INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

ANALYTICAL CHEMISTRY DIVISION COMMISSION ON SOLUBILITY DATA

SOLUBILITY DATA SERIES

Volume 48

ESTERS WITH WATER PART I: ESTERS 2-C TO 6-C

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES

Volume 48

ESTERS WITH WATER PART I: ESTERS 2-C TO 6-C

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U.K.	Pergamon Press Ltd., Headington Hill Hall, Oxford OX3 0BW, England
U.S.A.	Pergamon Press Inc., 660 White Plains Road, Tarrytown, New York 10591-5153, USA
KOREA	Pergamon Press Korea, KPO Box 315, Seoul 110-603, Korea
JAPAN	Pergamon Press Japan, Tsunashima Building Annex, 3-20-12 Yushima, Bunkyo-ku, Tokyo 113, Japan

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First edition 1992

Library of Congress Cataloging in Publication Data

The Library of Congress has catalogued this serial title as follows: Solubility data series.—Vol. 1—Oxford, New York: Pergamon, c 1979– v.; 28 cm. Separately catalogued and classified in LC before no. 18. ISSN 0191-5622 = Solubility data series. 1. Solubility—Tables—Collected works. QD543.S6629 541.3'42'05-dc19 85-641351 AACR 2 MARC-S

British Library Cataloguing in Publication Data

A catalogue record for this book is available from the British Library

ISBN 0 08 040496 0

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FOREWORD

If the knowledge is undigested or simply wrong, more is not better.

The Solubility Data Series is a project of Commission V.8 (Solubility Data) of the International Union of Pure and Applied Chemistry (IUPAC). The project had its origins in 1973, when the Analytical Chemistry Division of IUPAC set up a Subcommission on Solubility Data under the chairmanship of the late Prof. A. S. Kertes. When publication of the *Solubility Data Series* began in 1979, the Committee became a full commission of IUPAC, again under the chairmanship of Prof. Kertes, who also became Editor-in-Chief of the Series. The Series has as its goal the preparation of a comprehensive and critical compilation of data on solubilities in all physical systems, including gases, liquids and solids.

The motivation for the Series arose from the realization that, while solubility data are of importance in a wide range of fields in science and technology, the existing data had not been summarized in a form that was at the same time comprehensive and complete. Existing compilations of solubility data indeed existed, but they contained many errors, were in general uncritical, and were seriously out-of-date.

It was also realized that a new series of compilations of data gave educational opportunities, in that careful compilations of existing data could be used to demonstrate what constitutes data of high and lasting quality. As well, if the data were summarized in a sufficiently complete form, any individual could prepare his or her own evaluation, independently of the published evaluation. Thus, a special format was established for each volume, consisting of individual data sheets for each separate publication, and critical evaluations for each separate system, provided sufficient data from different sources were available for comparison. The compilations and, especially, the evaluation were to be prepared by active scientists who were either involved in producing new data, or were interested in using data of high quality. With minor modifications in format, this strategy has continued throughout the Series.

In the standard arrangement of each volume, the Critical Evaluation gives the following information:

(i) A text which discusses the numerical solubility information which has been abstracted from the primary sources in the form of compilation sheets. The text concerns primarily the quality of the data, after consideration of the purity of the materials and their characterization, the experimental method used, the uncertainties in the experimental values, the reproducibility, the agreement with accepted test values, and finally, the fitting of the data to suitable functions, along with statistical tests of the fitted data. (ii) A set of recommended data, whenever possible, including weighted averages and estimated standard deviations. If applicable, one or more smoothing equations which have been computed or verified by the evaluator are also given.

(iii) A graphical plot of the recommended data, in the form of phase diagrams where appropriate.

The Compilation part consists of data sheets which summarize the experimental data from the primary literature. Here much effort is put into obtaining complete coverage; many good data have appeared in publications from the late nineteenth and early twentieth centuries, or in obscure journals. Data of demonstrably low precision are not compiled, but are mentioned in the Critical Evaluation. Similarly, graphical data, given the uncertainty of accurate conversion to numerical values, are compiled only where no better data are available. The documentation of data of low precision can serve to alert researchers to areas where more work is needed.

A typical data sheet contains the following information:

- (i) list of components: names, formulas, Chemical Abstracts Registry Numbers;
- (ii) primary source of the data;
- (iii) experimental variables;
- (iv) compiler's name;
- (v) experimental values as they appear in the primary source, in modern units with explanations if appropriate;
- (vi) experimental methods used;
- (vii) apparatus and procedure used;
- (viii) source and purity of materials used;
 - (ix) estimated error, either from the primary source or estimated by the compiler;
 - (x) references relevant to the generation of the data cited in the primary source.

Each volume also contains a general introduction to the particular type of system, such as solubility of gases, of solids in liquids, etc., which contains a discussion of the nomenclature used, the principle of accurate determination of solubilities, and related thermodynamic principles. This general introduction is followed by a specific introduction to the subject matter of the volume itself.

The Series embodies a new approach to the presentation of numerical data, and the details continue to be influenced strongly by the perceived needs of prospective users. The approach used will, it is hoped, encourage attention to the quality of new published work, as authors become more aware that their work will attain permanence only if it meets the standards set out in these volumes. If the Series succeeds in this respect, even partially, the Solubility Data Commission will have justified the labour expended by many scientists throughout the world in its production.

January, 1989

J. W. Lorimer, London, Canada

PREFACE

This volume, one of a pair in the Solubility Data Series devoted to esters in water, includes solubility data for binary systems containing an ester and water published up through the end of 1988. The first volume contains the esters having two through six carbon atoms with water and the second volume contains esters having seven or more carbon atoms with water. With only rare exceptions, the compiled data and evaluations involve measurements made at constant pressure over rather restricted ranges of temperature. The limited ranges of pressure and temperature involved are to be expected in view of the liquid-liquid condition prescribed for the systems.

For the most part, the data presented show general patterns of behavior expected for the topic systems. While rather extensive data have been reported for many of the systems under consideration, no effort was made to attempt any detailed correlations of behavior or descriptions of trends beyond those presented by the evaluator in the evaluation sections.

The critical evaluations were all prepared by one author and an introductory section has been included to elaborate the philosophy and methodology followed in the evaluations. No attempts were made to extract thermodynamic parameters such as activity coefficients, enthalpies of solution, and the like from the reported data although much of the published work is sufficiently precise for such activities.

Every attempt was made to include all published data for the subject systems through the end of 1988. The editors would be grateful for any information concerning material which was overlooked in the preparation of this work.

The editors would like to express their appreciation to all those who have provided assistance in the volume preparation, especially to fellow members of the IUPAC Commission on Solubility Data and to those who have served as reviewers of this work.

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November 1991.

LIQUID-LIQUID SOLUBILITY: EVALUATION PHILOSOPHY AND METHODOLOGY

G.T. HEFTER

INTRODUCTION

Because of the differing ways in which it is possible to critically evaluate published solubility data it is worthwhile to present a coherent statement on the philosophy and procedures which have been used in this volume. Although this is a personal statement concerning the present volume, many of the ideas have been developed by myself as an evaluator for previous liquid-liquid volumes in the Solubility Data Series [1-3] and are shared, to some degree, by other evaluators.

EVALUATION PHILOSOPHY

The critical evaluation of data is, at least in part, a subjective process. Some physical scientists are uncomfortable with this notion but the history of science shows us it is undeniable. Because some subjective judgements are inevitably involved, it is vital that the evaluator's procedure should be as visible as possible. In this way, if the user does not agree with the evaluator's judgement or arguments or if new data become available it is possible, with a minimum of effort, to derive a new set of preferred or "best" values. For this reason the Critical Evaluations in this and those previous volumes to which I have contributed [1-3] have been, in essence, written like research papers with enough information provided for users to repeat or change the evaluation should they so desire.

The starting point for each Critical Evaluation is that the data compilation is complete, i.e., the data sheets include all the available data. This is an important premise because the addition of extra data may change the evaluation considerably. This is especially true of liquid-liquid systems since very few have been adequately studied over a wide temperature range and disagreements often exist between independent investigations.

In general, a "democracy of observers" is followed. That is, the data of all investigators are given equal weight irrespective of their reputation or location. This is justifiable in scientific terms because experience shows that real "errors" in liquid-liquid solubility data are much greater than individual authors' reported precisions. Thus, the benzene-water system, which is relatively simple and probably the most widely studied of all liquid-liquid systems [2], has solubilities which are known to an accuracy of about ± 2% (relative). The same estimated error is obtained regardless of whether a simple average of the available data is taken or whether a complex weighting procedure is used. This suggests that, at the present stage of development of liquid-liquid solubility determinations, equal weighting for all data is the most appropriate course of action. The exceptions to this rule are discussed below.

REJECTION OF DATA

The statement that all data are given equal weight must be qualified: some data are assigned zero weight, i.e., they are rejected. Data rejection is potentially dangerous, especially when few data are available. Nevertheless, since a critical evaluation is required, it has to be considered. The most important reasons for rejecting data are as follows.

1. The data disagree "significantly" from most other studies (especially if these are numerous). Significance is subjective but a criterion of

 $|\mathbf{s}_{obs} - \mathbf{s}_{av}| > 3\sigma_n$

- where s_{obs} is the reported solubility datum being considered for rejection
 - s_{av} is the arithmetic average (mean) of all other studies at the same temperature and pressure
 - σ_n is the standard deviation from the mean of these studies

has been generally, but not rigidly, applied [1-3].

It should be noted that this procedure can be invoked only once. That is, having rejected some points in a particular data set it is not statistically valid to recalculate a new value of σ_n and then reject further points. Strictly speaking this means that outlying data should be included in the original calculation of σ_n . However, the amount of available data does not always make this approach realistic and common sense must be applied.

- 2. Approximate data (one significant figure) are rejected when a reasonable amount of more precise data is available.
- 3. Data which are grossly inconsistent with chemical systematics or thermodynamic expectations are also rejected.
- 4. In keeping with the practice adopted in previous liquid-liquid solubility values, data originally presented in graphical form or in volume ratio units are also excluded. In the latter case, data are retained if appropriate density data are readily available to permit conversion to mass units. As density measurements are usually far more reliable than solubility data, the choice of density values is usually not critical.

It is appropriate to add here that data for a particular system coming from the same authors or the same laboratories have generally not been regarded as independent measurements and have therefore been subsumed into a single result (at each temperature).

THE EVALUATION FORMAT

The Critical Evaluations in this volume follow the format evolved in previous liquid-liquid solubility volumes [1-3]. In essence each Evaluation is divided into three parts. In the first part Table 1 lists all the available publications containing quantitative solubility data for the particular system. Broad experimental details such as temperature range, type of solubility measured ((1) in (2), (2) in (1) or mutual) and the method used are also included in Table 1. After mention of any other special features such as critical points, or any special types of investigation, further discussion is usually divided into two parts: the solubility of the organic in the aqueous phase, and that of water in the organic-rich phase. Since these two sections are handled in the same way they will be discussed together.

After listing rejected data, anomalies and caveats, all the available data (usually expressed as g/100g sln) are collected into Tables (usually Tables 2 & 3). To facilitate comparisons, data are interpolated (if necessary) to specific temperatures at 5K intervals near 298K, then 10 or 20K intervals. These temperatures are exact, i.e. 298.15, 303.15 ... K but for convenience are written 298, 303, ... K in the text. The nature of most liquid-liquid solubility data makes graphical interpolation the most appropriate approach [4]. Interpolated values are always designated with an asterisk (*). Very occasionally data are extrapolated but only over a short range (<5K) and only if the solubility curve is not changing sharply.

All the retained values at each temperature are then averaged and the mean and σ_n recorded in the Tables. Few of the systems in this volume have sufficient data to permit meaningful statistical analysis. The value of σ_n is therefore included only as a convenient measure of the spread of the experimental data.

"BEST" VALUES

The word "best", almost always in inverted commas (quotation marks), is used throughout the Critical Evaluations in this and previous liquid-liquid solubility volumes [1-3] in a specific way: to mean "best available estimate". It follows from what has been said above that "best" values are simply the arithmetic average (mean) of all the accepted data, including those obtained by interpolation and excluding rejected data. "Best" values are given in both g/100g sln and mole fraction units (x). RECOMMENDED VALUES

Solubilities are recommended only if two or more independent studies (including rejected data) agree to within \pm 5%(relative), i.e.,

 $|100\sigma_n/s_{av}| \leq 5$

and there are no other obvious problems. Recommended data are designated by (R) immediately following the numerical value.

For sparingly soluble systems this criterion may be too harsh and

 $|100\sigma_{\rm n}/s_{\rm av}| \leq 10 \text{ or } 20$

may be more appropriate [3]. Very few high molecular weight esters have been sufficiently well characterized to enable even these less restrictive criteria to be applied.

Data which are not "Recommended" are regarded as "Tentative". The likely accuracy of these data varies from system to system and from temperature to temperature but may be inferred from

1. σ_n

2. $100\sigma_{\rm n}/s_{\rm av}$

3. n (the number of independent measurements).

Occasionally there are definite reasons to suspect the available data are not reliable. Such data are 'labelled "Doubtful" and the detailed reasons for this classification given. Considerable care should be exercised in the use of such data.

Note that the mole fraction "best" solubilities in each table should be regarded as having the same status ("Recommended", "Tentative" or "Doubt-ful") and the same (relative) percentage uncertainties (where given) as the corresponding mass % solubilities.

GRAPHICS

In systems for which a reasonable amount of data exists, selected results are plotted graphically over the studied temperature range. Appropriate comments on the plots are made in the figure caption or in the text.

FITTING EQUATIONS

The use of fitting equations to smooth solubility data as a function of temperature is controversial and a topic in its own right which will not be discussed here. As in previous liquid-liquid solubility volumes [1-3], fitting equations are not generally given in the printed version of this volume. There are several reasons for this.

- 1. There is no single equation form which can be used for all systems.
- 2. The data for some systems are too scattered or poorly defined for realistic curve fitting.
- 3. Without special care empirical fitting equations may give misleading results (spurious extrema, etc.) when interpolating and can almost never be reliably used for extrapolation.

For certain systems where reliable data appear evident, fitting equations have been provided. Such equations come directly from the original works or from the efforts of the compilers in the course of their examination of reported data and preparation of smoothed value tables.

Users who wish to derive their own fitting equations are advised to do so with caution. It is suggested that the "best" values be used for this purpose, but it should be noted that this may create anomalies because of the way in which the "best" values are derived (see above). Where fitting equations are given in this volume they should be used only over the stated range.

xii

THERMODYNAMIC CONSISTENCY

Using standard relationships from thermodynamics it can be shown that:

$$\Delta_{sln}G = -RT \ln a_{sat}$$

$$\frac{\partial (\Delta_{sln} G/T)}{\partial T} = - \frac{\Delta_{sln} H}{RT^2}$$

and

$$\frac{\partial^2 (\Delta_{sln} G/T)}{\partial T^2} = \frac{\partial (\Delta_{sln} H)}{\partial T} = \Delta_{sln} C_p$$

where $\Delta_{gln}G$, $\Delta_{gln}H$ and $\Delta_{gln}C_p$ are respectively the Gibbs energy, enthalpy and heat capacity (at constant pressure) changes corresponding to the dissolution of the solute in the solvent and a_{gat} is the activity of the saturated solute in the solvent. If the solute is only sparingly soluble the thermodynamic parameters may be equated with their standard state values, and it should be noted that $\Delta_{gln}C_p$ may itself be temperature dependent.

Both $\Delta_{gln}H$ and $\Delta_{gln}C_p$, at least in principle, can be measured directly by separate calorimetric procedures [5,6] and therefore can serve as an independent check on the temperature dependence of published solubility data. This approach has been used with significant effect in evaluating hydrocarbon solubilities in water [2-3]. However, very few calorimetric data have been reported for ester-water systems and so this approach has not been utilized in the present volume.

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- G.T. Hefter, in A.F.M. Barton, Ed., Solubility Data Series, Vol. 15, Alcohols with Water (Pergamon Press, Oxford, 1984).
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- G.T. Hefter, unpublished paper presented at 1st Intl. Symp. Soly. Phenom., London, Canada, August, 1984.
- 5. S.O. Nilsson and I. Wadso, J. Chem. Thermodyn. <u>1984</u>, 16, 317.
- P. Picker, P.A. Leduc, P.R. Philip and J.E. Desnoyers, J. Chem. Thermodyn. 7, 3, 641.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Formic acid methyl ester	Rayman, J.	
(methyl formate); C ₂ H ₄ O ₂ ; [107-31-3]	Thesis, Budapest, <u>1906</u> .	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 303	G.T. Hefter	
EXPERIMENTAL VALUES: Solubility of formic acid me	ethyl ester in water	
t/°C g(1)/100g(2) g(1)/10 (ca	$\begin{array}{llllllllllllllllllllllllllllllllllll$	
0. 26.79	21.13 0.0744	
10. 28.60	22.24 0.0790	
20. 30.36	23.29 0.0835	
30. 32.51	24.53 0.0888	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved Volume was knot as small as possi-	 (1) Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated. (2) Not specified. 	
ble to minimize the error arising	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Winkler, L. <i>Z. Phys. Chem.</i> <u>1906</u> , 55, 360.	
	2. Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u> , Vol. 3, 387-98.	

<pre>COMPONENTS: (1) Acetic acid, trichloro-, methyl ester (methyl tri- chloroacetate); C₃H₃Cl₃O₂; [598-99-2] (2) Water; H₂O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 363	Z. Maczynska

Mutual solubility of trichloroacetic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	_	99.74		0.9750
9.5	-	99.79	-	0.9797
20.0	-	99.81	-	0.9816
29.6	0.09	• -	0.00009	-
39.8	0.09	99.70	0.00009	0.9712
49.8	0.04	99.65	0.00004	0.9665
60.0	0.05	99.52	0.00005	0.9546
70.5	0.06	99.29	0.00006	0.9342
80.1	0.03	99.28	0.00003	0.9333
90.2	0.03	98.97	0.00003	0.9070
std. de	v. 0.01	0.01		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The analytical method was used. (1) Source not specified, commer-Component (1) was equilibrated cial sample; purity 99%; used with component (2) at a given as received. temperature in a thermostat. Each layer was sampled with a syringe; (2) Not specified. (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. **REFERENCES:**

				·····
COMPONENTS:			ORIGINAL MEASUREMEN	ITS:
(1) Acetic acid, dichloro-, methyl			Stephenson, R.; St	uart, J.
ester (methyl dichloro-			J. Chem. Eng. Data	a 1986 <i>. 31</i> .
acetate); C ₃ H ₄ Cl ₂ O ₂ ; [116-54-1]			56-70.	
(2) Water;	H ₂ O; [7732-	18-5]		
VARIABLES:			PREPARED BY:	<u>, , , , , , , , , , , , , , , , , , , </u>
T/K = 273 -	363		Z. Maczynska	
EXPERIMENTAL	VALUES:			
Mutual	solubility o	f dichloroacet	cic acid methyl ester	r and water
	a(1)/1	00a sin	x. (compi	ler)
(2	-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase
0	1.09	99.78	0.00139	0.9828
9.6	0.86	99.73	0.00109	0.9790
20.1	0.33	99.68	0.00042	0.9751
29.6	0.33	99.63	0.00042	0.9714
39.5	0.35	99.52	0.00044	0.9631
50.0	0.37	99.49	0.00047	0.9609
60.0	0.36	99.40	0.00045	0.9543
70.3	0.37	99.27	0.00047	0.9448
79.9	0.46	98.60	0.00058	0.8987
90.2	0.44	98.20	0.00056	0.8730
std. dev.	0.04	0.01		
		AUXILIARY	INFORMATION	
			r	
METHOD/APPAR	ATUS/PROCEDU	RE:	SOURCE AND PURITY O	OF MATERIALS:
The analyti Component (cal method w 1) was equil	as used. ibrated	(1) Source not spe cial sample; p	ecified, commer- ourity 99%; used
with component	ent (2) at a	given stat Fach	as received.	
layer was s	ampled with	a syringe;	(2) Not specified.	
(1) was deto Weighed amon	ermined by a unt of aceto	dding a nitrile		
(or sometime	es propanol)	to the		
by a Gow-Ma	er sample an c thermal co	d measuring nductivity	ESTIMATED ERROR:	
gc the $(1)/(1)$	acetonitrile	peak ratio	Accuracy of method] 0.1 wt% or less
³³⁹⁰ A recorder-integrator).			for solubility, se	ee above.
A similar procedure but a higher				
Was used to determine (2) in the				
water layer.			REFERENCES:	•
ļ				
			<u></u>	

<pre>COMPONENTS: (1) Acetic acid, chloro-, methyl ester (methyl chloroacetate); C₃H₅ClO₂; [96-34-4] (2) Water; H₂O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 363	Z. Maczynska

Mutual solubility of chloroacetic acid methyl ester and water

t/°C	g(1)/100g sln		x ₁ (compiler)	
((2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	5.44	99.29	0.00946	0.9587
9.8	5.18	99.15	0.00898	0.9509
19.8	5.16	98.97	0.00895	0.9410
29.8	5.09	98.69	0.00882	0.9259
39.5	5.31	98.58	0.00922	0.9201
50.2	5.34	98.16	0.00928	0.8985
60.0	5.79	97.88	0.01010	0.8846
70.2	5.79	97.44	0.01010	0.8633
80.1	6.70	96.96	0.01178	0.8411
90.1	7.00	96.09	0.01234	0.8031
std. dev	7. 0.08	0.03		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:		EVALUATOR:
(1)	Acetic acid methyl ester; (methyl acetate); C2HcO2;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[79-20-9]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia
	· · · ·	January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the Acetic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> Acetic acid methyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Fuehner (ref 3)	293	(1) in (2)	titration
Hill (ref 4)	267-381	mutual	synthetic
Kendall and Harrison (ref 5)	278-357	(1) in (2)	synthetic
Murti et al. (ref 6)	303	mutual	titration
Venkataratnam et al. (ref 7)	303	mutual	titration
Lutugina and Kalyuzhnyi (ref 8)	293,330	mutual	titration
Beregovykh et al. (ref 9)	293-377	mutual	titration
Filip and Maciejewski (ref 10)	293	mutual	titration
Skrzecz (ref 11)	295-357	mutual	synthetic
Richon and Viallard (ref 12)	298	mutual	calorimetric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid methyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The approximate value of Traube (ref 1) at 293 K is excluded because more precise information is readily available (ref 3,5,8,9,11). The data of Rayman (ref 2), Murti et al. (ref 6) and Venkataratnam et al. (ref 7), all at 303 K, and of Lutugina and Kalyuzhnyi (ref 8) at 330 K are substantially higher (> $3\sigma_n$) than all other studies and are rejected. The data of Filip and Maciejewski (ref 10) at 293 K and Richon and Viallard (ref 12) at 298 K are substantially lower (> $3\sigma_n$) than all other values at these temperatures The data of Hill (ref 4) which are composite values and are also rejected.

(continued next page)

COMPONENTS:		EVALUATOR:
(1)	Acetic acid methyl ester;	G.T. Hefter, School of Mathematical
	(methyl acetate); C ₃ H ₆ O ₂ ;	and Physical Sciences,
	[79-20-9]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732+18-5]	Australia
1-1		January, 1989

based on published and unpublished data are also in disagreement with most other studies over most of the temperature range and are rejected.

The remaining data (Table 2) are in excellent agreement over a wide range of temperature enabling many of the average "Best" values to be Recommended. Selected data are plotted in Figure 1.

TABLE 2:	Recommended	(R) and	Tentati	ve Solubil	ities
of Ac	cetic acid met	hyl este	er (1) in	Water (2)	L

T/K	Solubilities			
	Reported values	"Best" values $(\pm \sigma_n)^a$		
	g(1)/100g sln	$g(1)/100g \ sln$ $10^2 x_1$		
273	24.95 (ref 2)	25.0 7.48		
278	24.7 [*] (ref 2), 22.6 (ref 5)	23.7 ± 1.1 7.02		
283	24.49 (ref 2), 22.6 [*] (ref 5)	23.5 ± 1.1 6.95		
293	24.18 (ref 2), 24.35 (ref 3), 22.8* (ref 5), 24.49 (ref 8), 24.0* (ref 11), 23.35 (ref 9)	23.9 ± 0.6 (R) 7.10		
298	22.9 [*] (ref 5), 23.35 [*] (ref 9), 23.05 [*] (ref 11)	23.1 ± 0.2 (R) 6.81		
303	23.0 [*] (ref 5), 23.4 [*] (ref 9), 22.32 [*] (ref 11)	22.9 ± 0.4 (R) 6.74		
313	23.2 [*] (ref 5), 23.4 (ref 9), 21.58 [*] (ref 11)	22.7 ± 0.8 (R) 6.67		
323	23.3 [*] (ref 5), 23.5 [*] (ref 9), 21.78 [*] (ref 11)	22.9 ± 0.8 (R) 6.74		
333	23.8 [*] (ref 5), 23.9 [*] (ref 9), 22.93 [*] (ref 11)	23.5 ± 0.4 (R) 6.95		
343	25.2 [*] (ref 5), 25.3 [*] (ref 9), 25.01 [*] (ref 11)	25.2 ± 0.2 (R) 7.57		
353	27.7 [*] (ref 5), 27.9 [*] (ref 9), 28.03 [*] (ref 11)	27.9 ± 0.1 (R) 8.60		
363	32.2 [*] (ref 9)	32.2 10.36		
373	36.5 [*] (ref 9)	36.5 12.27		

^a Obtained by averaging where appropriate.

(continued next page)

COMPONENTS:		EVALUATOR:	
(1) Acetic acid methyl ester; (methyl acetate); C ₂ H ₆ O ₂ ;		G.T. Hefter, School of Mathematical and Physical Sciences,	
	[79-20-9]	Murdoch University, Perth, W.A.,	
(2)	Water: H_O: [7732-18-5]	Australia	
		January, 1989	

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.



FIGURE 1. Selected data for the solubility of acetic acid methyl ester (1) in water (2): ref 4 (\bullet); ref 5 (\Box); ref 9 (X); ref 11 (O). Solid line is drawn through the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID METHYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid methyl ester (1) are summarized in Table 3 with the following exceptions. The data of Murti *et al.* (ref 6) and Venkataratnam *et al.* (ref 7) at 303 K and Lutugina and Kalyuzhnyi (ref 8) at 330 K are substantially higher than all other studies and are rejected.

The remaining data, mainly due to Hill (ref 4), Beregovykh et al. (ref 9) and Skrzecz (ref 11) are generally in reasonable agreement, especially the Values given in ref 4 and 11. At low (T < 293 K) and high (T > 373 K)

(continued next page)

COMPONENTS:		EVALUATOR:	
(1)	Acetic acid methyl ester;	G.T. Hefter, School of Mathematical	
(methyl acetate); C ₃ H ₆ O ₂ ;		and Physical Sciences,	
[79-20-9]		Murdoch University, Perth, W.A.,	
(2)	Water: H_O: [7732-18-5]	Australia	
		January, 1989	

temperatures only the data of Hill (ref 4) are available and must be considered tentative. Hill also reports the upper critical solution temperature of methyl acetate and water to be at 108 °C (381.2 K) at a composition of 52.5 g (1)/100 g sln ($x_1 = 0.212$).

Selected data for the solubility of water in methyl acetate are plotted in Figure 2.

TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid methyl ester (1)

T/K	Solubilities				
	Reported values	"Best" values (:	tσ _n) ^a		
	g(2)/100g sln	g(2)/100g sln	<i>x</i> ₂		
268	6.2 [*] (ref 4)	6.2	0.214		
273	6.4 [*] (ref 4)	6.4	0.219		
283	6.8 [*] (ref 4)	6.8	0.231		
293	7.5 [*] (ref 4), 7.41 (ref 8), 8.16 (ref 9), 7.77 (ref 10), 7.38 (ref 11)	7.6 ± 0.3 (R)	0.253		
298	8.0 [*] (ref 4), 8.15 [*] (ref 9), 8.03 (ref 11), 8.33 (ref 12)	8.1 ± 0.1 (R)	0.266		
303	8.7 [*] (ref 4), 8.20 [*] (ref 9), 8.73 (ref 11)	8.5 ± 0.2 (R)	0.276		
313	10.3 [*] (ref 4), 8.5 [*] (ref 9), 10.30 [*] (ref 11)	9.7 ± 0.8	0.306		
323	12.1 [*] (ref 4), 9.2 [*] (ref 9), 12.10 [*] (ref 11)	11.1 ± 1.4	0.339		
333	14.2 [*] (ref 4), 11.1 [*] (ref 9), 14.12 [*] (ref 11)	13.1 ± 1.4	0.382		
343	16.6 [*] (ref 4), 14.6 [*] (ref 9), 16.35 [*] (ref 11)	15.9 ± 0.9	0.437		
353	19.4 [*] (ref 4), 19.0 [*] (ref 9), 18.81 [*] (ref 11)	19.1 ± 0.2 (R)	0.493		
363	22.7 [*] (ref 4), 24.5 [*] (ref 9)	23.6 ± 0.9 (R)	0.560		
373	28.2 [*] (ref 4), 29.5 [*] (ref 9)	28.9 ± 0.7 (R)	0.626		
^a Obtain	ed by averaging where appropriate.	(continued	l next page)		

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COMPONENTS:	EVALUATOR:	
 Acetic acid methyl ester; (methyl acetate); C₃H₆O₂; 	G.T. Hefter, School of Mathematical and Physical Sciences,	
[79-20-9]	Murdoch University, Perth, W.A.,	
(2) Water: H ₂ O: [7732-18-5]	Australia	
	January, 1989	

-

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass solubilities.



FIGURE 2. Selected data for the solubility of water (2) in acetic acid methyl ester (1): ref 4 (\bullet); ref 9 (X); ref 11 (O). Solid line is drawn through the "Best" values from Table 3.

REFERENCES

- 1. Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u>, 17, 2294-316.
- 2. Rayman, J. Thesis, Budapest 1906.
- 3. Fuehner, H. Ber. Dtsch. Chem. Ges. <u>1924</u>, 57, 510-5.
- Hill, A. E. International Critical Tables (Washburn, E. W., Ed.), McGraw-Hill, New York, <u>1928</u>, Vol. 3, 387-98.
- 5. Kendall, J.; Harrison, E. Trans. Faraday Soc. <u>1928</u>, 24, 588-96.
- 6. Murti, P. S.; Venkataratnam, A.; Rao, C. V. J. Sci. Ind. Res. 1954, 13B, 392-6. (continued next page)

COMP	ONENTS:	EVALUATOR:
(1) (2)	Acetic acid methyl ester; (methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRIT	ICAL EVALUATION: (continued)	
REFE	RENCES (continued)	
7.	Venkataratnam, A.; Rao, J. R.; 7, 102-10.	Rao, C. V. <i>Chem. Eng. Sci.</i> <u>1957</u> ,
8.	Lutugina, N. V.; Kalyuzhnyi, V. 2626-33.	M. Zh. Prikl. Khim. <u>1959</u> , 32,
9.	Beregovykh, V. V.; Grishunin, A. L. A. Fiz. Khim. Osn. Rektifikat	V.; Balashov, M. I.; Serafimov, tsii <u>1970</u> , 103-12.
10.	Filip, S.; Maciejewski, Z. Cher	n. Stosow. <u>1972</u> , 16, 445-51.
11.	Skrzecz, A. Pol. J. Chem. <u>1980</u> , Thesis, I. Ch. F. PAN, Warszawa,	54, 1101-4; see also Skrzecz, A. <u>1979</u> .
12.	Richon, D.; Viallard, A. Fluid	Phase Equil. <u>1985</u> , 21, 279-93.
ACKN	CWLEDGEMENT	
	The Evaluator thanks Dr. Brian C.	lare for the graphics.
-		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Acetic acid methyl ester;	Traube, J.		
(methyl acetate); C ₃ H ₆ O ₂ ;	Ber. Dtsch. Chem. Ges. <u>1884</u> , 17, 2294-316		
(7) = 20 - 3	2234-310.		
VARIABLES:	PREPARED BY:		
T/K = 295	A. Skrzecz		
EXPERIMENTAL VALUES: The solubility of acetic acid methyl to be 1 part of methyl acetate in 3 p per cent and mole fraction, x_1 , value 25 g(1)/100g sln and 0.075.	ester in water at 22°C was reported parts of water. The corresponding mass as calculated by the compiler are		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The method was not specified.	(1) Not specified.		
	(2) Not specified.		
	ESTIMATED ERROR:		
	Soly. about ±1.5 g(1)/100g sln (compiler).		
	REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid methyl ester (methyl acetate); C₃H₆O₂; [79-20-9]</pre>	Rayman, J. <i>Thesis</i> , Budapest, <u>1906</u> .
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 303	G.T. Hefter

Solubility of acetic acid methyl ester in water

t/°c	g(1)/100g(2)	g(1)/100g solution (compiler)	x ₁ (compiler)
		·	
0.	33.24	24.95	0.0748
10.	32.43	24.49	0.0731
20.	31.89	24.18	0.0720
30.	31.73	24.09	0.0717

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

SOURCE AND PURITY OF MATERIALS:

- Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated.
- (2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

 Winkler, L. Z. Phys. Chem. <u>1906</u>, 55, 360.

COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Acetic acid methyl ester;	Fuehner, H.			
(methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9]	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.			
(2) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
T/K = 293	A. Skrzecz			
EXPERIMENTAL VALUES: The solubility of acetic acid methyl ester in water at 20°C was reported to be 25.37 vol%, 24.35 g(1)/100g sln. and 3.290 mol(1)/L sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.07259.				
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remain- ed transparent.	 (1) Source not specified, commer- cial product. (2) Not specified. 			
	ESTIMATED ERROR:			
	Soly. about ±0.5 g(1)/100g sln (compiler).			
	REFERENCES:			

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COMPONENT	s:		ORIGINAL MEASUREME	NTS:	
(1) Acetic acid methyl ester;			Hill, A. E.		
(methyl acetate); C ₃ H ₆ O ₂ ;			International Cri	tical Tables	
[79	-20-9]		(Washburn E.W.	Ed.) McGraw-Hill.	
(2) Wat	er; H ₂ O; [7732-	18-5]	(#431154111,1,		
			New York, <u>1928</u> ,	Vol. 3, 387-98.	
VARIABLES	······		PREPARED BY:		
T/K = 26	57 - 381		G.T. Hefter		
				· · · · · · · · · · · · · · · · · · ·	
EXPERIMEN	TAL VALUES: Mutual solubili	ty of acetic a	cid methyl ester ar	nd water	
t/°C	q(1)/1	00q sln	<i>x</i> , (comp	iler)	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
-6.55	25.5	93.8	0,0769		
0.0	25.0	93.6	0.0750	0.781	
10.	24.6	93.0	0.0735	0.764	
20.	24.2	91.8	0.0721	0.756	
25.	24.1	91.3	0.0717	0.743	
30.	24.0	90.8	0.0713	0.729	
40.	24.2	89.4	0.0721	0.672	
50.	24.6	87.7	0.0735	0.634	
60.	25.1	85.9	0.0754	0.597	
80.	27.5	80.6	0.0845	0.503	
90.	30.2	77.3	0.0952	0.453	
100.	35.2	71.8	0.117	0.382	
105.	40.3	66.0	0.141	0.321	
108. ((UCST) 52.5	-	0.212	-	
		AUXILIARY	INFORMATION		
METHOD/AI	PPARATUS/PROCEDU		SOURCE AND PURITY	OF MATERIALS:	
The data	annoar to be t				
and Morrow (unpublished) and were		Not specified.			
probably obtained by the synthetic					
were given in the article.					
		ESTIMATED ERROR:			
		Not specified.			
			REFERENCES:		

COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) Acetic acid methyl ester;		ster;	Kendall, J.; Harrison, L.E.	
(methyl acetate); C ₃ H ₆ O ₂ ;		1 ₆ 0 ₂ ;	Trans. Faraday Soc. <u>1928</u> , 24,	
[79-2	[79-20-9]		588-96.	
(2) Water	; H ₂ O; [7732-18-	-5]		
VARIABLES:			PREPARED BY:	
T/K = 278	- 357		Z. Maczynska	
EVDEDTUE			I	
Solubi	L VALUES: lity of acetic a	acid methvl	ester in water	
		······		
t/°C	<i>x</i> ₁	g(1)/100g	sln (compiler)	
5.0	0.0662	2	22.6	
21.0	0.0670	2	22.8	
35.0	0.0679	2	23.1	
58.0	0.0700	2	23.6	
58.9	0.0703	2	23.7	
60.1	0.0706	2	23.8	
69 1	0.0751	2	23.9	
70 5	0.0751	2	25.4	
71.9	0.0773	2	25.6	
83.5	0.0883	-	28.5	
		AUXILIARY :	INFORMATION	
METHOD/APPA	RATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
The synthe	tic method was u	ised.	(1) Source not specified,	
adopted, t	tube method (re he free space be	er 1) was eing kept	CP commercial sample; distilled; b.p. range 0.1°C. (2) Distilled.	
as small a:	s possible in or	der to		
in composi	tion at the high	ier		
cemperature	es.			
			ESTIMATED ERROR:	
			Solv. about $\pm 1 \alpha(1)/100\alpha$ sln	
			(compiler).	
			BEFEDENCES	
			1. Smith, A.; Eastlack, H.E. J. Am. Chem. Soc. <u>1916</u> , 38,	
			1269.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid methyl ester; (methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9]	Murti, P.S.; Venkataratnam, A.; Rao, C.V. J. Sci. Ind. Res. 1954, 13B.
(2) Water: $H_{2}O: [7732-18-5]$	392-6.
VADTABLES.	DDEDADED BV.
$\pi/K = 303^{-4}$	A Skrzecz
<pre>EXPERIMENTAL VALUES: The solubility of acetic acid methyl to be 26.1 g(1)/100g sln. The corresp calculated by the compiler is 0.0791. The solubility of water in acetic aci to be 9.7 g(2)/100g sln. The correspondence calculated by the compiler is 0.31. Presumably the measurments were m not reported in the paper.</pre>	ester in water at $30^{\circ}C^{a}$ was reported bonding mole fraction, x_{1} , value id methyl ester at $30^{\circ}C^{a}$ was reported bonding mole fraction, x_{2} , value hade at $30^{\circ}C$; the temperature was
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. Determinations were made either from the production of turbidity or from its disappearance. The data were reported together with the ternary system methyl acetate-water-acetic acid. No further details were reported	 British Drug House, laboratory reagent grade; distilled; b.p. 57.3°C, d 0.9274, n_D³⁰ 1.3570. Not specified.
in the paper.	ESTIMATED ERROR:
	Soly. about $\pm 3.6 g(1)/100g slnand \pm 0.9 g(2)/100g sln(compiler).$
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid methyl ester; (methyl acetate); C₃H₆O₂; [79-20-9]</pre>	Venkataratnam, A.; Rao, J.R.; Rao, C.V. Chem. Eng. Sci. <u>1957</u> , 7, 102-10.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXDEDIMENTAL VALUES.	L	

The solubility of acetic acid methyl ester in water at 30° C was reported to be 25.4 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0765.

The solubility of water in acetic acid methyl ester at 30° C was reported to be 11.4 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.346.

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The titration method described in Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system methyl acetate-water- acetone. No further details were reported in the paper.	<pre>Source AND PURITY OF MATERIALS: (1) British Drug House Ltd., laboratory reagent grade; distilled; b.p. 57.3°C, d³⁰ 0.9234, n³⁰ 1.3570. (2) Distilled; free of CO₂. (2) Distilled; free of CO₂. (3) REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. 1941, 33, 1240.</pre>			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Acetic acid methyl ester; (methyl acetate); C₃H₆O₂; [79-20-9]</pre>	Lutugina, N.V.; Kalyuzhnyi, V.M. <i>Zh. Prikl. Khim.</i> <u>1959</u> , <i>32</i> , 2526-33.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 293 and 330	A. Skrzecz		
EXPERIMENTAL VALUES: Mutual solubility of acetic	acid methyl ester and water		
$t/^{\circ}$ C x_1 (2)-rich phase (1)-rich ph	g(1)/100g sln (compiler) Nase (2)-rich phase (1)-rich phase		
20.0 0.0731 0.7525 56.8 ^a 0.104 0.544	24.49 ^b 92.59 ^c 32.30 ^d 83.10 ^e		
AUXILIAR	Y INFORMATION		
AUXILIAR	Y INFORMATION		
AUXILIAR METHOD/APPARATUS/PROCEDURE: The titration method was used. Bottles with both narrow and long necks were used at room tempera- ture. The apparatus with dephlegmator was used at the boiling temperature. The mixture was stirred by the boiling liquid. The data were reported together with the ternary system methyl acetate-water-chloroform.	Y INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Synthesized in laboratory; washed with Na ₂ CO ₃ (aq) and water, dried with CaCl ₂ , distilled three times; b.p. 56.8°C, n _D ³⁰ 1.3614. (2) Distilled. ESTIMATED ERROR: Soly. about ±0.6 ^b , ±0.1 ^c , ±10. ^d and ±3.6 ^e g(1)/100g sln (compiler).		

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COMPONENTS:			ORIGINAL MEASUREMENTS:			
(1) Acetic acid methyl ester; (methyl acetate); C ₂ H ₆ O ₂ ;			Beregovykh, V.V.; Grishunin, A.V.; Balashov, M.I.; Serafimov, L.A.			
(79	-20-9]	8-51	Fi	z. Khim. Osn. F <u>1970</u> , 103-12.	Rektifikatsii	
(2) Hat	.ei, 11 ₂ 0, [//32=1					
VARIABLES	5:		PRE	PARED BY:		
T/K = 29	93 - 377		Α.	Skrzecz		
EXPERIMEN M	TAL VALUES: Mutual solubility	y of acetic ac	id r	nethyl ester and	l water	
t/°c	q(1)/10)0q sln		x_1 (comp	viler)	
·	(2)-rich phase	(1)-rich phas	е	(2)-rich phase	(1)-rich phase	
20.0 ^a	23.35 ^b	91.84 ^c	_	0.06897	0.7324	
56.5	23.65 ^d	89.5 ^e		0.07005	0.6746	
78.9	27.50 ^f	81.5 ^g		0.08445	0.5172	
103.4	38.00	68.50		0.12972	0.3459	
		AUXILIARY :	NFO	RMATION	·····	
METHOD/AF	PARATUS/PROCEDU	RE:	SOU	RCE AND PURITY	OF MATERIALS:	
The titr The mutu Visually	ation method was al solubility was during titration	s used. as observed	(1) Source not sp n _D ²⁰ 1.3619, b	ecified; purifie .p. 56.3°C.	d;
ebullion were obt the boil	eter. The exact ained from a gra ing temperature	values aph of vs.	(2) Distilled.		
the vapo	r-liquid equilib	orium				
measurem the pape	ents were preser er.)	nted in	ESTIMATED ERROR:			
No furth in the p	er details were reported aper.	Sc	ly. about ±0.4 ^b ±1.3 ^d , ±0.4 ±0.1 ^g g(1) (compiler).	, ±0.7 ^c e, ±0.4 ^f and /100g sln		
			REFERENCES:			
		1.	Balashov, M.I. M.I.Kh.T., Mos	<i>Thesis,</i> skva, <u>1967</u> .		

COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) Acetic acid methyl ester; (methyl acetate); C₃H₆O₂; [79-20-9]</pre>	Filip, S.; Maciejewski, Z. <i>Chem. Stoso</i> w. <u>1972</u> , 16, 445-51.			
(2) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
T/K = 293	A. Skrzecz			
EXPERIMENTAL VALUES: The solubility of acetic acid methyl ester in water at 20°C was reported to be 13.65 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0370.				
The solubility of water in acetic acid methyl ester at 20°C was reported to be 7.77 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.257.				

AUXTLTARV	TNFORMATION	

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously.

SOURCE AND PURITY OF MATERIALS:

- (1) FOCH Gliwice; chemically pure grade; used as received.
- (2) Distilled.

ESTIMATED ERROR:

Soly. about ±10. g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).

REFERENCES:

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Acetic acid methyl ester; (methyl acetate); C₃H₆O₂; [79-20-9] (2) Water; H₂O; [7732-18-5] 	Skrzecz, A. Pol. J. Chem. <u>1980</u> , 54, 1101-4. Skrzecz, A. Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .	
VARIABLES:	PREPARED BY:	
T/K = 295 - 357	A. Skrzecz	

Mutual solubility of acetic acid methyl ester and water

T/K	<i>x</i> ₁		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	e (1)-rich phase
294.6	0.0698	_	23.58	
295.1	0.0697	-	23.55	-
296.5	-	0.7407	-	92.15
297.3	0.0687	-	23.27	-
304.5	-	0.7155	-	91.18
305.1	0.0653	-	22.32	-
316.1	-	0.6646	-	89.07
322.7	-	0.6417	-	88.05
331.0	0.0653	-	22.32	-
332.5	0.0660	-	22.51	-
333.6	-	0.5944	-	85.77
335.4	0.0687	-	23.27	-
336.3	0.0698	-	23.58	-
			(c	ontinued next pag

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The synthetic method of Alexejew (1) International Enzymes Limited, was used. pure grade; distilled; purity An ampoule with the solution of 99.99% by glc, 0.07 wt% water by the Karl Fischer method. fixed concentration was placed into a glass tube connected with a thermostat filled completely with (2) Distilled. distilled water. During the measurements the temperature of the bath was changed continuously and ESTIMATED ERROR: the appearance and disappearance of turbidity within the ampoule was Temp. $\pm (0.2-0.6)^{\circ}C$. observed visually. The amount of water in pure ester was taken into Soly. see above. account. **REFERENCES:**

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1)	Acetic acid methyl ester;	Skrzecz, A.	
(methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9]	Pol. J. Chem. <u>1980</u> , 54, 1101-4.		
(2)	Water; H ₂ O; [7732-18-5]	Skrzecz, A.	
		Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .	

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid methyl ester and water

T/K	x ₁		g(1)/100g sin	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
337.1	0.0710	_	23.91	-
341.2	-	0.5624	-	84.09
341.6	0.0746	-	24.90	-
345.5	0.0775	-	25.68	-
348.7	0.0802	-	26.39	-
350.8	-	0.5227	-	81.83
357.1	-	0.4980	-	80.31

Author's smoothing equations:

 $\begin{aligned} x_1 &= 0.093868 - 1.4651 \times 10^{-3} & (T/K - 273.15) + 1.708 \times 10^{-5} & (T/K - 273.15)^2 \\ & \text{st. dev.} &= 7.87 \times 10^{-4} & (2) \text{-rich phase} \\ x_2 &= 0.168783 + 3.6860 \times 10^{-3} & (T/K - 273.15) + 3.54 \times 10^{-6} & (T/K - 273.15)^2 \\ & \text{st. dev.} &= 2.40 \times 10^{-3} & (1) \text{-rich phase} \end{aligned}$

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid methyl ester;	Richon, D.; Viallard, A.
(methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9]	Fluid Phase Equilib. <u>1985</u> , 21, 279-93.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
The solubility of acetic acid methyl ester in water at 298.1 K was reported to be $x_1 = 0.0545$. The corresponding mass per cent value calculated by the compiler is 19.16 g(1)/100g sln. The solubility of water in acetic acid methyl ester at 298.1 K was reported to be $x_2 = 0.272$. The corresponding mass per cent value calculated by the compiler is 8.33 g(2)/100g sln.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The calorimetric method was used. The method was described by Richon (ref 1) and by Richon and Villard (ref 2).	<pre>(1) Carlo Erba (for analysis); purified by preparation gas chromatographic method; purity >99.5%, water content was</pre>

ETHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The calorimetric method was used. The method was described by Richon (ref 1) and by Richon and Villard (ref 2). No further details were reported in the paper.	 Carlo Erba (for analysis); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible. Distilled.
	ESTIMATED ERROR:
	Soly. about $\pm 4g(1)/100g$ sln and $\pm 0.2 g(2)/100g$ sln (compiler).
	REFERENCES:
	1. Richon, D. <i>Thesis</i> , University de Clermont-Ferrand, <u>1974</u> .
	 Richon, D.; Villard, A. Can. J. Chem. <u>1976</u>, 54, 2584.
COMPONENTS:	EVALUATOR:
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 Formic acid ethyl ester (ethyl formate); C₃H₆O₂; 	G.T. Hefter, School of Mathematical and Physical Sciences,
[109-94-4]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia
	January, 1989

Quantitative solubility data for the formic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> Formic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Rayman (ref 1)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 2)) 278-349	(1) in (2)	synthetic
Batmanova <i>et al</i> . (ref 3)	293,326	mutual	titration, analytical

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid ethyl ester (1) in water (2) are summarized in Table 2 except for the 293 K datum of Batmanova et al. (ref 3) which is significantly lower (> $3\sigma_n$) than the other available values (ref 1,2).

Over the temperature range $273 \le T \le 303$ K where independent data are available, the solubilities of Rayman (ref 1) and Kendall and Harrison (ref 2) are in good agreement. However, the average solubilities derived from these two studies have not been Recommended because they show a totally contradictory dependence of solubility on temperature (Figure 1). Thus although some reliance may be placed on the average "Best" values further studies are clearly necessary. These should include detailed consideration of the possibility of ester hydrolysis.

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СОМРО	NENTS:	EVALUATOR:
(1)	Formic acid ethyl ester (ethyl formate); C ₃ H ₆ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
([109-94-4]	Murdoch University, Perth, W.A., Australia
(2)	Water; H ₂ O; [7732-18-5]	January, 1989

TABLE 2: Tentative Solubilities of Formic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values ^a	
	g(1)/100g sln	g(1)/100g sln	$10^2 x_1$
273	9.34 (ref 1), 7.4 [*] (ref 2)	8.4 ± 1.0	2.2
283	9.07 (ref 1), 7.78 [*] (ref 2)	8.4 ± 0.6	2.18
293	8.58 (ref 1), 8.04 [*] (ref 2)	8.3 ± 0.3	2.15
298	8.06 [*] (ref 1), 8.16 [*] (ref 2)	8.1 ± 0.1	2.10
303	7.34 (ref 1), 8.29 [*] (ref 2)	7.8 ± 0.5	2.01
313	8.63 [*] (ref 2)	8.6	2.2
323	9.16 [*] (ref 2), 10 ^b (ref 3)	9.2	2.4
333	9.95 [*] (ref 2)	10	2.6
343	11.12 [*] (ref 2)	11	2.9

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.

^b 325.8 K; not included in "Best" value.

2. SOLUBILITY OF WATER (2) IN FORMIC ACID ETHYL ESTER (1)

Only the data of Batmanova *et al.* (ref 3) are available for the solubility of water in formic acid ethyl ester and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities although the comments in Part 1 above should be noted.

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Formic acid ethyl ester	Rayman, J.	
(ethyl formate); C ₃ H ₆ O ₂ ;	Thesis, Budapest, <u>1906</u> .	
[109-94-4]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 303	G.T. Hefter	
EXPERIMENTAL VALUES: Solubility of formic acid et	hyl ester in water	
	······································	
$t/^{5}C$ g(1)/100g(2) g(1)/10	$0g \text{ solution } x_1$	
(66	(compiler) (compiler)	
0. 10.30	9.34 0.0244	
10. 9.97	9.07 0.0237	
20. 9.39	8.58 0.0223	
30. 9.00	7.34 0.0189	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara-	 (1) Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated. 	
(ref 1). After a suitable period	(2) Not specified.	
of time, the volume of undissolved (1) was measured. This undissolved		
volume was kept as small as possi- ble to minimize the error arising		
from the solubility of (2) in (1).	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Winkler, L. <i>Z. Phys. Chem.</i> <u>1906</u> , 55, 360.	
	2. Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw-Hill, New York, <u>1928</u> , Vol. 3, 387-98.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Formic acid ethyl ester (ethyl formate); C₃H₆O₂; [109-94-4]</pre>	Kendall, J.; Harrison, L.E. <i>Trans. Faraday Soc.</i> <u>1928</u> , 24, 588-96.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 278 - 349	Z. Maczynska

Solubility of formic acid ethyl ester in water

t/°C	<i>x</i> ₁	g(1)/100g sln (compiler)
 5 0	0.0197	7 63
15.0	0.0107	7 92
12.9	0.0205	7.52
30.2	0.0215	8.29
38.0	0.0223	8.57
45.1	0.0231	8.86
50.0	0.0241	9.22
55.5	0.0249	9.51
63.9	0.0273	10.35
70.0	0.0295	11.11
75.5	0.0320	11.97

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C. (2) Distilled.</pre>
	ESTIMATED ERROR: Temp. ±(0.1-0.2)°C.
	REFERENCES: 1. Smith, A.; Eastlack, H.E. <i>J. Am. Chem. Soc.</i> <u>1916</u> , 38, 1269.

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COMPONENTS:			ORIGINAL MEASURE	MENTS:
<pre>(1) Formia (ethy. [109-] (2) Water</pre>	c acid ethyl 1 <i>formate</i>); 94-4] : H ₂ O: [7732	ester C ₃ H ₆ O ₂ ; -18-51	Batmanova, G.A. Grishunin, A. I.G.; Serafimo Gidroliz. Lesokl 24(8), 11-2.	; Balashov, M.I.; V.; Savinskaya, ov, L.A. him. Prom. <u>1971</u> ,
	, m ₂ 0, [7,52		DDEDADED DV.	
T/K = 293	and 326		A. Skrzecz	
EXPERIMENTA	L VALUES:		L	
M	utual solubi	lity of formic	acid ethyl ester	and water
t/°C	g(1)/	100g sln	x ₁ (cor	npiler)
(:	2)-rich phas	e (1)-rich phas	se (2)-rich phas	e (1)-rich phase
	6.1	97.1	0.0156	0.891
52.6 ^{b,c}	7.0	96.0	0.0180	0.854
52.6 ^{a,c}	13.9	95.5	0.0378	0.838
in tl 52.6	he paper; bo ⁹ C was taken	iling temperatu from Horsley (are of two-phase m	ixture equal to
		AUXILIARY	INFORMATION	
ETHOD/APPAI	RATUS/PROCED	URE:	SOURCE AND PURITY	OF MATERIALS:
The titration and analytical methods were used. In the titration method, the titrations were carried out in thermostated bottles using a magnetic stirrer at 20°C and in a heated flask with a magnetic stirrer and reflux condenser at the boiling temperature. In the analytical procedure, a two-phase mixture was placed into a heated flask attached to a reflux conden- ser, mixed for 1/2 h. at the boil-		 (1) Source not s distilled, o redistilled; n²⁰ 1.3605. (2) Distilled. 	specified; dried with CaCl ₂ an ; b.p. 54.13°C,	
		ESTIMATED ERROR: Not specified.		
analyzed by glc. A small amount of Water was also determined by the		1		

1. Horsley, L.E. Azeotropic Data III, Advances in Chemistry Series 116, American Chemical Society, Washington, <u>1973</u>.

REFERENCES:

Karl Fischer method. The data and methods were reported together with the ternary systems ethyl formate-water-ethyl acetate

and ethyl formate-water-ethanol.

30				
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Carbonic acid dimethyl ester		Stephenson, R.; Stuart, J.		
(dimethyl carbonate); C ₃ H ₆ O ₃ ; [616-38-6]		J. Chem. Eng. Da 56-70.	ata <u>1986</u> , 31,	
(2) Wat	er; H ₂ O; [7732-	18-5]		
VARIABLES			PREPARED BY:	
T/K = 27	73 - 353		Z. Maczynska	
EXPERIMEN Mu	TAL VALUES: Itual solubility	of carbonic a	cid dimethyl este	r and water
t/°C	g(1)/1 (2)-rich phase	00g sln (1)-rich phas	x ₁ (cor se (2)-rich phas	mpiler) e (1)-rich phase
9.8	12.5	97.84	0.0278	0.9006
20.5	12.7	97.39	0.0283	0.8818
29.7	12.4	96.79	0.0275	0.8577
50 0	13.5	95.90	0.0295	0.8239
60.4	14 3	,95.34	0.0303	0.8030
70 1	14.5	93.19	0.0323	0.7324
79.5	-	92.24 91.67	-	0.6876
std. dev. 0.1 0.06				
<u> </u>	<u> </u>	AUXILIARY :	INFORMATION	
METHOD/AP	METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY	OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		 (1) Source not a cial sample as received (2) Not specifie 	specified, commer- ; purity 99%; used ed.	
		ESTIMATED ERROR: Accuracy of meth for solubility,	nod 0.1 wt% or less, see above.	
		REFERENCES:		

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ORIGINAL MEASUREMENTS:
Apelblat, A.
J. Chem. Soc. B <u>1969</u> , 175-7.
PREPARED BY:
A. Skrzecz
thioic acid 0,0,0-trimethyl ester ^a at L sln. The corresponding value on a compiler is 8.8 g(2)/L sln. eported to be d_4^{25} 1.1904. s not specified. The C.A. number, 0,-trimethyl phosphorothioic acid
INFORMATION
SOURCE AND PURTTY OF MATERIALS:
 (1) Aldrich Chemical Co.; purified by method described in Alcock, Grimley, et al. (ref 1); d₄²⁵ 1.1919, n_D²⁵ 1.4535. (2) Not specified.
ESTIMATED ERROR:
Temp. ±0.1°C.
REFERENCES:
 Alcock, K.; Grimley, S.S.; Healy, T.V.; Kennedy, J.; McKay, H.A.C. Trans. Faraday Soc. <u>1956</u>, 52, 39.

СОМРО	NENTS:	EVALUATOR:
(1)	Acetic acid ethenyl ester (vinyl acetate); C ₄ H ₆ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[108-05-4]	Murdoch University, Perth, W.A.,
(2) Water: H_O: [7732-18-5]	Australia	
\ - /		January, 1989

Quantitative solubility data for the acetic acid ethenyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid ethenyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Smith (ref 1)	298	mutual	titration
Pratt and Glover (ref 2)	293	mutual	titration
Nakamura (ref 3) ·	293	mutual	analytical
Tikhonova et al. (ref 4)	293,339	mutual	analytical
Richon and Viallard (ref 5)	298	(1) in (2)	refractometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID ETHENYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid ethenyl ester (1) in water (2) are summarized in Table 2 except for the value reported by Pratt and Glover (ref 2) at 293 K which is much lower than other studies (ref 3,4) and is rejected.

The remaining data, mainly at 293 and 298 K, are in reasonable agreement although further studies are required before any values can be Recommended.

COMPONENT	S:	EVALUATOR:
(1) Ace (vi	tic acid ethenyl ester nyl acetate); C ₄ H ₆ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
[10	8-05-4]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia	
•		January, 1989

TABLE 2: Tentative Solubilities of Acetic acid ethenyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values	$(\pm \sigma_n)^a$
	g(1)/100g sln	g(1)/100g sln	10 ³ x ₁
293	2.3 (ref 3), 2.0 (ref 4)	2.15 ± 0.15	4.9
298	2.5 (ref 1), 2.67 (ref 5)	2.58 ± 0.09	5.5
339	1.2 (ref 4)	1.2 ^b	2.5

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.

^b Value should be regarded as very Tentative.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID ETHENYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid ethenyl ester (1) are summarized in Table 3. The data are in very poor agreement and further studies will be necessary before even Tentative values can be nominated.

TABLE 3: Reported Solubilities of Water (2) in Acetic acid ethenyl ester (1)

T/K	Reported solubilities	5
	g(2)/100g sln	$10^2 x_2$
293	1.08 (ref 2), 1.1 (ref 3), 0.1 (ref 4)	5.0 (ref 2), 5.0 (ref 3) 0.5 (ref 4)
298	0.1 (ref 1)	0.5 (ref 1)
339	12.3 (ref 4)	40 (ref 4)

COMPONENTS:	EVALUATOR:
 Acetic acid ethenyl ester (vinyl acetate); C₄H₆O₂; 	G.T. Hefter, School of Mathematical and Physical Sciences,
[108-05-4]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia January, 1989

REFERENCES

1. Smith, J. C. J. Phys. Chem. <u>1942</u>, 46, 229-32.

- Pratt, H. R. C.; Glover, S. T. Trans. Inst. Chem. Eng. <u>1946</u>, 24, 54-65.
- 3. Nakamura, A. Kogyo Kagaku Zosshi <u>1968</u>, 71, 319-21.

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- Tikhonova, N. K.; Timofeev, V. S.; Serafimov, L. A.; Tolkacheva, N. L. Izv. Vyssh. Ucheb. Zaved Khim. Khim. Tekhnol. <u>1970</u>, 13, 175-7.
- 5. Richon, D.; Viallard, A. Fluid Phase Equil. 1985, 21, 279-93.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethenyl ester (vinyl acetate); C₄H₆O₂; [108-05-4]</pre>	Smith, J.C. <i>J. Phys. Chem.</i> <u>1942</u> , 46, 229-32.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
EXPERIMENTAL VALUES:	

The solubility of acetic acid ethenyl ester in water at $25^{\circ}C$ was reported to be 2.5 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0053.

The solubility of water in acetic acid ethenyl ester at $25^{\circ}C$ was reported to be 0.1 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.005.

INFORMATION
SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethenyl ester	Pratt, H.R.C.; Glover, S.T.
(vinyl acetate); C ₄ H ₆ O ₂ ; [108-05-4]	Trans. Inst. Chem. Eng. <u>1946</u> , 24, 54-65.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid ethenyl ester in water at 20°C was reported to be 1.14 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00241. The solubility of water in acetic acid ethenyl ester at 20°C was reported to be 1.08 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.0496.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method was used. The data and methods were reported together with the ternary system acetic acid ethenyl ester- water-2-propanone (vinyl acetate- water-acetone).	 (1) Source not specified; commer- cial product; distilled; stabilized with 0.1% hydro- quinone. (2) Distilled.
	ESTIMATED ERROR:
	Temp. ±0.1°C.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethenyl ester (vinyl acetate); C₄H₆O₂; [108-05-4]</pre>	Nakamura, A. <i>Kogyo Kagaku Zasshi <u>1968</u>, 71,</i> 319-21.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

The solubility of acetic acid ethenyl ester in water at 20° C was reported to be 2.3 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0049.

The solubility of water in acetic acid ethenyl ester at $20^{\circ}C$ was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.050.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture was placed in a 1 L flask and stirred for 1 h. which was sufficient for equilibrium. Then, after 1/2 h. separation, sam- ples of both phases were analysed. Acetic acid ethenyl ester was ti- trated with 1.4 mole% Br ₂ in acetic acid. Water was determinated by the Karl Fischer method. Both volumet- ric and analytical methods gave similar results. The method and data were reported together with the ternary system acetic acid ethenyl ester-water-methanol.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Commercial product; distilled; impurities (wt%): ethanol 0.009, acids 0.001, non-volatile 0.001, water 0.005; d 0.934 g/cm³. (2) Purified on ion-exchange material; resistivity >4x10⁶ ohm. ESTIMATED ERROR: Temp. ±0.2°C. REFERENCES:</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Acetic acid ethenyl ester (vinyl acetate); C₄H₆O₂; [108-05-4] (2) Water; H₂O; [7732-18-5] 	Tikhonova, N.K.; Timofeev, V.S.; Serafimov, L.A.; Tolkacheva, N.L. Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. <u>1970</u> , 13, 175-7.	
VARTABLES:	PREPARED BY:	
$\pi/K = 293$ and 339	A. Skrzecz	
EXPERIMENTAL VALUES: Mutual solubility of acetic acid ethenyl ester and water		
$t/^{\circ}C$ $g(1)/100g sln$	x, (compiler)	
(2)-rich phase (1)-rich phas	e (2)-rich phase (1)-rich phase	
20 2.0 99.9	0.0043 0.995	
66.0 ^a 1.2 87.7	0.0025 0.599	
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used. Two-phases mixtures were placed in a thermostated apparatus with a mechanical stirrer, mixed and after separation the samples of both equilibrium phases were analyzed. Water was determined by the Karl Fischer method. The boiling temperature was measured in a Swietoslawski ebulliometer. Only the measurements for the ternary system were described. The data were reported together with the ternary system acetic acid ethenyl ester-water-acetic acid.	 Source not specified; purified; b.p. 72.5°C, physico-chemical properties were in agreement with literature data. Not specified. ESTIMATED ERROR: Not specified. 	
	REFERENCES:	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethenyl ester	Richon, D.; Viallard, A.
(vinyl acetate); C ₄ H ₆ O ₂ ;	Fluid Phase Equilib. <u>1985</u> , 21,
[108-05-4]	279-93.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid etheny: ported to be 0.0319 mol(1)/100g(2) an sponding mass per cent and mole fract compiler are 2.67 g(1)/100g sln and 0	Lester in water at 298.1 K was re- nd 2.74 g(1)/100g(2). The corre- cion, x_1 , values calculated by the 0.00570.
AUXILIARY	
METHOD / APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).	 (1) Merck (for synthesis); purified by preparation gas chromato- graphic method, the purity >99.5%; water content was negligible. (2) Distilled.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES: 1. Richon, D. <i>Thesis</i> , University de Clermont-Ferrand, <u>1974</u> .

COMPONENTS:	EVALUATOR:
<pre>(1) 2-Propenoic acid methyl ester (methyl acrylate); C₄H₆O₂; [96-33-3]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia March, 1990

Quantitative solubility data for the 2-propenoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> 2-Propenoic acid methyl ester (1) - Water (2) System			
Reference	T/K	Solubility	Method
Chubarov et al. (ref 1)	293	mutual	analytical
Filip and Maciejewski (ref 2)	288	mutual	titration
Dabrowski (ref 3)	288,298	(1) in (2)	turbidimetric
Richon and Viallard (ref 4)	298	(1) in (2)	refractometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-PROPENOIC ACID METHYL ESTER (1) IN WATER (2)

All the available solubility data for 2-propenoic acid methyl ester (1) in water (2) are summarized in Table 2. The data are in good agreement and the average values are Recommended although the temperature dependence of the averaged "Best" values is probably dubious.

of 2-Propenoic acid methyl ester (1) in Water (2)

Recommended (R) Solubilities

T/K	Solubilities		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	g(1)/100g sln	$g(1)/100g \ sln \ 10^2 x_1$	
288	5.29 (ref 2), 4.96 (ref 3)	5.1 ± 0.2 (R) 1.11	
293	5.4 (ref 1), 4.96 [*] (ref 3)	5.2 ± 0.2 (R) 1.13	
298	4.96 (ref 3), 5.47 (ref 4)	5.2 ± 0.3 (R) 1.13	

Obtained by averaging where appropriate.

a

TABLE 2:

COMPONENTS:	EVALUATOR:
<pre>(1) 2-Propenoic acid methyl ester (methyl acrylate); C₄H₆O₂; [96-33-3]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia March, 1990

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN 2-PROPENOIC ACID METHYL ESTER (1)

All the available data for the solubility of water (2) in 2-propenoic acid methyl ester (1) are summarized in Table 3. The data of Chubarov et al. (ref 1) and of Filip and Maciejewski (ref 2) although at slightly different temperatures, are in broad agreement, giving some confidence in the values reported which are regarded as Tentative.

> TABLE 3: Tentative Solubilities of Water (2) in 2-Propenoic acid methyl ester (1)

T/K	Reported Solubilities	
	g(2)/100g sln	<i>x</i> ₂
288	2.05 (ref 2)	0.091
293	2.3 (ref 1)	0.101

REFERENCES

 Chubarov, G. A.; Danov, S. M.; Logutov, V. I.; Brovkina, G. V. Zh. Prikl. Khim. <u>1979</u>, 52, 1082-5.

- 2. Filip, S.; Maciejewski, Z. Chem. Stosow. <u>1972</u>, 16, 445-51.
- 3. Dabrowski, L. Thesis, I. Ch. F. PAN, Warszawa, 1984.
- 4. Richon, D.; Viallard, A. Fluid Phase Equil. 1985, 21, 279-93.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) 2-Propenoic acid methyl ester (methyl acrylate); C₄H₆O₂; [96-33-3] (2) Water; H₂O; [7732-18-5] 	Chubarov, G.A.; Danov, S.M.; Logutov, V.I. Zh. Prikl. Khim. <u>1982</u> , 55, 1032-4.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

The solubility of 2-propenoic acid methyl ester in water at 20°C was reported to be 5.4 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0118.

The solubility of water in 2-propenoic acid methyl ester at 20°C was reported to be 2.3 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.101.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The sample was vigorously mixed for 3 min and analysed after separation. Water was determined using the Karl Fischer reagent. The concentration of 2-propenoic acid methyl ester was determined by the bromate method. The data and method were reported together with the ternary system 2-propenoic acid methyl ester-water-sulphuric acid. SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; used as received; n_D^{20} 1.3984.

(2) Twice distilled.

ESTIMATED ERROR:

Temp. ±0.5°C.

REFERENCES:

COMPONENTS (1) 2-Pi (mei [96- (2) Wate	S: ropenoic acid methyl ester thyl acrylate); C ₄ H ₆ O ₂ ; -33-3] er; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Filip, S.; Maciejewski, Z. <i>Chem. Stosow.</i> <u>1972</u> , 16, 445-51.
VARIABLES: T/K = 288	: B	PREPARED BY: A. Skrzecz
EXPERIMENT The solub ported to value cal	TAL VALUES: pility of 2-propenoic acid me p be 5.29 g(1)/100g sln. The lculated by the compiler is (withyl ester in water at 15° C was re- corresponding mole fraction, x_1 , 0.01155.

The solubility of water in 2-propenoic acid methyl ester at 15° C was reported to be 2.05 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.0909.

SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: (1) Source not specified; distilled; d_4^{20} 0.956, n_D^{20} 1.3984. The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant (2) Distilled. temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously. ESTIMATED ERROR: Not specified. **REFERENCES:**

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COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) 2-Propenoic acid methyl ester	Dabrowski. L.		
(methyl acrylate); C ₄ H ₆ O ₂ ;	Thesis Inst Dhys Chem Pol		
[96-33-3]	Acad. Sci., Warszawa, <u>1984</u> .		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 288 and 298	A. Skrzecz		
EXPERIMENTAL VALUES:			
Solubility of 2-propenoic acid methyl ester in water			
	X.		
	~1		
288.15 4.96	0.0108		
298.15 4.96	0.0108		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
The modified Othmer-White-Trueger	(1) Synthesized by esterification;		
method was used. The samples of known composition	distilled on a 70 TP column, washed with 20 % KOH and		
were slowly cooled to obtain the	several times with distilled		
was a little below the desired	water, 0.1 % of hydroquinone was added to protect		
temperature. After addition of a	polymerization.		
procedure was repeated.	(2) Twice distilled.		
the solubility at the desired temperature was obtained by an			
interpolation. All measurements were made in a thermostated vessel	ESTIMATED ERROR:		
of 50 cm^3 in the range $\pm 3^\circ\text{C}$ of the	Temp. $\pm 0.05^{\circ}$ C. Soly. ± 0.02 g(1)/100g sln.		
of the samples were measured with			
a mercury-in-glass thermometer. A magnetic stirrer was used. The	DEEEDENCES		
water included in ester was taken	REFERENCES;		
were reported together with the			
ternary system 2-propenoic acid methyl ester-water-2-propenoic acid			
(methyl acrylate- water-acrylic			

COMPONENTS: (1) 2-Propenoic acid methyl ester (methyl acrylate); $C_4H_6O_2$; [96-33-3] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Richon, D.; Viallard, A. <i>Fluid Phase Equilib</i> . <u>1985</u> , 21, 279-93.
VARIABLES: T/K = 298	PREPARED BY: A. Skrzecz

The solubility of 2-Propenoic acid methyl ester in water at 298.1 K was reported to be 0.0672 mol(1)/100g(2) and 5.79 g(1)/100g(2). The corresponding mass per cent and mole fraction, x_1 , values calculated by the compiler are 5.47 g(1)/100g sln and 0.01197.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) Merck (for synthesis); purified by preparation gas chromato- graphic method, the purity >99.5%; water content was negligible. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES: 1. Richon, D. Thesis, University de Clermont-Ferrand, 1974.</pre>		

COMPONENTS:		EVALUATOR:	
(1)	1,3-Dioxolan-2-one, 4-methyl-	G.T. Hefter, School of Mathematical	
	(propylene carbonate);	and Physical Sciences,	
	C ₄ H ₆ O ₃ ; [108-32-7]	Murdoch University, Perth, W.A.,	
(2)	Water: H_O: [7732-18-5]	Australia	
(2)		March, 1990	

Quantitative solubility data for the 4-methyl-1,3-dioxolan-2-one (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 4-Methyl-1,3-dioxolan-2-one (1) - Water (2) System

Reference	T/K	Solubility	Method
Catherall and Williamson (ref 1)	243-334	mutual	synthetic
Hong et al. (ref 2)	,223-344	mutual	titration

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 4-METHYL-1, 3-DIOXOLAN-2-ONE (1) IN WATER (2)

All the available data for the solubility of 4-methyl-1,3-dioxolan-2one (1) in water (2) are summarized in Table 2. Whilst agreement between the two studies (ref 1,2) in the middle temperature range is good and the average values are Recommended, they differ at more extreme temperatures, see Figure 1.

TABLE 2: Recommended (R) and Tentative Solubilities

	<u>Of 4-Methyl-1,3-dloxolan-2-one (1) in water (2)</u>		
T/K	Solubilities		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	g(1)/100g sln	$g(1)/100g \ sln \ 10^2 x_1$	
278	13 [*] (ref 1), 6 [*] (ref 2)	10 ± 4 1.9	
283	15 [*] (ref 1), 10 [*] (ref 2)	13 ± 3 2.6	
293	17 [*] (ref 1), 16 [*] (ref 2)	16.5 ± 0.5 (R) 3.4	
298	17.5 [*] (ref 1), 17.8 [*] (ref 2)	17.7 ± 0.2 (R) 3.7	



COMPONENTS:		EVALUATOR:
(1)	1,3-Dioxolan-2-one, 4-methyl- (propylene carbonate);	G.T. Hefter, School of Mathematical and Physical Sciences,
	C ₄ H ₆ O ₃ ; [108-32-7]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia
		March, 1990

2. SOLUBILITY OF WATER (2) IN 4-METHYL-1,3-DIOXOLAN-2-ONE (1)

All the available data for the solubility of water (2) in 4-methyl-1,3-dioxolan-2-one (1) are summarized in Table 3. In general the data are in only fair agreement and show a very different dependence on temperature. Further studies are required before any of the average "Best" values can be Recommended. The data are also plotted in Figure 2.

T/K	Solubilities		
	Reported values	"Best" values	$(\pm \sigma_n)^a$
	g(2)/100g sln	g(2)/100g sln	<i>x</i> ₂
243b	1.0 [*] (ref 1), 1.2 [*] (ref 2)	1.1 ± 0.1	0.06
253 ^b	2.0 [*] (ref 1), 2.2 [*] (ref 2)	2.1 ± 0.1	0.11
263 ^b	2.8 [*] (ref 1), 3.3 [*] (ref 2)	3.1 ± 0.3	0.15
273	3.3 [*] (ref 1), 4.3 [*] (ref 2)	3.8 ± 0.5	0.18
283	4.0 [*] (ref 1), 5.2 [*] (ref 2)	4.6 ± 0.6	0.21
293	5.4 [*] (ref 1), 6.1 [*] (ref 2)	5.8 ± 0.4	0.26
298	7.0 (ref 1), 6.9 (ref 2)	7.0 ± 0.1	0.30
303	9.2 [*] (ref 1), 8.0 [*] (ref 2)	8.6 ± 0.6	0.35
313	14.1 [*] (ref 1), 10.6 [*] (ref 2)	12 ± 2	0.44
323	21.1 [*] (ref 1), 13.8 [*] (ref 2)	17 ± 4	0.54
333	18.4 [*] (ref 2)	18	0.55
343	36.0 [*] (ref 2)	36	0.76

<u>TABLE 3: Tentative Solubilities</u> of Water (2) in 4-Methyl-1,3-dioxolan-2-one (1)

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

^b Solid-liquid equilibrium.

(continued next page)

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COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) 1,3-Dioxolan-2-one, 4-methyl-			Catherall, N.F.;	Williamson, A.G.	
(pr	opylene carbonat	te);	J. Chem. Eng. Dat	ta <u>1971</u> , 16,	
с ₄ н	₆ 0 ₃ ; [108-32-7]		335-6.	335-6.	
(2) Wat	er; H ₂ O; [7732-1	18-5]			
VARIABLES	5:	<u> </u>	PREPARED BY:		
T/K = 24	3 - 334		A. Skrzecz		
EXPERIMEN	TAL VALUES:				
Mu 	tual solubility	of 4-methyl-	1,3-dioxolan-2-one	and water	
Mu t/°C	g(1)/10	of 4-methyl-	1,3-dioxolan-2-one a	and water	
Mu t/°C	g(1)/10 (2)-rich phase	of 4-methyl- 00g sln (1)-rich pha	1,3-dioxolan-2-one (x ₁ se (2)-rich phase	and water (1)-rich phase	
Mu t/°C -30.1 ^a	g(1)/10 (2)-rich phase 	of 4-methyl- 00g sln (1)-rich pha 	1,3-dioxolan-2-one a x ₁ se (2)-rich phase 	(1)-rich phase	
Mu t/°C -30.1 ^a -15.5 ^a	g(1)/10 (2)-rich phase - -	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5	1,3-dioxolan-2-one (x ₁ se (2)-rich phase - - -	(1)-rich phase 0.9854 0.8732	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a	g(1)/10 (2)-rich phase - - 5.0	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 -	1,3-dioxolan-2-one x ₁ se (2)-rich phase - - - 0.0092	(1)-rich phase 0.9854 0.8732	
Mu t/°C -30.1 ^a -15.5 ^a ~0.6 ^a 0.	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0.	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 -	1,3-dioxolan-2-one (x ₁ se (2)-rich phase - - 0.0092 0.	(1)-rich phase 0.9854 0.8732 -	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a 0. 1.5	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0. 10.0	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 - - -	1,3-dioxolan-2-one (x ₁ se (2)-rich phase - - 0.0092 0. 0.0192	(1)-rich phase 0.9854 0.8732 - - -	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a 0. 1.5 20.1	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0. 10.0 -	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 - - - 94.6	1,3-dioxolan-2-one x ₁ se (2)-rich phase 0.0092 0. 0.0192 -	and water (1)-rich phase 0.9854 0.8732 - - - 0.7556	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a 0. 1.5 20.1 25.0	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0. 10.0 - 17.5	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 - - 94.6 93.0	1,3-dioxolan-2-one (x ₁ se (2)-rich phase - - 0.0092 0. 0.0192 - 0.0361	(1)-rich phase 0.9854 0.8732 - - 0.7556 0.7010	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a 0. 1.5 20.1 25.0 30.1	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0. 10.0 - 17.5 19.6	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 - - 94.6 93.0 -	1,3-dioxolan-2-one (x ₁ se (2)-rich phase - - 0.0092 0. 0.0192 - 0.0361 0.0412	(1)-rich phase 0.9854 0.8732 - - 0.7556 0.7010 -	
Mu t/°C -30.1 ^a -15.5 ^a -0.6 ^a 0. 1.5 20.1 25.0 30.1 41.6	g(1)/10 g(1)/10 (2)-rich phase - - 5.0 0. 10.0 - 17.5 19.6 -	of 4-methyl- 00g sln (1)-rich pha 99.0 97.5 - - 94.6 93.0 - 85.0	1,3-dioxolan-2-one a x ₁ se (2)-rich phase - 0.0092 0. 0.0192 - 0.0361 0.0412 -	(1)-rich phase 0.9854 0.8732 - - 0.7556 0.7010 - 0.5000	

_

0.3343

59.7	47.8	-	0.1391
61.1	57.5	-	0.1926
a	Solid-liquid	equilibrium.	

-

56.1

74.0

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The cloud-point method at temper- atures above 0°C and the cooling curves method at low temperature were used. For the cloud-point method, mixtures of known composi- tion, sealed in 5-mm pyrex tubes, were immersed in a water bath at a temperature above the unmixing temperature and cooled at about 0.5°C/min. The cloud point temper- atures were measured with a mercu- ry-in-glass thermometer and the means of several observations were presented. In the cooling curves procedure, Cooling curves were measured on mixtures prepared by weight in 25 cm ³ test tubes and cooled slow- ly in a dry ice-acetone bath. Tem- peratures were measured with a thallium amalgam thermometer.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Koch Light "puriss"-grade; purity >99%; dried over a Linde molecular sieve, grade 5A. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Temp. ±0.1°C^b and ±0.2°C^c. b Cloud-point method. c Cooling curves method. REFERENCES:</pre>

COMPONENTS:			ORIGINAL MEASUREMENTS:		
<pre>(1) 1,3-Dioxolan-2-one, 4-methyl- (propylene carbonate);</pre>			Hong, C.S.; Waksi Finston, H.; Fr	ak, R.; ied, V.	
C ₄ H ₆ O ₃ ; [108-32-7]			J. Chem. Eng. Dat 146-8.	a <u>1982</u> , 27,	
(2) Wat	er; H ₂ O; [7732-1	18-5]			
ARIABLES	:		PREPARED BY:		
T/K = 22	3 - 344		A. Skrzecz		
XPERIMEN Mu	TAL VALUES: tual solubility	of 4-methyl-1	,3-dioxolan-2-one a	und water	
t/°C	g(1)/10)0g sln	x_1 (comp	iler)	
	(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase	
-50.2 ^a	_	100.00		1.0000	
-28.1 ^a	-	98.76	-	0.9336	
-1.8 ^a	10.11	-	0.01946	-	
-0.9 ^a	5.13	-	0.00945	-	
0.0	0.00	-	0.00000	-	
7.5	-	94.94		0.7680	
25.0	17.8	93.1	0.03681	0.7042	
27.1	20.46	-	0.04342	_	
40.1	_	89.34	-	0.5966	
62.6	_	79.76	-	0.4102	
67.2	39.41	_	0.10296	-	
71.0	_	59.58	-	0.2064	
a So	lid-liquid equil	ibrium.	<u> </u>		
- <u></u>					
		AUXILIARY I	NFORMATION		
ETHOD/AP	PARATUS/PROCEDU	RE:	SOURCE AND PURITY	OF MATERIALS:	
The titr water sa 4-methyl	ation method was mples were titra -1,3-dioxolan-2-	s used. The ited with one and	(1) Jefferson Che purified by r low-pressure	mical Co., Inc.; epeated distillation;	
4-methyl-1,3-dioxolan-2-one samples were titrated with water at various temperatures. The turbidity point was found to be reproducible within one very small drop (0.015 cm ³). No			d_4^{25} 1.2004.		
			(2) Not specified; d ₄ ³ 0.9986.		
the pape	aetalls were rep r.	oortea in	ESTIMATED ERROR:		
			Soly. <±0.3 g(1)/ (accuracy).	100g sln	
		-	REFERENCES:		
			_		

COMPONENTS:		EVALUATOR:
(1)	Ethanedioic acid dimethyl	G.T. Hefter, School of Mathematical
	ester (dimethyl oxalate);	and Physical Sciences,
	C ₄ H ₆ O ₄ ; [553-90-2]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732-18-5]	Australia
(2)		January, 1989

Quantitative solubility data for the ethanedioic acid dimethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Ethanedioic acid dimethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Skrabal (ref 1)	273-327	mutual	thermal
Dehn (ref 2)	'R.T. ^a	(1) in (2)	gravimetric
Kendall and Harrison (ref 3)	273-369	(1) in (2)	synthetic

^a R.T. - room temperature (sic).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ETHANEDIOIC ACID DIMETHYL ESTER (1) IN WATER (2)

All the available solubility data for ethanedioic acid dimethyl ester (1) in water (2) are summarized in Table 2. As can be seen, the independent studies are not in good agreement. The data of Kendall and Harrison (ref 3) have been chosen as the best available because solubilities reported by these authors in well characterized systems are generally reliable. Nevertheless, it should be noted that the experimental results of Kendall and Harrison (ref 3) for this system are rather scattered.

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COMPONENTS:		EVALUATOR:
(1)	Ethanedioic acid dimethyl ester (dimethyl oxalate);	G.T. Hefter, School of Mathematical and Physical Sciences,
	C ₄ H ₆ O ₄ ; [553-90-2]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

TABLE 2: Tentative Solubilities of Ethanedioic acid dimethyl ester (1) in Water (2)

T/K	Solubi	lities	
-	Reported values	"Best" valu	es ^a
	g(1)/100g sln	g(1)/100g sln	10 ² x1
273	4 ^b (ref 1), 2.60* (ref 3)	3	0.5
283	7.13 [*] (ref 3)	7	1.1
293	5.82 ^c (ref 2), 12.4 [*] (ref 3)	12	2.0
298	15.3 [*] (ref 3)	15	2.6
303	18.1 [*] (ref 3)	18	3.2
313	23.9 [*] (ref 3)	24	4.6
323	16 ^d (ref 1), 29.4 [*] (ref 3)	29	5.9
333	34.3 [*] (ref 3)	34	7.3
343	38.3 [*] (ref 3)	38	8.5
353	40.9 [*] (ref 3)	41	9.6
a Rour	nded values of ref 3.		
^b 272.	.7 K.		
c Roon	n temperature.		
^d 321	к.		
2. SOI The	LUBILITY OF WATER (2) IN ETHANEDIO e only datum available for the solu	IC ACID DIMETHYL EST ability of water (2)	ER (1) in ethane-
dioic ac	cid dimethyl ester (1) is that of s	Skrabal (ref 1) and s reader is referred to	so no Critical
Data She	eet for the experimental solubility	······	
REFERENC	CES		
1. Skr	cabal, A. Monatsch. Chem. <u>1917</u> , 38	3, 25-9.	
2. Del	2. Dehn, W. M. J. Am. Chem. Soc. <u>1917</u> , 39, 1399-404.		
3. Ker	ndall, J.; Harrison, E. Trans. Fa	araday Soc. <u>1928</u> , 24,	, 588-96.

r			······································		
COMPONENTS:			ORIGINAL MEASUREM	ENTS:	
(1) Ethanedioic acid dimethyl		Skrabal, A.			
ester (dimethyl oxalate);		Monatsch. Chem.	<u>1917</u> , 38, 25-9.		
C ₄ H ₆ O ₄	; [553-90-2]				
(2) Water;	H ₂ O; [7732-18	-5]		<u> </u>	
VARIABLES:			PREPARED BY:		
T/K = 273 -	- 327		Z. Maczynska		
EXPERIMENTAI	VALUES:		<u>1</u>		
Mutual	. solubility of	ethanedioic	acid dimethyl est	er and water	
t/°C	g(1)/100	g sln	<i>x</i> ₁ (com)	piler)	
(2)-rich phase (1)-rich phas	e (2)-rich phase	(1)-rich phase	
-0.5ª	4		0.006	-	
48 ^b	16	94	0.028	0.71	
53.5 ^c	-	100	-	1.00	
<u></u>		AUXILIARY J	INFORMATION		
METHOD/APPAR	ATUS/PROCEDURE	:	SOURCE AND PURITY	OF MATERIALS:	
The thermal	analysis metho	od was	(1) Not specified.		
used. No de the paper.	tails were rep	orted in	(2) Not specified.		
			ESTIMATED ERROR:		
			Not specified.		
			REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethanedioic acid dimethyl	Dehn, W.M.
ester (dimethyl oxalate); C ₄ H ₆ O ₄ ; [553-90-2]	J. Am. Chem. Soc. <u>1917</u> , 39, 1399-1404.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = room temperature	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of ethanedioic acid d: perature ^a was reported to be 6.18 g(1 percentage and mole fraction, x ₁ , val 5.82 g(1)/100g sln and 0.00934. ^a room temperature was reported to	imethyl ester in water at room tem- .)/100g(2). The corresponding mass ues calculated by the compiler are be 20-25°C.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Excess of the substance and 5 mL of	(1) Not specified.
which when stoppered were shaken or let stand until equilibria were established. The solution was then filtered into weighed crucibles and reweighed. After drying in a vacuum desiccator or on a water bath, the	(2) Not specified.
crucibles were again weighed and the loss of solvent calculated.	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Ethanedioic acid dimethyl	Kendall, J.; Harrison, L.E.	
ester (dimethyl oxalate);	Trans, Faraday Soc. 1928, 24.	
C ₄ H ₆ O ₄ ; [553-90-2]	588-96.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
$\pi/K = 273 - 369$	Z Maczynska	
1/1 210 305		
EXPERIMENTAL VALUES:		
Solubility of ethanedioic acid dime	thyl ester in water	
t/°C x ₁ g(1)/100g	sln (compiler)	
0.1 0.00541	3 44	
	7.62	
19.5 0.01853 1	1.01	
27.1 0.0268 1	5.3	
31.9 0.0336 1	8.6	
44.4 0.0536 2	7.1	
49.2 0.0607 2	9.8	
51.0 0.0646 3	1.2	
53.0 0.0691 3	2.7	
75.0 0.0861 3	8.2	
79.3 0.0889 3	9.0	
96.1 0.1022 4	2.7	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The synthetic method was used. The	(1) Source not specified,	
sealed tube method (ref 1) was adopted, the free space being kept	CP commercial sample; distilled: b.p. range 0.1°C.	
as small as possible in order to	m.p. 54.35°C.	
composition at the higher tempera-	(2) Distilled.	
tures.		
	ESTIMATED ERROR	
	Temp. $\pm (0.1-0.2)$ °C.	
	REFERENCES:	
	1 Smith A · Fastlack H F	
	J. Am. Chem. Soc. <u>1916</u> , 38,	
	1269.	
]	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 Acetic acid 2-bromoethyl ester (2-bromoethyl acetate); C₄H₇BrO₂; [927-68-4] Water; H₂O; [7732-18-5] 	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. <i>J. Chem. Eng. Data</i> <u>1982</u> , 27, 451-4.	
VARIABLES: T/K = 298	PREPARED BY: A. Skrzecz	

The solubility of acetic acid 2-bromoethyl ester in water at $25^{\circ}C$ was reported to be 0.212 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 25.9 g(1)/L sln.

AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of water reservoir using compressed air at 5 psi. The solute concentration in the aqueous phase was analyzed by a high-pressure liquid chromato- graphic technique described in Devoe, Miller and Wasik (ref 1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; purity >99% by glc. (2) Not specified. (2) Not specified. ESTIMATED ERROR: Temp. ±0.1°C. Soly. ±1.0%. REFERENCES: 1. DeVoe, H.; Miller, M.M.; Wasik, S.P. J. Res. Nat. Bur. Stand. 1981, 86, 361.</pre>			

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid, chloro-, ethyl	Stephenson, R.; Stuart, J.
ester (ethyl chloroacetate);	J. Chem. Eng. Data <u>1986</u> , 31,
C ₄ H ₇ ClO ₂ ; [105-39-5]	56~70.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska

Mutual solubility of chloroacetic acid ethyl ester and water

t∕°C	g(1)/100g sln		x ₁ (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
	2.49	00 53	0.00374	0.9689
9.0	2.50	99.43	0.00375	0.9625
19.8	2.00	99.33	0.00299	0.9561
30.8	1.90	99.19	0.00284	0.9474
39.9	1.88	99.11	0.00281	0.9424
50.0	1.92	98.83	0.00287	0.9254
60.1	1.97	98.55	0.00294	0.9090
70.2	2.11	98.24	0.00316	0.8913
80.1	2.19	97.99	0.00328	0.8775
90.5	2.33	97.54	0.00349	0.8535
std. de	v. 0.01	0.01		-,,

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Propanoic acid, 2-chloro-, methyl ester (methyl 2-chloropropionate); C₄H₇ClO₂; [17639-93-9] Water; H₂O; [7732-18-5] 	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
VARIABLES: $T/K = 273 = 364$	PREPARED BY:
1/K = 2/3 = 304	

Mutual solubility of 2-chloropropanoic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0		99.58		0.9721
10.0	2.42	99.47	0.00363	0.9650
19.8	2.29	99.40	0.00343	0.9606
29.7	1.66	99.32	0.00247	0.9555
40.3	1.62	99.24	0.00241	0.9505
50.2	1.69	99.17	0.00252	0.9461
60.1	1.81	99.08	0.00270	0.9406
70.3	1.91	98.46	0.00285	0.9038
80.2	1.98	98.63	0.00296	0.9137
90.5	2.13	97.96	0.00319	0.8759
std. der	v. 0.01	0.02		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 97%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:
COMPONENTS:		EVALUATOR:	
(1)	Acetic acid ethyl ester	G.T. Hefter, School of Mathematical	
	(ethyl acetate); C ₄ H ₈ O ₂ ;	and Physical Sciences,	
	[141-78-6]	Murdoch University, Perth, W.A.,	
(2)	Water: H_O: [7732-18-5]	Australia	
(-)		January, 1989	

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid ethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Mohr (ref 1)	RT ^a	(1) in (2)	titration
Marsson (ref 2)	291	mutual	cloud point
Traube (ref 3)	• 295	(1) in (2)	unspecified
Bancroft (ref 4)	293	mutual	titration
Euler (ref 5)	301	(1) in (2)	analytical
Rayman (ref 6)	273-303	(1) in (2)	volumetric
Bonner (ref 7)	273	mutual	titration?
Seidell (ref 8)	283-313	mutual	titration
Merriman (ref 9)	273-333	mutual	synthetic, analytical
Euler and Svanberg (ref 10)	291	(1) in (2)	unspecified
Fuehner (ref 11)	293	(1) in (2)	titration
Glasstone and Pound (ref 12)	273-323	(1) in (2)	analytical
Kendall and Harrison (ref 13)	273-323	(1) in (2)	synthetic
Jones (ref 14)	293	mutual	synthetic?
Schlesinger and Kubasowa (ref 15)	288-323	(1) in (2)	synthetic
Mion (ref 16)	273-303	mutual	turbidimetric
Park and Hofmann (ref 17)	298	mutual	unspecified
Doolittle (ref 18)	293	mutual	unspecified
Lloyd et al. (ref 19)	298	mutual	titration
Beech and Glasstone (ref 20)	273-313	mutual	synthetic?
Shanley and Greenspan (ref 21)	RT ^a	(2) in (1)	unspecified
Griswold et al. (ref 22)	290-344	mutual	synthetic
Sohoni and Warhadpande (ref 23)	303	mutual	synthetic
			(continued next pa

COMPONENTS:		EVALUATOR:		
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989		
CRITICAL EVALUATION: (continue	:d)			
Reference	T/K	Solubility	Method	
Altshuller and Everson (ref 24)	292-313	(1) in (2)	synthetic	
Garner and Ellis (ref 25)	303	(1) in (2)	titration	
Gayler and Pratt (ref 26)	288-303	mutual	titration, analytical	
Jones and McCants (ref 27)	311	mutual	titration	
Rao and Rao (ref 28)	303	mutual	titration	
Venkataratnam <i>et al</i> . (ref 29)	303	mutual	titration	
Rao et al. (ref 30)	308	mutual	titration	
Akita and Yoshida (ref 31)	298,343	mutual	titration, analyical	
Zheleznyak and Brounshtein (ref 32)	298,323	mutual	analytical	
Pai and Sane (ref 33)	273,303	mutual	turbidimetric	
Nakamura (ref 34)	303	mutual	analytical	
Batmanova <i>et al</i> . (ref 35)	293,344	mutual	titration, analytical	
Iguchi and Fuse (ref 36)	298	mutual	titration	
Krupatkin and Shcherbakova (ref 37)	298	mutual	titration	
Utkin et al. (ref 38)	298,313	mutual	titration	
Aleksandrova et al. (ref 39)	293	mutual	titration	
Filip and Maciejewski (ref 40)	293	mutual	titration	
Mertl (ref 41)	293-343	mutual	titration	
Sadovnikova <i>et al</i> . (ref 42)	293	mutual	unspecified	
Woycicka et al. (ref 43)				
Van Zandijcke and Verhoeye (ref 44)	343	mutual	GLC	
Tare et al. (ref 45)	303	(1) in (2)	titration	
Sugi and Katayama (ref 46)	333	mutual	cloud point	
Alvarez and Neila (ref 47)	298	mutual	titration?	
			(continued next page)	

COMPONENTS:		EVALUATOR:	
 Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] Water; H₂O; [7732-18-5] 		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989	
CRITICAL EVALUATION: (continue	d)		
Reference	T/K	Solubility	Method
Skrzecz and Maczynski (ref 48)	286-364	mutual	synthetic
Tewari et al. (ref 49)	298	(1) in (2)	GLC
Ouyang et al. (ref 50)	323	mutual	GLC
Richon and Viallard (ref 51)	298,318	mutual	calorimetric, refractometric
Stephenson and Stuart (ref 52)	273-344	mutual	GLC

^a RT - room temperature.

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Data available in the article by Hill (ref 53), which are composite values based on published and unpublished data, have been omitted because of the ready availability of other good quality data. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exceptions.

The data of Marsson (ref 2), Traube (ref 3), Euler (ref 5), Fuehner (ref 11) and Doolittle (ref 18) at ca. 293 K, Iguchi and Fuse (ref 36) at 298 K, and Garner and Ellis (ref 25) at 303 K are all substantially lower (> $3\sigma_n$) than other studies and have therefore been rejected. Similarly, the data of Van Zandijcke and Verhoeye (ref 44) at 343 K and Ouyang et al. (ref 50) are substantially higher (> $3\sigma_n$) than other studies and have also been rejected. The data of Mohr (ref 1, unspecified temperature), Bancroft (ref 4, v/v units), Euler and Svanberg (ref 10), and Tewari et al. (ref 49, w/v units) have been excluded from consideration because of the abundance of other good quality data.

The remaining data, the most substantial set for any ester-water system, are generally in good agreement enabling the average "Best" values to be Recommended over a wide range. Selected data for the solubility of acetic acid ethyl ester in water are plotted in Figure 1.

(continued next page)

COMPONENTS:		EVALUATOR:
(1)	Acetic acid ethyl ester	G.T. Hefter, School of Mathematical
	(ethyl acetate); C ₄ H ₈ O ₂ ;	and Physical Sciences,
	[141-78-6]	Murdoch University, Perth, W.A.,
(2)	Water: H.O: [7732-18-5]	Australia
, ,		January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (R) and Tentative Solubilities of Acetic acid ethyl ester (1) in Water (2)

ĺ	T/K	Solubilit	ies		
		Reported values	"Best"	values (±	$\sigma_n)^a$
		g(1)/100g sln	g(1)/100g	sln	$10^2 x_1$
	273	9.86 (ref 6), 9.80 (ref 7), 10.08 (ref 9), 10.40 (ref 12), 9.41 (ref 13), 10 (ref 16), 9.67 (ref 20), 9.29 (ref 33), 9.71 (ref 52)	9.8 ± 0.3	(R)	2.17
	283	8.84 (ref 6), 9.15 (ref 8), 8.81 (ref 9), 8.96 (ref 12), 8.19 (ref 13), 8.8* (ref 16), 8.61 (ref 20), 8.2* (ref 48), 8.60* (ref 52)	8.7 ± 0.3	(R)	1.91
	293	7.94 (ref 6), 8.27 (ref 8), 7.86 (ref 9), 7.85 (ref 12), 7.28 (ref 13), 8.53 (ref 14), 7.77 (ref 15), 7.8* (ref 16), 7.75 (ref 20), 7.68* (ref 22), 7.77 (ref 24), 7.74* ^b (ref 26), 8.51 (ref 32), 7.86 (ref 35), 8.70 (ref 39), 8.22 (ref 40), 7.31 (ref 41), 8.9 (ref 42), 8.1* (ref 48), 7.70* (ref 52)	8.0 ± 0.4	(R)	1.74
	298	7.59* (ref 6), 7.90 (ref 8), 7.48 (ref 9), 7.39 (ref 12), 6.84 (ref 13), 7.43 (ref 15), 7.4* (ref 16), 7.9 (ref 17), 7.56 (ref 19), 7.42* (ref 20), 7.30* (ref 22), 7.42 (ref 24), 7.48* ^b (ref 26), 7.47 (ref 37), 6.9 (ref 38), 6.99 (ref 41), 7.48 (ref 43), 7.3 (ref 47), 8.0* (ref 48), 7.50 (ref 51), 7.21* (ref 52)	7.4 ± 0.3	(R)	1.61
	303 ^c	7.23 (ref 6), 7.61 (ref 8), 7.15 (ref 9), 7.06 (ref 12), 6.58 (ref 13), 7.14 (ref 15), 7.1 (ref 16), 7.10" (ref 20), 7.1" (ref 22), 7.10 (ref 23), 7.15 (ref 24), 7.22" ^D (ref 26), 7.22 (ref 28), 7.4 (ref 29), 7.5 (ref 31), 6.70 (ref 33), 6.7 (ref 34), 6.5" (ref 38), 6.68" (ref 41), 7.56" (ref 45), 7.5" (ref 48), 7.20" (ref 51), 6.76" (ref 52)	7.1 ± 0.3	(R)	1.54
				(continued	next page)

COMPC	DNENTS:	EVALUATOR:
(1)	Acetic acid ethyl ester (ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRITI	CAL EVALUATION: (continued)	
т/к	Sol	ubilities
	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(1)/100g sln	g(1)/100g sln $10^2 x_1$
313 ^đ	7.17 (ref 8), 6.63 (ref 9), 6.50 (ref 12), 6.10 (ref 13 6.70 (ref 15), 6.52 (ref 20 6.8* (ref 22), 6.65 (ref 24 5.8 (ref 38), 5.95* (ref 41 6.7* (ref 48), 6.70* (ref 5 6.34* (ref 52)	6.5 ± 0.4 1.40),),),), 1),
323	6.04 (ref 12), 5.65 (ref 13 6.43 (ref 15), 6.6 [*] (ref 22 6.93 (ref 32), 5.72 [*] (ref 4 6.0 [*] (ref 48), 6.18 [*] (ref 5), 6.2 ± 0.4 1.33), 1), 2)
333	6.4 [*] (ref 22), 5.40 [*] (ref 4 5.52 (ref 46), 5.8 [*] (ref 48 6.04 (ref 52)	1), 5.8 ± 0.4 1,24),
343	6.3 [*] (ref 22), 6.2 [*] (ref 31) 6.3 ^e (ref 35), 5.14 [*] (ref 4) 6.1 [*] (ref 48), 5.89 [*] (ref 5)), 6.0 ± 0.4 1.29 1), 2)
353	6.5 [*] (ref 48)	6.5 1.40
363	8.4 [*] (ref 48)	8.4 1.84

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.

^b Average of results from two separate methods.

^c Data from ref 5 at 301 K omitted for representational convenience.

^d Data from ref 27 at 311 K omitted for representational convenience.

e 343.6 K.

(continued next page)



COMPONENTS:	EVALUATOR:
 Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; 	G.T. Hefter, School of Mathematical and Physical Sciences,
[141-78-6]	Murdoch University, Perth, W.A.,
(2) Water: H ₂ O: [7732-18-5]	Australia
	January, 1989

CRITICAL EVALUATION: (continued)

The remaining data are generally in good agreement enabling the averaged "Best" values to be Recommended over quite a range. Selected data are plotted in Figure 2.

TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid ethyl ester (1)

T/K	Solubilities	
	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(2)/100g sln	$g(2)/100g \ sln x_2$
273	2.28 (ref 9), 2.26'(ref 16), 2.3 (ref 20), 2.38 (ref 33), 2.13 (ref 52)	2.27 ± 0.08 (R) 0.102
283	2.61 (ref 9), 2.60 [*] (ref 16), 2.49 (ref 52)	2.57 ± 0.05 (R) 0.114
293	2.98 (ref 9), 3.07 (ref 14), 3.05 (ref 16), 2.8 (ref 20), 3.1* (ref 22), 3.02 ^b (ref 26), 3.0 (ref 35), 2.96 (ref 41), 2.87* (ref 52)	2.98 ± 0.09 (R) 0.130
298	3.19 (ref 9), 3.28 [*] (ref 16), 3.0 (ref 17), 3.24 (ref 19), 3.2 [*] (ref 22), 3.22 ^b (ref 26), 3.1 (ref 38), 3.17 [*] (ref 48), 3.08 [*] (ref 52)	3.16 ± 0.08 (<i>R</i>) 0.138
303	3.42 (ref 9), 3.52 (ref 16), 3.5* (ref 22), 3.50 (ref 23), 3.47 ^b (ref 26), 3.47 (ref 28), 3.5 (ref 29), 3.25 (ref 33), 3.7 (ref 34), 3.4* (ref 38), 3.40 (ref 41), 3.60* (ref 48), 3.28* (ref 52)	3.46 ± 0.11 (<i>R</i>) 0.149
313	3.98 (ref 9), 4.0 [*] (ref 22), 3.9 (ref 38), 3.88 (ref 41), 3.98 (ref 48), 3.68 [*] (ref 52)	3.90 ± 0.11 (R) 0.166
323	4.46 (ref 9), 4.5 [*] (ref 22), 4.40 (ref 41), 4.54 [*] (ref 48), 4.23 (ref 50), 4.03 [*] (ref 52)	4.36 ± 0.18 (R) 0.195
333	5.02 (ref 9), 5.1 [*] (ref 22), 5.00 [*] (ref 41), 4.985 (ref 46), 5.24 [*] (ref 48)	5.07 ± 0.09 (R) 0.207

^a Obtained by averaging where appropriate.

^b Average of two independent determinations.

(continued next page)

COMPONENTS:		EVALUATOR:
(1)	Acetic acid ethyl ester	G.T. Hefter, School of Mathematical
	[141-78-6]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION: (continued)

T/K	Solubilities		
	Reported values	"Best" values $(\pm \sigma_n)^a$	
	g(2)/100g sln	g(2)/100g sln x ₂	
343	5.8 [*] (ref 22), 6.0 (ref 31), 5.8 ^c (ref 35), 5.61 (ref 41), 6.38 ^d (ref 44), 6.02 (ref 48)	5.9 ± 0.2 (R) 0.235	
353	6.82 [*] (ref 48)	6.8 0.263	
363	7.59* (ref 48)	7.6 0.286	

° 343.6 K.

^d 343.4 K.

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.



COMPONENTS: EVALUATOR: G.T. Hefter, School of Mathematical Acetic acid ethyl ester (1) (ethyl acetate); C₄H₈O₂; and Physical Sciences, Murdoch University, Perth, W.A., [141-78-6] Australia Water; H₂O; [7732-18-5] (2) January, 1989 CRITICAL EVALUATION: (continued) REFERENCES 1. Mohr Arch. Pharm. 1851, 65, 1-16. Marsson, T. Arch. Pharm. 1853, 74, 290-6. 2. 3. Traube, J. Ber. Dtsch. Chem. Ges. 1884, 17, 2294-316. Bancroft, W. D. Phys. Rev. 1895, 3, 114-36. 4. Euler, H. Z. Phys. Chem. 1899, 31, 360-9. 5. Rayman, J. Thesis, Budapest 1906. 6. 7. Bonner, W. D. J. Phys. Chem. 1910, 14, 738-89. Seidell, A. Hygienic Lab. Bull. 1910, No. 67, 98 pp. (U.S. Govt. 8. Printing Office, Washington, DC). 9. Merriman, R. W. J. Chem. Soc. 1913, 103, 1774-89. Euler, H.; Svanberg, O. Ark. Kem. Mineral. Geol. 1917, 6(14), 10. 1-14. 11. Fuhner, H. Ber. Dtsch. Chem. Ges. 1924, 57, 510-5. Glasstone, S.; Pound, A. J. Chem. Soc. 1925, 127, 2260-7. 12. 13. Kendall, J.; Harrison, E. Trans. Faraday Soc. 1928, 24, 588-96. 14. Jones, D. C. J. Chem. Soc. <u>1929</u>, 799-813. 15. Schlesinger, N.; Kubasowa, W. Z. Phys. Chem. 1929, 142A, 25-36. 16. Mion, M. C.R. Hebd. Seances Acad. Sci. 1931, 193, 1330-3. 17. Park, J. G.; Hofmann, H. E. Ind. Eng. Chem. 1932, 24, 132-4. Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79. 18. 19. Lloyd, B. A.; Thompson, S. O.; Ferguson, J. B. Canad. J. Res. 1937, 15B, 98-102. 20. Beech, D. G.; Glasstone, S. J. Chem. Soc. 1938, 67-73. 21. Shanley, E. S.; Greenspan, F. P. Ind. Eng. Chem. 1947, 39, 1536-43. 22. Griswold, J.; Chu, P. L.; Winsauer, W. O. Ind. Eng. Chem. 1949, 49, 2352-8. 23. Sohoni, V. B.; Warhadpande, U. R. Ind. Eng. Chem. 1952, 44, 1428-9. 24. Altshuller, A. P.; Everson, H. E. J. Am. Chem. Soc. 1953, 75, 1727. 25. Garner, P. H.; Ellis, S. R. M. Chem. Eng. Sci. 1953, 2, 282-6. 26. Gayler, R.; Pratt, H. R. C. Trans. Inst. Chem. Eng. 1953, 31, 78-93. (continued next page)

COMPONENTS:		EVALUATOR:	
(1)	Acetic acid ethyl ester (<i>ethyl acetate</i>); C ₄ H ₈ O ₂ ; [141-78-6] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia	
		January, 1989	
CRIT	ICAL EVALUATION: (continued)		
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		(continued next page)	

COMPONENTS:	EVALUATOR:
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRITICAL EVALUATION: (continued)	
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McGraw-Hill, New York <u>1928</u> , Vol. 3, 387-98. ACKNOWLEDGEMENT The Evaluator thanks Dr. Brian Clare for the graphics.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester	Mohr
(ethyl acetate); C ₄ H ₈ O ₂ ;	Arch. Pharm. <u>1851</u> , 65, 1-16.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
$T/K = room temperature^{a}$	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl e 3 g(1)/34.2 g(2) and 2.655 g(1)/31.04 percentage and mole fraction, x ₁ , val 8.06 g(1)/100g sln, 7.878 g(1)/100g s ^a No information about temperature;	ester in water was reported to be 45 g(2) ^a . The corresponding mass ues calculated by the compiler are 31n and 0.01762, 0.01719 respectively. 6 probably below room temperature.
AUXILIARY INFORMATION	
	SOURCE AND PURTTY OF MATERIALS.
The titration method was used	(1) Source not specified. distill-
A known mass of ester was titrated	(i) d_{4}^{20} 0.8889.
became homogeneous.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	· · · · · · · · · · · · · · · · · · ·
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid ethyl ester	Marsson, T.	
(ethyl acetate); $C_4H_8O_2$;	Arch. Pharm. 1853. 74. 290-6.	
[141-78-6]	Alen: Indin: <u>1000</u> , 74, 250 01	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 290.5	A. Szafranski and G.T. Hefter	
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 17.5° C was reported to be 7.86 g(1)/100g sln. The corresponding mole fraction, x_1 , value cal- culated by the compiler is 1.72×10^{-2} . The solubility of water in acetic acid ethyl ester at 17.5° C was reported to be 2.835 g(2)/100g sln. The corresponding mole fraction, x_2 , value cal- culated by the compiler is 1.25×10^{-1} .		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The cloud point method was used. No further details were provided.	 (1) Synthesized (details not provided) and distilled; middle fraction shaken with water, dried over CaCl₂, redistilled; b.p. range 78.0-78.5°C. (2) Distilled (no details given). 	
	ESTIMATED ERROR:	
	Temp. ±0.1 ^o C. Soly. ±1.4% rel., (1) in (2). ±0.5% rel., (2) in (1).	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid ethyl ester	Traube, J.	
(ethyl acetate); $C_4H_8O_2$;	Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,	
	2294-316.	
(2) water; n ₂ 0; [//32-10-5]		
VARIABLES:	PREPARED BY:	
T/K = 295	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 22°C was reported to be 1 part of ethyl acetate in 17-20 parts of water. The corresponding mass percent and mole fraction, x_1 , values calculated by the compiler are 5.2 g(1)/100g sln and 0.011.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Soly. ±0.4 g(1)/100g sln.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Bancroft, W.D. <i>Phys. Rev.</i> <u>1895</u> , 3, 114-36.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 20° C was reported to be 0.926 mL(1)/10mL(2). The solubility of water in ethyl acetate at 20° C was reported to be 0.294 mL(2)/10mL(1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. 10 mL of solvent in a test tube was titrated with the second component until the solution became cloudy.

SOURCE AND PURITY OF MATERIALS:

- Source not specified; dried over CaCl₂, distilled.
- (2) Not specified.

ESTIMATED ERROR:

Soly. ±0.01 mL.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Euler, H. <i>Z. Phys. Chem.</i> <u>1899</u> , 31, 360-69.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 301	A. Skrzecz
EXPERIMENTAL VALUES:	

The solubility of acetic acid ethyl ester in water at 28° C was reported to be 0.825 mol(1)/L(2). The corresponding mass per cent and mole fraction, x_1 , values calculated by the compiler are 6.80 g(1)/100g sln and 0.0147.

Density of water $d_4^{28} = 0.9962$ (ref 1) was used in the calculation.

AUXILIARY INFORMATION	
<pre>PARATUS/PROCEDURE: Trical method was used. Tre of 15 mL of (1) with of (2) was shaken for thermostated vessel. aration, the water-rich analyzed by saponifica- a known excess of alkali with standard acid. ESTIMATED ERROR: Soly. about ±0.5 g(1)/100g sln (compiler). REFERENCES: 1. Selected Values of Properties of Hydrocarbons and Related Compounds, API Research Project 44, Thermodynamics Research Center, Texas A and M University, Texas, <u>1973</u>.</pre>	
<pre>PARATUS/PROCEDURE: Source AND PURITY stical method was used. (1) Not specified (2) was shaken for thermostated vessel. aration, the water-rich analyzed by saponifica- a known excess of alkali which was then back with standard acid. ESTIMATED ERROR: Soly. about ±0.5 (compiler) REFERENCES: 1. Selected Value of Hydrocarboi Compounds, AP: 44, Thermodyn. Center, Texas University, Texas</pre>	

COMPONENTS:		ORIGINAL MEAS	SUREMENTS:
(1) Acetic	c acid ethyl ester	Rayman, J.	
(ethy) [141-7	l acetate); C ₄ H ₈ O ₂ 78-6]	; Thesis, Buda	apest, <u>1906</u> .
(2) Water;	H ₂ O; [7732-18-5]		
VARIABLES:		PREPARED BY:	
T/K = 273 -	- 303	G.T. Hefter	
EXPERIMENTAL VALUES:			
Sc	olubility of aceti	c acid ethyl ester in t	water
t/°C	g(1)/100g(2)	g(1)/100g solution	<i>x</i> ₁
		(compiler)	(compiler)
0.	10.94	9.86	0.0219
10.	9.70	8.84	0.0194

7.94

7.23

0.0173

0.0157

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possi- ble to minimize the error arising from the solubility of (2) in (1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated. (2) Not specified. ESTIMATED ERROR: Not specified.</pre>	
	REFERENCES: 1. Winkler, L. Z. Phys. Chem. <u>1906</u> , 55, 360.	

20.

30.

8.63

7.79

.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Bonner, W.D. <i>J. Phys. Chem.</i> <u>1910</u> , 14, 738-89.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES: T/K = 273	PREPARED BY: A. Skrzecz

The solubility of acetic acid ethyl ester in water at 0°C was reported to be 1.086 g(1)/10g(2). The corresponding mass per cent and mole fraction, x_1 , values calculated by the compiler are 9.80 g(1)/100g sln and 0.0217.

The solubility of water in acetic acid ethyl ester at $0^{\circ}C$ was reported to be 0.301 g(2)/10g(1). The corresponding mass per cent and mole fraction, x_2 , values calculated by the compiler are 2.92 g(2)/100g sln and 0.128.

AUXILIARY 1	AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: Presumably the titration method was used. Only the measurements for the ternary systems were described.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.		
	ESTIMATED ERROR: Soly. about ±0.8 g(1)/100g sln and ±0.6 g(2)/100g sln (compiler).		
	REFERENCES:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	Seidell, A. <i>Hygienic Lab. Bull. <u>1910</u>, No. 67, 98 pp. (US Govt. Printing Office, Washington, DC).</i>
VARIABLES:	PREPARED BY:
T/K = 283 - 313	G.T. Hefter

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g sln	x ₁ (compiler)
10.	9.15	0.0202
15.	8.71	0.0191
20.	8.27	0.0181
25.	7.90 '	0.0172
30.	7.61	0.0166
35.	7.39	0.0161
40.	7.17	0.0156

Extrapolated data down to 0°C and up to 55°C are given also. The solubility of water in acetic acid ethyl ester at 25°C was reported to be 4.8 cm³(2)/100cm³(1) and 5.38 g(2)/100g(1) giving 5.10 g(2)/100g sln. and a mole fraction, x_2 , value of 0.208 as calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. Por- tions of distilled water (50 cm^3) at approximately the desired tempera- ture were titrated to opalescence with (1). The exact temperature of the mixture was noted immediately after the saturation point was reached. The solubility of (2) in (1) appears to have been obtained by an analogous procedure	 (1) Kahlbaum, dried for 24h. over CaCl₂, filtered, and distilled; b.p. 75-76°C, d²⁵₂₅ 0.8915 g/cm³. (2) Distilled; no other details given.
Sy an analogous procedure.	ESTIMATED ERROR:
	soly. not stated.
	temp. not stated.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Merriman, R.W. <i>J. Chem. Soc.</i> <u>1913</u> , <i>103</i> , 1774-89.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 333	A. Skrzecz

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/10	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
0 ^a	10.08	97.72	0.02241	0.8976	
1.6	-	97.64	-	0.8943	
5 ^a	9.40	97.56	0.02077	0.8910	
7.1	-	97.49	-	0.8882	
10 ^a	8.81	97.39	0.01937	0.8841	
13.3	-	97.29	-	0.8801	
15 ^a	8.30	97.21	0.01817	0.8769	
17.7	-	97.10	-	0.8726	
20 ^a	7.86	97.02	0.01714	0.8694	
20.0	-	97.04	-	0.8702	
25 ^a	7.48	96.81	0.01626	0.8612	
25.9	-	96.74	-	0.8585	
30 ^a	7.15	96.58	0.01550	0.8524	
^a Author's smoothed results.			(con	tinued next pag	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic and analytical methods were used. The (2)-rich phase was determined by the cloud point method. A mixture of 100g of (1) and a required amount of (2) was warmed until clearness; then, it was allowed to cooled to produce a turbidity. The reported temperature was the mean of the two observations. Each experiment was repeated several times. The (1)-rich phase was determined at constant temperature in a sealed bulb of 75 mL capacity. Samples of known composition were shaken until constant volume of the layers was reached (<2 h.) and then the phase Composition was calculated using mass balance, density and phase volume.

SOURCE AND PURITY OF MATERIALS:

- Prepared and purified in laboratory; purity not specified.
- (2) Not specified.

ESTIMATED ERROR:

REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Acetic acid ethyl ester		Merriman, R.W.		
(et	hyl acetate); C ₄	H ₈ O ₂ ;	J. Chem. Soc. <u>19</u>	<u>13, 103, 1774-89.</u>
[14	1-78-6]			
(2) Wat	er; H ₂ O; [7732-1	.8-5]		
EXPERIMEN	TAL VALUES: (co	ontinued)		
	Mutual solubili	ity of acetic	acid ethyl ester ar	nd water
			<u></u>	
t/°C	g(1)/10	00g sln	x_1 (comp	iler)
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
33.4	_	96.40		0.8456
35 ^a	6.87	96.34	0.01486	0.8433
36.7	-	96.28	-	0.8411
39.6	-	96.10	-	0.8344
40 ^a	6.63	96.08	0.01431	0.8337
40.7	-	96.04	-	0.8322
45 ^a	-	95.81	-	0.8238
46.0	-	95.78	-	0.8227
50 ^a	-	95.54	-	0.8141
53.1	-	95.38	-	0.8085
55 ^a	-	95.26	-	0.8043
58.0	-	95.10	-	0.7987
60 ^a	-	94.98	-	0.7946

^a Author's smoothed results.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Euler, H.; Svanberg, O. <i>Ark. Kem. Mineral. Geol. <u>1917</u>, 6(14), 1-14.</i>
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES: T/K = 291	PREPARED BY: A. Szafranski and G.T. Hefter

The solubility of acetic acid ethyl ester in water at 25° C was reported to be 7.3 g(1)/100g(2). The corresponding mass percent and mole fraction, x_1 , values calculated by the compiler are 6.8 g(1)/100g sln and 0.0147.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The experimental procedure was as described in (ref 1). The satura- composition was approached from both sides and the excess of (1) was kept to a minimum. No further details were provided.	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified.	
	ESTIMATED ERROR: Not specified.	
	REFERENCES: 1. Euler, H. Z. Phys. Chem. <u>1899</u> , 31, 360-9.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	Fuehner, H. Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 20° C was reported to be 7.00 vol%, 6.44 g(1)/100g sln and 0.731 mol(1)/L sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.01388.

AUXILIARY INFORMATION

The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial product.
- (2) Not specified.

ESTIMATED ERROR:

Soly. about ±1.3 g(1)/100g sln (compiler).

REFERENCES:

COMPONENTS: (1) Acetic acid ethyl ester (ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Glasstone, S.; Pound, A. J. Chem. Soc. <u>1925</u> , 127, 2660-7.	
VARIABLES:	PREPARED BY:	
T/K = 273 - 323	A. Skrzecz	

Solubility of acetic acid ethyl ester in water

t∕°C	g(1)/100g(2)	<pre>mol(2)/mol(1)</pre>	g(1)/100g sln (compiler)	x ₁ (compiler)
0	10.40	<u> </u>	9.42	0.02082
10	8.96	-	8.22	0.01779
20 ^a	7.85	-	7.28	0.01580
25	7.39	-	6.88	0.01488
25 ^b	-	66.15	6.88	0.01489
30 ^a	7.06	-	6.59	0.01423
37	6.65	-	6.24	0.01341
40 ^a	6.50	-	6.10	0.01312
50	6.04	-	5.70	0.01220
50 ^b	_	80.98	5.70	0.01220

^a Authors' graphically interpolated data.

^b The method was not specified.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The water with a slight excess of ester was shaken at a temperature below the one measured and placed into a thermostat bath. The mixture was saturated in the course of one to two hours at the measured temperature. The saturated solution (3 to 8 g) was transferred to a stoppered bottle, weighed and hydrolyzed with standard NaOH. The residue was always tested to make sure that no acetic acid remained.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Synthesized as described in Roberts (ref 1); distilled over CaCl₂ and then several times over P₂O₅. (2) Not specified. ESTIMATED ERROR: Soly. about ±(0.4-0.6) g(1)/100g sln (compiler).</pre>	
	REFERENCES: 1. Roberts, J. Soc. Chem. Ind. <u>1924</u> , 43, 295T.	

MPONENTS:		ORIGINAL MEASUREMENTS:
1) Aceti	c acid ethyl	ester Kendall, J.; Harrison, L.E.
(ethy [141-	l acetate); C 78-6]	4 ^H 8 ^O 2; Trans. Faraday Soc. <u>1928</u> , 24, 588-96.
2) Water; H ₂ O; [7732-18-5]		18-5]
RIABLES:		PREPARED BY:
/K = 273	- 323	Z. Maczynska
PERIMENTA Solubi 	L VALUES: lity of aceti x ₁	c acid ethyl ester in water g(1)/100g sln (compiler)
PERIMENTA Solubi t/°C	L VALUES: lity of aceti 	c acid ethyl ester in water g(1)/100g sln (compiler)
PERIMENTA Solubi t/°C	L VALUES: lity of aceti 	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41
PERIMENTA Solubi t/°C 0.0 10.0	L VALUES: lity of aceti $\frac{x_1}{0.0208}$ 0.0179	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19
PERIMENTA Solubi t/°C 0.0 10.0 20.0	L VALUES: lity of aceti 	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19 7.28
PERIMENTA Solubi t/°C 0.0 10.0 20.0 25.0	L VALUES: lity of aceti 	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19 7.28 6.84
PERIMENTA Solubi t/°C 0.0 10.0 20.0 25.0 30.0	L VALUES: lity of aceti .0.0208 0.0179 0.0158 0.0148 0.0142	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19 7.28 6.84 6.58
PERIMENTA Solubi t/°C 0.0 10.0 20.0 25.0 30.0 37.0	L VALUES: lity of aceti 	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19 7.28 6.84 6.58 6.23
PERIMENTA Solubi t/°C 0.0 10.0 20.0 25.0 30.0 37.0 40.0	L VALUES: lity of aceti 0.0208 0.0179 0.0158 0.0148 0.0142 0.0134 0.0131	c acid ethyl ester in water g(1)/100g sln (compiler) 9.41 8.19 7.28 6.84 6.58 6.23 6.10

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The synthetic method was used. The sealed tube method of Smith and Eastlack (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.	 SOURCE AND PURITY OF MATERIALS: (1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C. (2) Distilled. 	
	ESTIMATED ERROR: Temp. ±(0.1-0.2) ^o C (authors). Soly. about ±0.5 g(1)/100g sln (compiler).	
	REFERENCES: 1. Smith, A.; Eastlack, H.E. J. Am. Chem. Soc. <u>1916</u> , 38, 1269.	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester	Jones, D.C.
(ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	J. Chem. Soc. <u>1929</u> , 799-813.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
<i>T</i> /K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl of be 8.53 g(1)/100g sln and $x_1 = 0.016$. The solubility of water in acetic acid be 3.07 g(2)/100g sln and $x_2 = 0.152$.	ester in water at 20°C was reported to id ethyl ester at 20°C was reported to
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the synthetic method	(1) Not specified.
was used as described in Jones and Betts (ref 1). No further details were reported in the paper.	(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.7 g(1)/100g sln and ±0.07 g(2)/100g sln (compiler).
	REFERENCES:
	1. Jones, D.C.; Betts, H.F. <i>J. Chem. Soc.</i> <u>1928</u> , 1177.

		<u> </u>		
COMPONENTS:		ORIGINAL I	ORIGINAL MEASUREMENTS:	
(1) Acetic acid ethyl ester		Schlesing	Schlesinger, N.; Kubasowa, W.	
(ethyl acetate); C ₄ H ₈ O ₂ ;		Z. Phys.	Chem. <u>1929</u> , 142A, 25-36.	
[141-78	3-6]			
(2) Water;	H ₂ O; [7732-18-5]			
VARIABLES:		PREPARED I	PREPARED BY:	
T/K = 288 - 323		A. Skrzed	CZ	
PYDEDTMENUDAT			·····	
EAPERIMENTAL	VALUES:	d ethyl ester	in water	
	authors' smoo	thed data	in water	
t/°c	g(1)/100g(2) g(1)/100g sln	x_1	
		(compiler)	(compiler)	
15	8.864	8.14	0.01780	
20	8.420	7.17	0.01696	
30	7.692	7.14	0.01548	
35	7.408	6.90	0.01492	
40	7.177	6.70	0.01446	
45	7.000	6.54	0.01411	
50	6.875	6.43	0.01386	
g(1)/100g(2) = 10.515 - 0.12605 (t/°C) + 0.001065 (t/°C) ²				
AUXILIARY INFORMATION				
METHOD/APPARA	TUS/PROCEDURE:	SOURCE AND	O PURITY OF MATERIALS:	
The synthetic method described by Alexejev (ref 1) was used. Measure- ments were carried out in ampoules containing water and 0.10-0.15g of ester. The measurements were re- peated several times.		(1) Source - range	ce not specified; b.p. 2 76.6-77.1°C at 753 mm Hg.	
		f (2) Not s	specified.	
		ESTIMATED	ERROR:	
		Temp +0	1°C	
		Soly. ±0. (co	01 g(1)/100g sln ompiler).	
		REFERENCES	5: 	
		1. Alexej <u>1886</u> ,	ew, W. Wied. Ann. Phys. 28, 306.	

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Ac (e [1	etic acid ethyl (thyl acetate); C 41-78-6]	ester 4H ₈ O ₂ ;	Mion, M. Compt. Rend. <u>193</u>	1 <u>1</u> , <i>193</i> , 1330-3.
(2) Wa	ter; H ₂ 0; [7732-1	18-5]		
VARIABLE	s:	I	PREPARED BY:	
T/K = 2	73 - 303		A. Skrzecz	
EXPERIME	NTAL VALUES:			
	Mutual solubil:	ity of acetic ad	cid ethyl ester ar	nd water
t/°c	g(1)/100g sln		x ₁ (comp	viler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	10. ^a	97.74 ^b	0.0222	0.8984
15	8.3 ^b	97.18 ^b	0.0182	0.8757

96.48^c

0.0154

0.8486

30

7.1^b

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The turbidity method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-ethanol. No fur- ther details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; used as received; d²⁰ 0.9244. (2) Not specified. ESTIMATED ERROR: Soly. about ±1.^a, ±0.1^b and ±0.02^c g(1)/100g sln (compiler). REFERENCES: </pre>	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid ethyl ester	Park, J.G.; Hofmann, H.E.	
(ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	Ind. Eng. Chem. <u>1932</u> , 24 132-4.	
(2) Water; H ₂ O; [7732-18-5]	1	
VARIABLES:	PREPARED BY:	
T/K = 298	Z. Maczynska	
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was reported to be 7.9 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0172. The solubility of water in acetic acid ethyl ester at 25°C was reported to be 3.0 g(2)/100g sln. The corresponding mole fraction, x_2 , value calcu- lated by the compiler is 0.131.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Nothing was specified in the paper.	 (1) Source not specified, CP reagent grade; containing no alcohol; used as received. (2) Not specified. 	
	ESTIMATED ERROR:	

soly.	about ±0.4 g(1)/100g sln
	and $\pm 0.2 g(2) / 100g sln$
	(compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 6.92 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0150.

The solubility of water in acetic acid ethyl ester at $20^{\circ}C$ was reported to be 11.01 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.377.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commer- cial product; purity 85%, b.p. range 70-80°C, d_4^{20} 0.886.
	(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.9 g(1)/100g sln and ±7 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Lloyd, B.A.; Thompson, S.O.; Ferguson, J.B. <i>Can. J. Res.</i> <u>1937</u> , 15B, 98-102.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	G.T. Hefter	
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25° C was reported be 7.56 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 1.64 x 10^{-2} . The solubility of water in acetic acid ethyl ester at 25° C was reported be 3.24 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 1.41 x 10^{-1} . Note: The values are the same as those given in (ref 1) but apparently were confirmed experimentally by the authors.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The titration method was used. A two component sample was placed in a long tube with a small stoppered side-arm in a thermometer. The sys- tem was rotated so that the vapor phase moved from end-to-end and so stirred the liquid. One com- ponent was then added from a small weight burette to adjust the compo- sition.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; CP grade washed with H₂O and distilled; d²⁰₄ = 0.9006. (2) Not specified. (2) Not specified. ESTIMATED ERROR: Temp. ±0.1°C. Soly. Not stated. REFERENCES: 1. Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u>, Vol. 3, 387-98.</pre>	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (<i>ethyl acetate</i>); C ₄ H ₈ O ₂ ; [141-78-6]	Beech, D.G.; Glasstone, S. J. Chem. Soc. <u>1938</u> , 67-73.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 313	A. Skrzecz

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g(2)	g(1)/1	100g sln	<i>x</i> ₁ (co	mpiler)
		(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
		<u> </u>			
0 ^{a,b,c}	10.70 ± 0.05	9.67 ^d	-	0.0214	-
0 ^c	-	9.6	97.7	0.0213	0.897
20 ^{a,b,c}	8.40 ± 0.04	7.75 ^d		0.0169	-
20 [°]	-	7.8	97.2	0.0170	0.877
40 ^{a,b,c}	6.97 ± 0.04	6.52 ^d	-	0.0141	-

d Calculated by the compiler.

AUXILIARY 1	INFORMATION
METHOD/APPARATUS/PROCEDURE: Presumably the synthetic method was used. Only the measurements for the ternary system were described.	<pre>NFORMATION SOURCE AND PURITY OF MATERIALS: (1) a Synthesized; dried over K₂CO₃, refluxed with P₂O₅, distilled; b.p. range 77.0-77.2°C. b Source not specified; kept over CaCl₂, distilled, frac- tion boiling at 74-76°C re- fluxed with P₂O₅ and dis- tilled. C Source not specified; washed three times with NaCl aq. and twice with H₂O,kept over CaCl₂, distilled. (2) Not specified. ESTIMATED ERROR: Soly. see above. REFERENCES:</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester	Shanley, E.S.; Greenspan, F.P.
$(ethyl acetate); C_4H_8O_2;$	Ind. Eng. Chem. <u>1947</u> , 39, 1536-43.
$(2) \text{Wator: } H \cap (7722 - 19 - 51)$	
(2) water, n ₂ 0; [//32-10-5]	
VARIABLES:	PREPARED BY:
T/K = room temperature	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in acetic act reported to be 3.5 g(2)/100g(1). The fraction, x_2 , values calculated by th 0.146.	id ethyl ester at room temperature was corresponding mass per cent mole ne compiler are 3.4 g(2)/100g sln and
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified. No further details were reported in	(1) Not specified.
the paper.	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (<i>ethyl acetate</i>); C ₄ H ₈ O ₂ ; [141-78-6]	Griswold, J.; Chu, P.L.; Winsauer, W.O. Ind. Eng. Chem. <u>1949</u> , 41, 2352-8.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 290 - 344	A. Skrzecz

t/°C	g(1)/10	0g sln	x_1 (comp	iler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
17.0	7.92	-	0.01728	
19.0	-	96.99	-	0.8682
27.0	7.23	-	0.01569	-
27.5	7.18	-	0.01557	-
40.9	-	95.95	-	0.8289
57.3	-	95.00	-	0.7953
68.2	-	94.35	-	0.7735
70.4	6.3	-	0.0136	-

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The synthetic method was used. A rotating cage containing the glass ampoule (ca. 10 mL) with a sample was warmed and cooled in a water bath until the cloud point appeared and disappeared over a 0.2°C temperature range. The average temperature was taken.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, anhydrous reagent grade; distilled; d_4^{25} 0.89428, n_D^{25} 1.37012. (2) Distilled; d_4^{25} 0.99707.	
	ESTIMATED ERROR: Temp. ±0.1 [°] C (authors). Soly. better than ±0.1 g(1)/100g sln (compiler).	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Sohoni, V.R.; Warhadpande, U.R. Ind. Eng. Chem. <u>1952</u> , 44, 1428-9.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 303	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 30° C was reported to be 7.10 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.01539.

The solubility of water in acetic acid ethyl ester at 30° C was reported to be 3.50 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1507.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The synthetic method described by Taylor (ref 1) was used. The data and method were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, analytical reagent grade; d^{30} 0.8939, n_D^{30} 1.3700. (2) Distilled; d_4^{30} 0.9957, n_D^{30} 1.3320.
	ESTIMATED ERROR:
	Soly. about ±0.1 g(1)/100g sln and ±0.02 g(2)/100g sln (compiler).
	REFERENCES:
	1. Taylor, S.F. <i>J. Phys. Chem.</i> <u>1897</u> , 1, 461.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Altshuller, A.P.; Everson, H.E. J. Am. Chem. Soc. <u>1953</u> , 75, 1727.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 292 - 313	Z. Maczynska

Solubility of acetic acid ethyl ester in water

t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x ₁ (compiler)
19.2	8.34	7.70	0.01677
20.4	8.31	7.67	0.01670
20.5	8.29	7.66	0.01667
21.3	8.26	7.63	0.01661
22.0	8.22	7.60	0.01653
22.6	8.14	7.53	0.01637
22.7	8.12	7.51	0.01633
23.0	8.11	7.50	0.01631
23.4	8.10	7.49	0.01629
24.7	8.05	7.42	0.01612
25.1	8.03	7.41	0.01611
25.4	8.02	7.41	0.01611
25.4	8.03	7.41	0.01611
			(continued next

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method as described in Weissberger (ref 1) was used. The solubilities of acetic acid ethyl ester agreed to within $\pm 0.1^{\circ}$ C when determined by heating and then by cooling. (The appearance of turbidity may be detected within about 0.2°C range usually.) Temperature was measured with a 0.05°C, thermometer which gave agreement to within 0.01°C with the sodium sulphate transition point. Each solubility value was determined twice or thrice.

SOURCE AND PURITY OF MATERIALS:

- (1) Mallinckrodt reagent analytical grade; 0.06% water asdetermined by Karl Fischer reagent; redistilled from a column of 24 theoretical plates; n_D^{24} 1.3697.
- (2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1^oC (authors).
Soly. about ±(0.05-0.1)
 g(1)/100g sln (compiler).

REFERENCES:

 Weissberger, A. Physical Methods of Organic Chemistry, Vol.1, Part I, Interscience Publishers, Inc., New York, <u>1939</u>, p.319.
COMPONENTS:			EVALUATOR:		
(1) Partia said sthul satau					
(1) Acetic acta ethyl ester		AIUSHUITEI	, A.P.; Everson, n.E	•	
(echy1	$acecate; c_4n_80_2;$,	J. Am. Chei	n. Soc. <u>1953</u> , 75, 1	727.
	5-0J				
(2) Water; H ₂ O; [7732-18-5]					
EXPERIMENTAL	VALUES: (contin	ued)			
So	lubility of aceti	c acid et	hyl ester in	water	
t/°C	g(1)/100g(2)	g(1)/10	Og solution	X1	
	5(-//5(-/	(co	ompiler)	(compiler)	
25.4	8.00	7	.41	0.01609	
25.9	7.93	7	.35	0.01596	
26.0	7.93	7	.35	0.01596	
26.3	7.94	7	.36	0.01598	
27.0	7.89	7	.31	0.01588	
28.0	7.80	7	.24	0.01570	
28.1	7.81	. 7	.24	0.01572	
28.4	7.82	7	.25	0.01574	
28.7	7.81	7	.24	0.01572	
29.7	7.71	7	.16	0.01552	
29.9	7.71	7	.16	0.01552	
30.0	7.72	7	.17	0.01554	
30.0	7.69	7	.14	0.01548	
30.1	7.69	7	.14	0.01548	
31.2	7.60	7	.06	0.01530	
31.8	7.58	7	.05	0.01526	
31.9	7.58	7	.05	0.01526	
31.9	7.57	7	.04	0.01524	
32.0	7.51	6	.99	0.01512	
32.8	7.49	6	.97	0.01508	
33.0	7.46	6	.94	0.01502	
33.8	7.40	6	.89	0.01491	
34.0	7.38	6	.87	0.01487	
36.8	7.32	6	.82	0.01475	
37.8	7.25	6	.76	0.01461	
39.9	7.15	6	.67	0.01441	
39.9	7.15	6	.67	0.01441	

(continued next page)

COMPONENTS:		EVALUATOR:	
(1) Aceti (ethy [141-	c acid ethyl ester <i>1 ac</i> etate); C ₄ H ₈ O ₂ 78-6]	Altshuller	, A.P.; Everson, H.E. m. <i>Soc</i> . <u>1953</u> , 75, 1727.
(2) Water	; H ₂ O; [7732-18-5]		
The smo	othed solubility o	of acetic acid ethyl e	ster in water
t/°C	g(1)/100g(2)	g(1)/100g solution (compiler)	x ₁ (compiler)
20	8.42	7.77	0.01693
25	8.04	7.42	0.01612

7.15

6.88

6.65

0.01550

0.01489

0.01435

Authors'	smoothing	equation:	

7.70

7.39

7.12

30

35

40

 $g(1)/100g(2) = (9.522 \pm 0.018) - (0.0618 \pm 0.0006) t/°C$

COMPO	DNENTS:	ORIGINAL	MEASUP	REMENTS	:
(1)	Acetic acid ethyl ester	Garner,	F.H.;	Ellis,	S.R.M.
	(athul agateta), OILO,				

(2)	(ethyl acetate); $C_4H_8O_2$; [141-78-6] Water; H_2O ; [7732-18-5]	Chem. Eng. Sci. <u>1953</u> , 2, 282-6.
VARIA	BLES:	PREPARED BY:
T/K	= 303	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 30°C was reported to be 1.7 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0035.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described in Garner, Ellis and Roy (ref 1) was used. The weighed amount of miscible mixture was placed into the test tube and titrated to turbidity. The apparatus was a thin-walled glass tube with a glass stirrer and thermometer inside, placed in a thermostat. Only the measurements for the ternary systems were described. The data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.

SOURCE AND PURITY OF MATERIALS:

- (1) Source not specified, analytical grade; distilled; b.p. 77.1°C, n_D^{20} 1.3700.
- (2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C (authors). Soly. about $\pm 5 g(1)/100g sln$ (compiler).

REFERENCES:

1. Garner, F.H.; Ellis, S.R.M.; Roy, U.N.G. Chem. Eng. Sci. <u>1953</u>, 2, 14.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl	ester Gayler, R.; Pratt, H.R.C.
(ethyl acetate); ([141-78-6]	4 ^H 8 ^O 2; Trans. Inst. Chem. Eng. <u>1953</u> , 31, 78-93.
(2) Water; H ₂ O; [7732·	18-5]
VARIABLES:	PREPARED BY:
T/K = 288 - 303	A. Skrzecz

	Mutual solubil:	ity of acetic ac	id ethyl ester an	nd water
t/°C	g(1)/10	00g sln	x_1 (comp	oiler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
15 ^a	8.22	97.04	0.01798	0.8702
15 ^b	8.05	97.26	0.01759	0.8789
20 ^a	7.86	96.87	0.01714	0.8635
20 ^b	7.62	97.10	0.01659	0.8726
25 ^a	7.58	96.69	0.01649	0.8566
25 ^b	7.38	96.87	0.01603	0.8635
30 ^a	7.32	96.40	0.01589	0.8456
30 ^b	7.11	96.65	0.01541	0.8551

^a Titration method.

^b Analytical method.

AUXILIARY INFO	ORMATION
METHOD/APPARATUS/PROCEDURE: SOU The titration and analytical (1) methods were used. In the titration method, the component (1) or (2) was added in stages from a finely calibrated 5 mL burette to a (2) thermostated 100 mL sample of the second component and shaken. The procedure was continued until a faint cloudiness persisted in the sample. In the analytical procedure, the (2) in the ester phase was determined by the Karl Fischer iodometric titration. The (1) in the water phase was determined by hydrolysis of duplicate samples of 5 g each with 0.2N alcoholic KOH for 2 h. Also, a third blank sample was refluxed at the same time. The samples were titrated with 0.2N HCl using phenolphthal- ein as an indicator.	<pre>DURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial product; distilled and dried; purity not specified. (2) Distilled. (2) Distilled. (3) Distilled.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester	Jones, J.H.; McCants, J.F.
(ethyl acetate); C ₄ H ₈ O ₂ ;	Ind. Eng. Chem. <u>1954</u> , 46, 1956-62.
[141-78-6]	
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 311	A. Skrzecz
EXPERIMENTAL VALUES:	
The solubility of acetic acid ethyl e	ester in water at 100 ⁰ F was reported
to be 7.0 g(1)/100g sln. The correspo	onding values of temperature Kelvin
and mole fraction, x_1 , calculated by	the compiler are 311 K and 0.015.
The colubility of water in acetic aci	d other at 100°E was reported
to be 4.6 g(2)/100g sln. The correspo	onding values of temperature Kelvin
and mole fraction, x_2 , calculated by	the compiler are 311 K and 0.19.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The organic-rich phase composition	(1) Commercial Solvents, 99% undenatured, n _D ⁰ 1.3717;
was obtained by adding water (first rapidly and then dropwise) to the	used as received.
glass-stoppered flask and agitated.	(2) Distilled; $n_{\rm D}^{20}$ 1.3330.
reached when the cloud persisted	
The water-rich phase was obtained	ESTIMATED ERROR:
were reported in the paper.	more to 200 (suthord)
	Soly. about ± 0.2 g(1)/100g sln and
	±0.7 g(2)/100g sin (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Rao, G.J.R.; Rao, C.V. <i>J. Sci. Ind. Res.</i> <u>1955</u> , 14B, 444-8.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES: T/K = 303	PREPARED BY: Z. Maczynska		

The solubility of acetic acid ethyl ester in water at 30° C was reported to be 7.22 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.01566.

The solubility of water in acetic acid ethyl ester at 30° C was reported to be 3.47 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1495.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-propanoic acid. No further details were reported in the paper.	 SOURCE AND PURITY OF MATERIALS: (1) Merck; b.p. 77.1°C, d³⁰ 0.8885; used as received. (2) Distilled and boiled; free from CO₂.
	ESTIMATED ERROR: Temp. ±0.1 ^o C (authors). Soly. about ±0.3 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).
	REFERENCES:

ONE	NT.	5:		

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Venkataratnam, A.; Rao, J.R.; Rao, C.V. Chem. Eng. Sci. <u>1957</u> , 7, 102-10.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 303	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 30° C was reported to be 7.4 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0161.

The solubility of water in acetic acid ethyl ester at 30° C was reported to be 3.5 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.151.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl esterwater-2-propanone (ethyl acetatewater-acetone).

SOURCE AND PURITY OF MATERIALS:

- (1) British Drug House Ltd., analytical grade; used as received; b.p. $77.1^{\circ}C$, d^{30} 0.8885, n^{30} 1.3680.
- (2) Distilled; free of CO₂.

ESTIMATED ERROR:

Soly. about ±0.1 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Rao, M.V.R.; Rao, K.S.; Rao, C.V. J. Sci. Ind. Res. <u>1961</u> , 20B, 379-81.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 308	Z. Maczynska

The solubility of acetic acid ethyl ester in water at 35° C was reported to be 8.9 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0196.

The solubility of water in acetic acid ethyl ester at $35^{\circ}C$ was reported to be 3.5 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.151.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-formic acid. No further details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) BDH, laboratory reagent grade; used as received. (2) Not specified. ESTIMATED ERROR: Soly. about ±1.9 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler). REFERENCES:</pre>
······	

COMPONENTS:		ORIGINAL MEASUREME	NTS:
(1) Acetic acid	l ethyl ester	Akita, K.; Yoshid	a, F.
(ethyl ace) [141-78-6]	cate); C ₄ H ₈ O ₂ ;	J. Chem. Eng. Dat 484-90.	a <u>1963</u> , 8,
(2) Water; H ₂ O;	[7732-18-5]		
VARIABLES:	· · · · · · · · · · · · · · · · · · ·	PREPARED BY:	
T/K = 298 and 34 p/kPa = 101.325	13 (1 atm)	A. Skrzecz	
EXPERIMENTAL VALU	JES:	J	
Mutual solubil	lity in the system of	acetic acid ethyl e	ester and water
t/°c	g(1)/100g sln	X1	
(2)-ric	ch phase (1)-rich phas	se (2)-rich phase	(1)-rich phase
25 7.	.5 ^a 97.8 ^b	0.016	0.899
70 6.	2 ^a 94.0 ^a	0.013	0.762
	AUXILIARY 1	INFORMATION	
METHOD/APPARATUS/	PROCEDURE:	SOURCE AND PURITY	OF MATERIALS:
The synthetic me 25°C. The analyt used at 70°C. Th ported together system acetic ac water-methanol. were reported in	ethod was used at ical method was e data were re- with the ternary bid ethyl ester- No further details a the paper.	 (1) Source not sp reagent grade column 150 cm McMahlon pack n_D⁵ 1.3697, b (2) Not specified 	ecified, special ; distilled with in height, with ing; d ²⁵ 0.8945, .p. 77.1°C.
		ESTIMATED ERROR:	
		Soly. about ±0.05 g(1)/100g s	^a and ±1.0 ^b ln (compiler).
		REFERENCES:	

	<u></u>			
COMPONEN	ITS:		ORIGINAL MEASUREME	INTS:
(1) Ac	etic acid ethyl est	ter	Zheleznyak, A.S.;	Brounshtein, B.I.
(e	thyl acetate); C ₄ H ₆	,o ₂ ;	Zh. Prikl. Khim.	<u>1965</u> , 38, 694-6.
(a) Wa		51	2	
(2) Wa	ссег; н ₂ 0; [//з2-18-	-5]		
VARIABLE	S:		PREPARED BY:	
T/K = 2	98 and 323		A. Skrzecz	
EXPERIME	NTAL VALUES: Mutual solubility	y of acetic	acid ethyl ester a	nd water
t/°C	g(1)/100	ısln	x. (com	viler)
	(2)-rich phase ()	1)-rich phas	e (2)-rich phase	(1)-rich phase
20	8.51	96.70	0.01866	0.8570
50	6.93	96.08	0.01500	0.8336
		AUXILIARY :	INFORMATION	
METHOD/A	PPARATUS/PROCEDURE	:	SOURCE AND PURITY	OF MATERIALS:
The ana The sam 2.5 h.	lytical method was ples were thermosta and then both phase	used. ated for es were	(1) Source not sp analytical gr received.	ecified, ade; used as
analyze the Kar of este The dat	d. Water was detern 1 Fischer method. 5 er analysis was not a and method were 1	nined by The method reported. reported	(2) Distilled.	
with th ethyl e	e ternary system ac ster-water-acetic a	cetic acid acid.		
			ESTIMATED ERROR:	b = = b
			Temp. ±0.1°C (aut Soly. better than sln (compil	nors). 1 ±0.7 g(1)/100g .er).
			REFERENCES:	

	7 0.	
COMPONEN	TS:	ORIGINAL MEASUREMENTS:
(1) Ac	etic acid ethyl ester	Pai, M.U.; Sane, A.G.
(e [1	41-78-61	Indian J. Technol. <u>1966</u> , 4, 373-5.
(2) Wa	ter; H ₂ O; [7732-18-5]	
VARIABLE	S:	PREPARED BY:
T/K = 2	73 and 303	A. Skrzecz
EXPERIME	NTAL VALUES: Mutual solubility of aceti	c acid ethyl ester and water
t/°c	g(1)/100g sln	x, (compiler)
	(2)-rich phase (1)-rich ph	ase (2)-rich phase (1)-rich phase
o	9.29 97.62	0.0205 0.8935
30	6.70 96.75	0.0145 0.8589
METHOD/A	PPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The tur Othmer, was use determi pered f The dat with th ethyl e	bidity method described in White and Trueger (ref 1) d. Mutual solubilities were ned in a 25 mL glass stop- lask placed in a thermostat. a were reported together e ternary system acetic acid ster-water-ethylacetoace-	 (1) Union Carbide, technical grade; treated with anhydrous K₂CO₃, distilled; purity 99.8%, b.p. 77.0°C, d²⁰ 0.9001. (2) Twice distilled.
tate.		ESTIMATED ERROR:
		Temp. ±0.1 ^o C (authors). Soly. about ±0.5 g(1)/100g sln (compiler).
		REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger,E. Ind. Eng. Chem. <u>1941</u> , 33, 1240.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]	Nakamura, A. <i>Kogyo Kagaku Zasshi <u>1968</u>, 71(10),</i> 1577-80.
VARIABLES:	PREPARED BY:
T/K = 303	A. SKrzecz

The solubility of acetic acid ethyl ester in water at 30° C was reported to be 6.7 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0145.

The solubility of water in acetic acid ethyl ester at 30° C was reported to be 3.7 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.158.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture was placed in a 1 L flask and stirred for 1 h. which was sufficient for equilibrium. Then, after 1/2 h. separation, samples of both phases were analysed. The ester was analysed by saponification with 2N NaOH and reverse titration with 2N NAOH and reverse titration with 2N HCL. Water was determined by the Karl Fischer method. The method and data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial product; distilled; purity 99.20% wt, impurities: 0.63% water, 0.08% ethyl alcohol, 0.06% vinyl acetate, 0.02% toluene, 0.01% unknown. (2) Purified on ion-exchange material; resistivity >4x10⁶ ohm. ESTIMATED ERROR: Temp. ±0.3^oC (author). Soly. about <3% (relative error of (1) author), ±0.5 g(1)/ 100g sln and ±0.2 g(2)/100g sln (compiler). REFERENCES:</pre>

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	Batmanova, G.A.; Balashov, M.I.; Grishunin, A.V.; Savinskaya, I.G.; Serafimov, L.A.
(2) Water; H ₂ O; [7732-18-5]	Gidroliz. Lesokhim. Prom. <u>1971</u> , 24(8), 11-2.
VARIABLES:	PREPARED BY:
T/K = 293 and 344	A. Skrzecz
EXPERIMENTAL VALUES: Mutual solubility of acetic	acid ethyl ester and water
t/°C g(1)/100g sln (2)-rich phase (1)-rich phas	x ₁ (compiler) se (2)-rich phase (1)-rich phase
20 ^a 7.86 ^d 97.0 ^d 70.40 ^{b,c} 6.3 ^d 94.2 ^e	0.01714 0.869 0.0136 0.769
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration and analytical methods were used. In the titration method, the titrations were carried out in thermostated bottles using a magnetic stirrer at 20°C and in a heated flask with a magnetic stir- rer and reflux condenser at the boiling temperature. In the analyt- ical procedure, a two-phase mixture	 (1) Source not specified, chemical- ly pure grade; used as receiv- ed. (2) Distilled.
attached to a reflux condenser, mixed for 1/2 h. at the boiling temperature, separated and analyzed by glc. A small amount of water was also determined by the Karl Fischer method.	Soly. about ±0.05 ^d and ±0.2 ^e g(1)/100g sln (compiler).
The data and methods were reported together with the ternary system formic acid ethyl ester-water- acetic acid ethyl ester.	REFERENCES: 1. Skrzecz, A.; Maczynska, Z. <i>Pol. J. Chem.</i> <u>1980</u> , 54, 2383.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid ethyl ester (ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	Iguchi, A.; Fuse, K. <i>Kagaku Kogaku <u>1971</u>, 35(9),</i> 1035-7.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

The solubility of acetic acid ethyl ester in water at $25^{\circ}C$ was reported to be 6.11 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.01313.

The solubility of water in acetic acid ethyl ester at $25^{\circ}C$ was reported to be 2.54 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1131.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The samples were titrated with the second component to obtain turbid- ity. The method and data were re- reported together with the ternary system acetic acid ethyl ester- water-acetic acid. No further details were reported in the paper.	 (1) Source not specified, commercial grade of high purity, used as received. (2) Not specified. ESTIMATED ERROR: Temp. ±0.1°C. Soly. about ±1.4 g(1)/100g sln and ±1.0 g(2)/100g sln (compiler).
	REFERENCES:

(1) Acetic acid ethyl ester (ethyl acetate); $C_4H_8O_2$; [141-78-6]Krupatkin, I.L.; Shcherbakova $Zh. Prikl. Khim. 1971, 44, 34$ (2) Water; H_2O ; [7732-18-5]PREPARED BY: A. SkrzeczVARIABLES: $T/K = 298$ PREPARED BY: A. SkrzeczEXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at $25^{\circ}C$ was report be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value call lated by the compiler is 0.01623.The solubility of water in acetic acid ethyl ester at $25^{\circ}C$ was report be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value call ated by the compiler is 0.1537.	<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] VARIABLES: T/K = 298 EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x₁, value lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x₂, value lated by the compiler is 0.1537.</pre>	COMPONENTS:	ORIGINAL MEASUREMENTS:
$[141-78-6]$ (2) Water; H20; $[7732-18-5]$ VARIABLES: $T/K = 298$ PREPARED BY: $T/K = 298$ A. SkrzeczEXPERIMENTAL VALUES:The solubility of acetic acid ethyl ester in water at 25°C was reportbe 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value cated by the compiler is 0.01623.The solubility of water in acetic acid ethyl ester at 25°C was reportbe 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value cated by the compiler is 0.1537.	<pre>[141-78-6] (2) Water; H₂O; [7732-18-5] VARIABLES: T/K = 298 EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x₁, value lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x₂, value lated by the compiler is 0.1537.</pre>	 Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; 	Krupatkin, I.L.; Shcherbakova Zh. Prikl. Khim. <u>1971</u> , 44, 3
(2) water, n_20 , $(7732-18-5)$ VARIABLES:T/K = 298PREPARED BY:A. SkrzeczEXPERIMENTAL VALUES:The solubility of acetic acid ethyl ester in water at 25°C was reportbe 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value calllated by the compiler is 0.01623.The solubility of water in acetic acid ethyl ester at 25°C was reportbe 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value calllated by the compiler is 0.1537.	<pre>(2) water, h₂0, [//32-18-5] VARIABLES: T/K = 298 EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x₁, value lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x₂, value lated by the compiler is 0.1537.</pre>	[141-78-6]	
VARIABLES:PREPARED BY: $T/K = 298$ A. SkrzeczEXPERIMENTAL VALUES:A. SkrzeczThe solubility of acetic acid ethyl ester in water at 25°C was reportbe 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value calllated by the compiler is 0.01623.The solubility of water in acetic acid ethyl ester at 25°C was reportbe 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value calllated by the compiler is 0.1537.	VARIABLES:PREPARED BY: $T/K = 298$ A. SkrzeczEXPERIMENTAL VALUES:The solubility of acetic acid ethyl ester in water at 25°C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value lated by the compiler is 0.01623.The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value lated by the compiler is 0.1537.		
T/K = 298 EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was report be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value cal- lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was report be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value cal- lated by the compiler is 0.1537.	T/K = 298 A. Skrzecz EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value lated by the compiler is 0.1537.	VARIABLES:	PREPARED BY:
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was repor- be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value cal- lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was repor- be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value cal- lated by the compiler is 0.1537.	EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25° C was rep be 7.47 g(1)/100g sln. The corresponding mole fraction, x_1 , value lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25° C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value lated by the compiler is 0.1537.	T/K = 298	A. Skrzecz
lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25° C was report be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value cal lated by the compiler is 0.1537.	lated by the compiler is 0.01623. The solubility of water in acetic acid ethyl ester at 25°C was rep be 3.58 g(2)/100g sln. The corresponding mole fraction, x_2 , value lated by the compiler is 0.1537.	The solubility of acetic acid ethy be 7.47 g(1)/100g sln. The correst	yl ester in water at 25°C was report ponding mole fraction, x ₁ , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corresp lated by the compiler is 0.1537.	acid ethyl ester at 25°C was report ponding mole fraction, x_2 , value cal
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corresp lated by the compiler is 0.1537.	acid ethyl ester at 25 ^o C was report ponding mole fraction, x_2 , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corres lated by the compiler is 0.1537.	acid ethyl ester at 25 ⁰ C was report ponding mole fraction, x ₂ , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corresp lated by the compiler is 0.1537.	acid ethyl ester at 25 ⁰ C was report ponding mole fraction, x ₂ , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corresp lated by the compiler is 0.1537.	acid ethyl ester at 25 ⁰ C was report ponding mole fraction, x ₂ , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corresp lated by the compiler is 0.1537.	acid ethyl ester at 25 ⁰ C was report ponding mole fraction, x ₂ , value ca
		The solubility of water in acetic be 3.58 g(2)/100g sln. The corres lated by the compiler is 0.1537.	acid ethyl ester at 25 ⁰ C was repor ponding mole fraction, x ₂ , value ca

AUXILIARY INFORMATION		
AUXILIARY METHOD/APPARATUS/PROCEDURE: The titration method was used. Only the measurements for the ternary systems were described. The amount of water in the pure ester was taken into account. The data were reported together with the ternary system acetic acid ethyl ester-water-phosphoric acid.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Source not specified, chemical reagent; d_4^{20} 0.9020. (2) Twice distilled. ESTIMATED ERROR: Temp. ±0.1 ^o C (authors). Soly. about ±0.05 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler). REFERENCES:	
	KEI EKENCED.	

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COMPONEN	TS:	-	ORIGINAL MEASUREME	NTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂;</pre>		Utkin, G.K.; Zamy Andronnikov, N.	atina, V.K.; V.; Golikov, L.V.	
[141-78-6] (2) Water; H ₂ O; [7732-18-5]		Gidroliz. Lesokhim. Prom. <u>1971</u> , 24(8), 9-10.		
VARIABLES:		PREPARED BY:		
T/K = 2	98 and 313		A. Skrzecz	
EXPERIME	NTAL VALUES:		I,	
Mutual solubility of acetic acid ethyl ester and water			d water	
t/°C g(1)/100g sln		x_1 (comp	iler)	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase
25	6.9 ^a	96.9 ^b	0.0149	0.865
40	5.8 ^a	96.1 ^b	0.0124	0.834
AUXILIARY INFORMATION				
METHOD/AI	PPARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:
The titration method was used. One-phase mixture was titrated and mixed in a thermostated apparatus with a reflux condenser for 1 h. until an opalescence appeared. Only the measurements for the ternary systems were described. The data were reported together with the ternary system acetic acid ethyl ester-water-propionic acid.		 (1) Source not spanned analysis; disting at 77 used; purity 9 0.001%, without d²⁰ 0.9002. (2) Distilled; without and another analysis and another analysis and another analysis and another analysis and another a	ecified, pure for tilled, fraction .0-77.5°C was 99.5%, dry residue ut ashes, thout CO ₂ .	
		ESTIMATED ERROR:		
		Soly. about ±0.7 ^a g(1)/100g si	and ±0.1 ^b ln (compiler).	
			REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Aleksandrova, M.V.; Sadovnikova, L. V.; Martynov, V.V. Sb. Nauch. Tr. Ivanov. Energ. Inst. <u>1972</u> , 14, 146-54.
(2) Water; H ₂ O; [7732-18-5]	Sadovnikova, L.V.; Aleksandrova, M. V.; Serafimov, L.A. Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. <u>1972</u> , 15, 1183-5.
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.70 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.01911.

The solubility of water in acetic acid ethyl ester at 20° C was reported to be 2.25 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1012.

AUXTLTARY	INFORMATION
TOVIDIUNI	THEORGHITCH

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water-acetic acid. No further details were reported in the paper.	 (1) Source not specified; purified; n_D²⁰ 13724. (2) Not specified.
	ESTIMATED ERROR:
	Temp. $\pm 0.1^{\circ}$ C (authors). Soly. about ± 0.9 g(1)/100g sln and ± 0.7 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Acetic aci (ethyl ace [141-78-6]	d ethyl ester etate); C ₄ H ₈ O ₂ ;	Filip, S.; Maciejewski, Z. <i>Chem. Stoso</i> w. <u>1972</u> , 16, 445-51.
(2) Water; H ₂ O	; [7732-18-5]	
VARIABLES:		PREPARED BY:
T/K = 293		A. Skrzecz

The solubility of acetic acid ethyl ester in water at 20°C was reported to be 8.22 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0180.

The solubility of water in acetic acid ethyl ester at 20°C was reported to be 4.9 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.20.

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubility, weighed amounts of one component (ca. 50g) were titrated with the second component in a constant temperature bath. Titrations were performed using a burette graduated in 0.1-mL divisions. The samples were stirred vigorously. SOURCE AND PURITY OF MATERIALS:

- (1) FOCH Gliwice; chemically pure grade; used as received.
- (2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.4 g(1)/100g sln and ±1.9 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂;</pre>	Mertl, I. Collect. Czech. Chem. Commun.
[141-78-6]	<u>1972</u> , 37, 366-74.
VADIABLES.	DEEDADED BV.
T/K = 293 - 343	A. Skrzecz

Mutual solubility of acetic acid ethyl ester and water

t/°C	C g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
20-	7.31	97.04	0.01587	0.8/02
40	6.27	96.12	0.01349	0.8351
55	5.49	95,24	0.01174	0.8036
70 ^b	5.14	94.39	0.01096	0.7748

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. To determine the solubilities, the selected component was added from a burette to the weighed sample in a vessel with a magnetic stirrer until a slight turbidity appeared and disappeared. The jacket of the vessel was connected by an insulated tube with a thermostat. A reflux condenser prevented the solution from evaporating. The observation was facilitated by shielding the vessel and by using intense illumination. SOURCE AND PURITY OF MATERIALS:

- (1) Lachema Brno, laboratory grade; triple distilled with acetic anhydride in a 40 plate bubble-cap glass column; b.p. 77.06°C, d²⁰₄ 0.90057, n²⁰_D 1.37242.
- (2) Not specified.

ESTIMATED ERROR:

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	<pre>Sadovnikova, L.V.; Komarova, V.F.; Aleksandrova, M.V.; Serafimov, L.A. Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. <u>1972</u>, 15(12),</pre>
VARIABLES: T/K = 293	PREPARED BY: Z. Maczynska

The solubility of acetic acid ethyl ester in water at 20° C was reported to be 8.9 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0196.

The solubility of water in acetic acid ethyl ester at 20° C was reported to be 2.25 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1012.

AUXILIARY	INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified. The data were reported together with the ternary system acetic acid ethyl ester-water-2-methylpropanoic acid.	(1) Not specified.(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±1.1 g(1)/100g sln and ±0.8 g(2)/100g sln (compiler).
	REFERENCES:

	n
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Woycicka, M.; Richon, D.; Viallard, A. C.R. Acad. Sci. (Paris) Ser. C
(2) Water; H ₂ O; [7732-18-5]	<u>1973</u> , 276, 983-6.
VARIABLES:	PREPARED BY:
T/K = 298	G.T. Hefter
The mole fraction, x_1 , solubility of 25°C was reported to be 0.0162 ₅ . The culated by the compiler is 7.475 g(1) The mole fraction, x_2 , solubility of 25°C was reported to be 0.145. The co culated by the compiler is 2.66 g(2),	acetic acid ethyl ester in water at corresponding mass percent value cal- /100g sln. water in acetic acid ethyl ester at prresponding mass percent value cal- '100g sln.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A calorimetric method was used. Mutual solubility was determined from plots of excess enthalpy (H^E) against composition. The H^E values were derived from heats of mixing measurements made in a Seteram "CRMT" microcalorimeter.	 (1) Source not specified; purified by preparative gas chromato- graphy.
	(2) Distilled.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Van Zandijcke, F.; Verhoeye, L. J. Appl. Chem. Biotechnol. <u>1974</u> , 24, 709-29.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 343	A. Skrzecz
1	

The solubility of acetic acid ethyl ester in water at 70.25° C was reported to be $x_1 = 0.025$. The corresponding mass per cent value calculated by the compiler is 11.1 g(1)/100g sln.

The solubility of water in acetic acid ethyl ester at 70.25° C was reported to be $x_2 = 0.250$. The corresponding mass per cent value calculated by the compiler is 6.38 g(2)/100g sln.

METHOD/APPARATUS/PROCEDURE: SOURCE	LON
The boiling liquid, in equilibrium with its vapor, was delivered into a thermostated vessel where the phase separation occurred at the boiling point. Samples of the two phases were taken for glc analysis. The temperature of the vessel was controlled automatically and was equal to the boiling temperature. Temp. : Soly. a REFERENCE	AND PURITY OF MATERIALS: urce not specified; p. 77.15°C, d_4^{25} 0.8945, ⁵ 1.3698. t specified. ED ERROR: $\pm 0.05^{\circ}$ C (authors). about ± 4.8 g(1)/100g sln and ± 0.4 g(2)/100g sln (compiler). CES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Tare, J.P.; Puranik, S.A.; Kher, M.G. Indian Chem. Eng. <u>1976</u> , 18(4), 27-30.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 303	Z. Maczynska
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl e be 7.56 g(1)/100g sln. The correspond lated by the compiler is 0.0164.	ester in water at 30° C was reported to ding mole fraction, x_1 , value calcu-
AUXILIARY 1	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method as described by Othmur, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl ester- water-furfural. No further details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) B.D.H., analar grade; distil- led; purity not specified. (2) Not specified. (2) Not specified. ESTIMATED ERROR: Temp. ±0.5°C (authors), Soly. about ±0.3 g(1)/100g sln (compiler). REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. 1941, 33, 1240.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Sugi, H.; Katayama, T. <i>J. Chem. Eng. Jpn.</i> <u>1978</u> , <i>11</i> , 167-72.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 333	A. Skrzecz	

The solubility of acetic acid ethyl ester in water at 60° C was reported to be $x_1 = 0.0118$. The corresponding mass per cent value calculated by the compiler is 5.52 g(1)/100g sln.

The solubility of water in acetic acid ethyl ester at 60° C was reported to be $x_2 = 0.2042$. The corresponding mass per cent value calculated by the compiler is 4.985 g(2)/100g sln.

AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE: The cloud-point method as described by Sugi, Nitta and Katayama (ref 1) was used. The data were reported together with the ternary system acetic acid ethyl ester-water- acetonitrile.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Merck Uvasol, spectrograde; purity 99.7%, d²⁵ 0.89453; used as received. (2) Deionized, distilled. ESTIMATED ERROR: Temp. ±0.01°C (authors). Soly. about ±0.1 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler). REFERENCES: 1. Sugi, H.; Nitta, T.; Katayama, T. J. Chem. Eng. Jpn. <u>1976</u>, 9, 12.</pre>

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid ethyl ester	Alvarez, J.R.; Neila, J.J.	
(ethyl acetate); C ₄ H ₈ O ₂ ;	An. Quim. <u>1978</u> , 74, 326-32.	
[141-78-6]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	2. Maczynska	
EXPERIMENTAL VALUES: The solubility of acetic acid ethyl ester in water at 25°C was reported be 7.3 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0159. The solubility of water in acetic acid ethyl ester at 25°C was reported be 3.6 g(2)/100g sln. The corresponding mole fraction, x_2 , value calcu- lated by the compiler is 0.154.		
AUXILTARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: Presumably the titration method was used. The data were reported together with the ternary system acetic acid ethyl ester-water- phenol. No further details were reported in the paper.	(1) Source not specified, commer- cial product; used as received; $d_4^{21.8}$ 0.8943, n_D^{20} 1.3724. (2) Twice distilled over KMnO ₄ .	
	ESTIMATED ERROR: Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler). REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid ethyl ester (<i>ethyl acetate</i>); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	<pre>Skrzecz, A.; Maczynski, A. Pol. J. Chem. <u>1979</u>, 53, 715-8. Skrzecz, A. Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u>.</pre>
VARIABLES: T/K = 286 - 364	PREPARED BY: A. Skrzecz

Mutual solubility of acetic acid ethyl ester and water

T/K	<i>x</i> 1	<i>x</i> ₁		g(1)/100g sln	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
285.8	0.0178	-	8.14	_	
299.2	0.0176	-	8.06	-	
307.1	0.0152	-	7.02	-	
307.9	-	0.8401	-	96.25	
311.6	0.0145	-	6.71	-	
318.6	0.0136	-	6.32	-	
320.2	0.0133	-	6.18	-	
322.7	-	0.8116	-	95.47	
327.7	0.0124	-	5.79	-	
332.2	-	0.7902	-	94.85	
343.0	0.0133	-	6.18	-	
344.7	-	0.7575	-	93.86	
346.2	-	0.7536	-	93.73	
			(con	tinued next pag	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew was used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. The amount of water in pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

- (1) Lachema Chemapol, pure for analysis grade; distilled; purity 99.99% by glc, 0.07 wt% water by the Karl Fischer method.
- (2) Distilled.

ESTIMATED ERROR:

Temp. $\pm (0.2-0.6)^{\circ}C.$ Soly. see above.

REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1)	Acetic acid ethyl ester	Skrzecz, A.; Maczynski, A.	
	(ethyl acetate); C ₄ H ₈ O ₂ ; [141-78-6]	Pol. J. Chem. <u>1979</u> , 53, 715-8.	
(2) Water; H ₂ O; [7732-18-5]	Skrzecz, A.		
	Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .		

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid ethyl ester and water

x	L	g(1)/100g sln	
(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0.0145		6.71	_
0.0158	-	7.28	-
-	0.7114	-	92.34
	x ₁ (2)-rich phase 0.0145 0.0158 -		$ \begin{array}{cccccccccccccccccccccccccccccccccccc$

Author's smoothing equations:

 $x_1 = 0.02175 - 3.081 \times 10^{-4} (T/K - 273.15) + 2.784 \times 10^{-6} (T/K - 273.15)^2$ st. dev. = 5.5 x 10⁻⁴ (2)-rich phase

 $x_2 = 0.09360 + 1.6981 \times 10^{-3} (T/K - 273.15) + 5.0221 \times 10^{-6} (T/K - 273.15)^2$ st. dev. = 2.19 x 10⁻³ (1)-rich phase

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] (2) Water; H₂O; [7732-18-5] 	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. <i>J. Chem. Eng. Data</i> <u>1982</u> , 27, 451-4.	
VARIABLES: T/K = 298	PREPARED BY: A. Skrzecz	

EXPERIMENTAL VALUES:

The solubility of acetic acid ethyl ester in water at $25^{\circ}C$ was reported to be 0.726 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 64.0 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.	 (1) Source not specified; purity >99% by glc. (2) Not specified.
	ESTIMATED ERROR: Temp. ±0.1 ^o C. Soly. ±1.0%.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Ouyang, F.; Wang, G.; Gao, W. Hua Kung Hsueh Pao <u>1985</u> , (1), 110-18.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 323	J. Fu

The proportion of acetic acid ethyl ester in the water-rich phase equilibrium at 50° C was reported to be 7.58 g(1)/100 g sln. The corresponding mole fraction solubility, x_1 , is 0.0165.

The proportion of water in the ester-rich phase at 50° C was reported to be 4.23 g(2)/100 g sln. The corresponding mole fraction solubility, x_2 , is 0.1778.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An analytical method was used. Sample mixtures in an equilibrium cell immersed in a constant temperature water bath were stirred with a magnetic agitator to be emulsified. Then, the mixture was settled for 4 h. and samples withdrawn from the upper and lower layers were analyzed by gas chromatograph.

SOURCE AND PURITY OF MATERIALS:

- CP reagent; fractionated before use and no other impurity peaks except that of ethyl acetate in chromatogram.
- (2) Twice distilled; b.p. 100.00°C.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:				
1) Ace	Acetic acid ethyl ester		Richon, D.;	Viallard, A	Α.	
(et [14	chyl aceta 1-78-6]	te); C ₄ H ₈ O	9 ₂ ;	Fluid Phase 279-93.	Equilib. <u>1</u>	<u>1985</u> , 21,
(2) Wat	er; H ₂ 0;	[7732-18-5	5]			
ARIABLES	5:			PREPARED BY:		
r/K = 29	8 and 318			A. Skrzecz		
(PERIME)	ITAL VALUE	S:		<u>.</u>		
T/K	TAL VALUE Mutual so mol(1)/ 100g(2)	S: olubility g(1)/ 100g(2)	of acetic	acid ethyl es	ter and wate g(1)/100c (compile	er g sln er)
T/K	Mutual so mol(1)/ 100g(2)	S: olubility g(1)/ 100g(2)	of acetic x (2)-r. ph.	acid ethyl es 1 (1)-r. ph.	g(1)/100g (compile (2)-r. ph.	er g sln er) (1)-r. ph.
T/K 298.1 ^a	mol(1)/ 100g(2)	S: olubility g(1)/ 100g(2) 	of acetic x (2)-r. ph. 0.01625	acid ethyl es 1 (1)-r. ph. 0.885	g(1)/1000 (compile (2)-r. ph. 7.475 ^d	er g sln er) (1)-r. ph.
XPERIMEN 	TAL VALUE Mutual so mol(1)/ 100g(2) - 0.0923	S: olubility g(1)/ 100g(2) - -	of acetic x (2)-r. ph. 0.01625 0.01636 ^c	acid ethyl es 1 (1)-r. ph. 0.885 -	g(1)/100g (compile (2)-r. ph. 7.475 ^d 7.521 ^d	er g sln er) (1)-r. ph. 97.41 ^e
XPERIMEN T/K 298.1 ^a 298.1 ^b 298.1	TAL VALUE: Mutual so mol(1)/ 100g(2) - 0.0923 -	S: olubility g(1)/ 100g(2) - - 8.13	of acetic x (2)-r. ph. 0.01625 0.01636 ^c 0.01635 ^c	acid ethyl es 1 (1)-r. ph. 0.885 - -	ter and wate g(1)/100g (compile (2)-r. ph. 7.475 ^d 7.521 ^d 7.519 ^d	er g sln er) (1)-r. ph. - 97.41 ^e -

a Calorimetric method.

^b Refractometric method.

c Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The calorimetric and differential refractometric methods were used. The calorimetric method was described in the thesis of Richon (ref 1) and by Richon and Villard (ref 2). For the refractometric measurements, a Phoenix model 1-2000T differential refractometer from Texas Instruments was used, and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

- (1) Merck (for analysis); purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.
- (2) Distilled.

ESTIMATED ERROR:

Soly. about $\pm 0.03^{d}$, $\pm 0.6^{e}$ and $\pm 0.1^{f}$ g(1)/100g sln (compiler).

REFERENCES:

 Richon, D. Thesis, University de Clermont-Ferrand, <u>1974</u>.
 Richon, D.; Villard, A. Can. J. Chem. <u>1976</u>, 54, 2584.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6]</pre>	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 344	Z. Maczynska

Mutual solubility of acetic acid ethyl ester and water

t/°C	g(1)/100g sln		x1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	9.71	97.87	0.0215	0.9038
9.8	8.62	97.52	0.0189	0.8894
20.2	7.79	97.12	0.0170	0.8733
29.7	6.81	96.74	0.0147	0.8585
39.5	6.28	96.36	0.0135	0.8440
50.0	6.20	95.96	0.0133	0.8292
59.9	6.06	95.77	0.0130	0.8223
70.5	5.88	95.56	0.0126	0.8148

std. dev. 0.05 0.02

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial sample; purity 99.9%; used as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formic acid 1-methylethyl	Stephenson, R.; Stuart, J.
ester (isopropyl formate);	J. Chem. Eng. Data <u>1986</u> , 31,
$C_4 H_8 O_2; [625-55-8]$	56-70.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 333	Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of water in formic acid 1	-methylethyl ester
t/°C g(1)/100g sln x	(compiler)
0 98.95	0.9506
9.6 98.67	0.9381
19.7 98.34	0.9237
30.7 98.24	0.9194
40.0 97.83	0.9021
49.9 96.97	0.8674
60.2 96.40	0.8455
AUXILIARY 1	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a	 (1) Source not specified, commer- cial sample; purity 96%; used as received. (2) Not specified.
weighed amount of acetonitrile (or sometimes propanol) to the	
organic layer sample and measuring by a Gow-Mac thermal conductivity	ESTIMATED ERROR:
gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP	Accuracy of method 0.1 wt% or less, for solubility, see above.
A similar procedure but a higher boiling material (e.g. 1-hexanol)	
was used to determine (2) in the water layer.	REFERENCES:

COMPONENTS:		EVALUATOR:	
(1)	Formic acid propyl ester (propyl formate); C ₄ H ₈ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[110-74-7]	Murdoch University, Perth, W.A.,	
(2) Water: H ₂ O: [7732-18-5]	Australia		
(-)		January, 1989	

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the

<u>Formic acid pro</u>	pyl ester	(1) - Water (2) S	System
Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 3)	272-318	(1) in (2)	synthetic
Rius and Alfonso (ref 4)	273-333	mutual	analytical, Karl Fischer
Stephenson and Stuart (ref 5)	273-343	(2) in (1)	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid propyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Traube (ref 1) which is significantly lower (> $3\sigma_n$) than all other studies and is therefore rejected. The remaining studies, especially those of Rayman (ref 2) and Kendall and Harrison (ref 3) are in good agreement and a number of values are Recommended. Selected data are plotted in Figure 1. However, it is pertinent to note that Stephenson and Stuart (ref 5) who usually report mutual solubility data were unable to do so for this system because of substantial hydrolysis of the ester in the aqueous phase. Other authors do not appear to have experienced similar problems.

(continued next page)

СОМРС	DNENTS:	EVALUATOR:
(1)	Formic acid propyl ester (propyl formate); C ₄ H ₈ O ₂ ; [110-74-7]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2:Recommended (R) and Tentative Solubilitiesof Formic acid propyl ester (1) in Water (2)

T/K	Solubilities	
	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(1)/100g sln	$g(1)/100g \ sln \ 10^3 x_1$
273	3.39 (ref 2), 3.54 [*] (ref 3), 3.09 (ref 4)	3.3 ± 0.2 (R) 6.9
283	3.00 (ref 2), 3.04 [*] (ref 3), 2.80 [*] (ref 4)	2.95 ± 0.10 (R) 6.18
293	2.79 (ref 2), 2.82 [*] (ref 3), 2.63 [*] (ref 4)	2.75 ± 0.08 (R) 5.75
298	2.75 (ref 2), 2.76 [*] (ref 3), 2.56 (ref 4)	2.69 ± 0.09 (R) 5.62
303	2.70 (ref 2), 2.71 [*] (ref 3), 2.50 [*] (ref 4)	2.64 ± 0.10 (R) 5.52
313	2.61 [*] (ref 3), 2.44 (ref 4)	2.52 ± 0.09 (R) 5.26
323	2.49 [*] (ref 4)	2.5 5.2
333	2.70 (ref 4)	2.7 5.6

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN FORMIC ACID PROPYL ESTER (1)

All the available data for the solubility of water (2) in formic acid propyl ester (1) are summarized in Table 3. Only two independent studies are available (ref 4,5) and the data are not in good agreement (see Figure 2) especially at higher temperatures. Consequently, no values have been Recommended and further investigation of this system is clearly justified with particular attention being given to the possibilities of ester hydrolysis.

(continued next page)




		EVALUATION .	
(1) (2)	DNENTS: Formic acid propyl ester (propyl formate); C ₄ H ₈ O ₂ ; [110-74-7] Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematica and Physical Sciences, Murdoch University, Perth, W.A., Australia	
CRIT	ICAL EVALUATION: (continued)		
REFE	RENCES		
1.	Traube, J. Ber. Dtsch. Chem. Ges	5. <u>1884</u> , 17, 2294-316.	
2.	Rayman, J. <i>Thesis</i> . Budapest, <u>190</u>	<u>06</u> .	
3.	Kendall, J.; Harrison, E. Trans	s. Faraday Soc. <u>1928</u> , 24, 588-96.	
••	. Rius, A.; Alfonso, C. An. Fis. Quim. Ser. B. <u>1955</u> , 51, 649-58.		
j.	Stephenson, R.; Stuart, J. J. C	Chem. Eng. Data <u>1986</u> , 31, 56-70.	
OWN			
CRIV	The Furlington thanks Dr. Drive al	and for the monthing	
	The Evaluator thanks br. Brian Cl	lare for the graphics.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Formic acid propyl ester (propyl formate); C₄H₈O₂; [110-74-7]</pre>	Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u> , 17, 2294-316.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 295	A. Skrzecz

The solubility of formic acid propyl ester in water at $22^{\circ}C$ was reported to be 1 part of formic acid propyl ester in 46 parts of water. The corresponding mass percent and mole fraction, x_1 , values calculated by the compiler are 2.13 g(1)/100g sln and 0.0044.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Not specified.
	(2) Not specified.
	ESTIMATED EDDOD.
	Not specified.
	REFERENCES:
	_

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Formic acid propyl ester	Rayman, J.	
(propyl formate); C ₄ H ₈ O ₂ ;	Thesis, Budapest, 1906.	
[110-74-7]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 303	G.T. Hefter	
EXPERIMENTAL VALUES:		
Solubility of formic acid p	ropyl ester in water	
t/°C g(1)/100g(2) g(1)/10	Dog solution x_1	
(C	ompiler) (compiler)	
0. 3.51	3.39 0.00712 3.00 0.00629	
20. 2.87	2.79 0.00584	
30. 2.77	2.70 0.00564	
AUXILIARY		
METHOD/APPARATUS/PROCEDURE: The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possi-	 SOURCE AND PURITY OF MATERIALS: (1) Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated. (2) Not specified. 	
from the solubility of (2) in (1).	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Winkler, L. Z. Phys. Chem. <u>1906</u> , 55, 360.	
	2. Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u> ,	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Formic acid propyl ester	Kendall, J.; Harrison, L.E.	
(propyl formate);	Trans, Faraday Soc. 1928, 24.	
C ₄ H ₈ O ₂ ; [110-74-7]	588-96.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 272 - 318	Z. Maczynska	
FYDERTMENTAL VALUES:	I	
Solubility of formic acid propyl	ester in water	
$\frac{1}{1000}$	sln (compiler)	
-1.0 0.00760	3.61	
4.0 0.00695 3	3.31	
6.0 0.00670 3	9.19	
12.5 0.00620 2	2.96	
20.0 0.00589 2	2.82	
34.0 0.00555 2	5.60	
45.0 0.00555 2		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The synthetic method was used. The sealed tube method (ref 1) was adopted, the free space being kept as small as possible in order to avoid any significant change in composition at the higher temperatures.	 (1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C. (2) Distilled. 	
	ESTIMATED ERROR:	
	$T_{emp} + (0, 1 - 0, 2)^{\circ}C$	
	Temp. ±(0.1-0.2)°C.	
	REFERENCES:	
	1. Smith, A.; Eastlack, H.E. J. Am. Chem. Soc. <u>1916</u> , 38, 1269.	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Formic acid propyl ester (propyl formate); C₄H₈O₂; [110-74-7] 	Rius, A.; Alfonso, C. An. Fis. Quim. Ser B. <u>1955</u> , 51, 649-58.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 333	G.T. Hefter	
EXPERIMENTAL VALUES: Mutual solubility of formic acid propyl ester and water		
$+/^{0}$ $a(1)/100a sln x a(2)/100a sln x$		

0. 3.09 0.00650	0.82	0.0387	
25. 2.56 0.00535	1.26	0.0586	
40. 2.44 0.00510	1.54	0.0709	
60. 2.70 0.00565	2.17	0.0978	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Appropriate quantities of components (1) and (2) were thermostatted separately to avoid ester hydrolysis. Then, they were combined and shaken in a separatory funnel and the two layers were analyzed. The ester was determined by a micro-saponification technique using 2M NaOH in a 50% methanol/water solution. The water was determined by Karl Fischer titrations using electrometric endpoint detection.

SOURCE AND PURITY OF MATERIALS:

- (1) Prepared from formic acid (85%, CP, Probus) and 1-propanol; free acid < 0.1%; water content < 0.1%.</pre>
- (2) Distilled from KMnO₄.

ESTIMATED ERROR:

Temp. ±0.02°C (25°C) - ±0.1°C (60°C) Soly. ±0.5% rel., (1). ±0.4% rel., (2).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Formic acid propyl ester	Stephenson, R.: Stuart, J.	
(propyl formate); C ₄ H ₈ O ₂ ;	I Chom Eng Data 1996 21	
[110-74-7]	56-70.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 344	Z. Maczynska	
EXPERIMENTAL VALUES:		
Solubility of water in formic ac	id propyl ester	
t/°C g(1)/100g sln	x ₁ (compiler)	
0 98.93	0.9497	
9.5 98.68	0.9386	
20.3 98.42	0.9272	
31.0 98.09	0.9130	
40.3 97.73	0.8980	
50.1 96.99 61.0 96.26	0.8682	
70.6 94.75	0.7867	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each	(1) Source not specified, commer- cial sample; purity 96%; used as received.	
layer was sampled with a syringe;		
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the	(2) Not specified.	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity	(2) Not specified. ESTIMATED ERROR:	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator).	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above.</pre>	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was word to determine (2) in the	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above.</pre>	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>	
(1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>(2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>	

COMPONENTS:		EVALUATOR:	
(1)	Propanoic acid methyl ester (methyl propionate); C ₄ H ₈ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,	
	[554-12-1]	Murdoch University, Perth, W.A.,	
(2) Water: H_O: [7732-18-5]	Australia		
(-,,, [December, 1988	

CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

Propanoic acid	methyl ester	(1) - Water (2) System
Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Kendall and Harrison (ref 3)	271-316	(1) in (2)	synthetic
Bomshtein et al. (ref 4)	293-343	mutual	titration
Richon and Viallard (ref 5)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 6)	273-343	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of propanoic acid methyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Traube (ref 1) which is much lower $(>3\sigma_n)$ than all other values (ref 2-6) and is therefore rejected.

The remaining data (ref 2-6) are generally in good agreement, enabling the average values to be Recommended over most of the temperature range studied, even though the temperature dependence of individual studies varies markedly. Selected data are plotted in Figure 1.

COMPONENTS:		EVALUATOR:
(1)	Propanoic acid methyl ester (<i>methyl propionate</i>); C ₄ H ₈ O ₂ ; [554-12-1]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia December, 1988

CRITICAL EVALUATION: (continued)

TABLE 2:Recommended (R) and Tentative Solubilitiesof Propanoic acid methyl ester (1) in Water (2)

T/K	Solubilit	ies
	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(1)/100g sln	$g(1)/100g \ sln \ 10^2 x_1$
273	8.46 (ref 2), 8.48 [*] (ref 3), 7.80 (ref 6)	8.3 ± 0.4 (R) 1.81
283	7.30 (ref 2), 7.38 [*] (ref 3), 6.89 (ref 6)	7.2 ± 0.2 (R) 1.56
293	6.50 (ref 2), 6.77 [*] (ref 3), 6.18 (ref 4), 6.25 (ref 6)	6.4 ± 0.2 (R) 1.38
298	6.22* (ref 2), 6.59* (ref 3), 5.6* (ref 4), 5.98 (ref 5), 5.98* (ref 6)	6.1 ± 0.3 (R) 1.31
303	5.93 (ref 2), 6.46 [*] (ref 3), 5.29 (ref 4), 5.72 [*] (ref 6)	5.9 ± 0.5 1.26
313	6.24 [*] (ref 3), 5.16 (ref 4), 5.36 [*] (ref 6)	5.6 ± 0.5 1.20
323	5.07 (ref 4), 5.11 (ref 6)	5.1 ± 0.1 (R) 1.09
333	5.02 (ref 4), 4.96 (ref 6)	5.0 ± 0.1 (R) 1.06
343	4.98 (ref 4), 4.90 (ref 6)	4.9 ± 0.1 (R) 1.04

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID METHYL ESTER (1)

Only Bomshtein *et al.* (ref 3) and Stephenson and Stuart (ref 5) have reported the solubility of water (2) in propanoic acid methyl ester (1). Their data are summarized in Table 3 and plotted in Figure 2. In general the agreement between the two studies is poor and the solubilities show quite different temperature dependences. Further study of this system is clearly warranted and the "Best" values must be regarded as very Tentative.



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COMPONENTS:		EVALUATOR:
(1)	Propanoic acid methyl ester (methyl propionate);	G.T. Hefter, School of Mathematical and Physical Sciences,
$C_4H_8O_2$	$C_4H_8O_2$; [554-12-1] Water: H_O: [7732-18-5]	Murdoch University, Perth, W.A., Australia
(2)		December, 1988

CRITICAL EVALUATION: (continued)

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.



COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid methyl ester	Traube, J.	
(methyl propionate); C ₄ H ₈ O ₂ ; [554-12-1]	Ber. Dtsch. Chem. Ges. <u>1884</u> , 17, 2294-316.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 295	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid meth ported to be 1 part of propanoic acid water. The corresponding mass percent calculated by the compiler are 5.2 g	byl ester in water at 22° C was re- a methyl ester in 17-20 parts of a and mole fraction, x_1 , values (1)/100g sln and 0.011.	
AUXILIARY		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Soly. $\pm 0.4 \text{ g(1)}/100 \text{g sln.}$	
	REFERENCES:	

<u> </u>			1		
COMPONENTS:			ORIGINAL MEASUREMENTS:		
(1) Propanoic acid methyl ester		Rayman, J	•		
(methyl propionate); C ₄ H ₈ O ₂ ;		Thesis, B	udapest, <u>1906</u> .		
[554-:	12-1]				
(2) Water	; H ₂ O; [7732-18-5]				
VARIABLES:			PREPARED B	Y:	
T/K = 273 ·	- 303		G.T. Heft	er	
EXPERIMENTAL	L VALUES:		L		
Sol	lubility of propan	oic acid	methyl este	er in water	
t/°C	g(1)/100g(2)	g(1)/10	0g solution	<i>X</i> 1	
		(cc	ompiler)	(compiler)	
			7.00		
10.	8.46		6.80	0.0170	
20.	6.50		6.10	0.0131	
30.	5.93		5.60	0.0119	
AUXILIARY I		NFORMATION			
METHOD/APPARATUS/PROCEDURE:			SOURCE AND	PURITY OF MATER	RIALS:
The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possi-		(1) Kahlba salt v CuSO ₄ ;	aum or Merck; wa water; dried ove ; purity not sta	ashed with er CaCl ₂ or ited.	
		(2) Not sp	pecified.		
ble to mini from the so	mize the error ari lubility of (2) ir	lsing n (1).	ESTIMATED ERROR:		
from the solubility of (2) in (1).		Not specified.			
		ľ	REFERENCES:		······
			1. Winkler <u>1906</u> , 5	c, L. Z. Phys. 55, 360.	Chem.
			2. Hill, A cal Tab McGraw Vol. 3,	A.E. Internation ples (Washburn, Hill, New York, 387-98.	al Criti- E.W., Ed.) <u>1928</u> ,

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COMPONENTS:	<u></u>		ORIGINAL MEASUREMENTS:
(1) Propanoic acid methyl ester		ester	Kendall, J.; Harrison, L.E.
(methyl C ₄ H ₈ O ₂ ;	<pre>propionate); [554-12-1]</pre>		Trans. Faraday Soc. <u>1928</u> , 24, 588-96.
(2) Water;	H ₂ O; [7732-18-	5]	
VARIABLES:			PREPARED BY:
T/K = 271 - 316			Z. Maczynska
EXPERIMENTAL Solubilit	VALUES: y of propanoic	acid methy	yl ester in water
t/°c	<i>x</i> ₁	g(1)/100g	sln (compiler)
-2.1	0.0195		3.87
1.0	0.0180	8	3.23
11.5	0,0158	-	7.28
14.9	0.0153	•	7.06
20.0	0.0147	· ·	5.80
27.1	0.0140	(5.49
32.5	0.0138		5.41
·····		<u></u>	
		AUXILIARY	INFORMATION
METHOD/APPARA	TUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:
The synthetic The sealed to adopted, the as small as p avoid any sid composition a tures.	c method was u ube method (re free space be possible in or gnificant chan at the higher	sed. f 1) was ing kept der to ge in tempera-	 (1) Source not specified, CP commercial sample; distilled; b.p. range 0.1°C. (2) Distilled.
			ESTIMATED ERROR: Temp. ±(0.1-0.2) ^o C.
			REFERENCES: 1. Smith, A.; Eastlack, H.E. J. Am. Chem. Soc. <u>1916</u> , 38, 1269.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Propanoic acid methyl ester	Bomshtein, A.L.; Trofimov, A.N.;	
(methyl propionate); C ₄ H ₈ O ₂ ;	Serafimov, L.A.	
[554-12-1] (2) Water; H₂O; [7732-18-5]	Zh. Prikl. Khim. <u>1978</u> , 51, 1280-2.	
VARIABLES:	PREPARED BY:	
T/K = 293 - 343	A. Skrzecz	

Mutual solubility of propanoic acid methyl ester and water

t/°C	x ₁ (2)-rich phase	(1)-rich phase	g(1)/100g sl (2)-rich phase	n (compiler) (1)-rich phase
20	0.0133	0.9529	6.18	99.00
30	0.0113	0.8927	5.29	97.60
40	0.0110	0.8571	5.16	96.70
50	0.0108	0.8308	5.07	96.00
60	0.0107	0.8023	5.02	95.20
70	0.0106	0.7785	4.98	94.50

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The titration method was used at constant temperature. No further details were reported in the paper.	 SOURCE AND PURITY OF MATERIALS: (1) Source not specified; distilled; without impurities by glc, b.p. 79.8°C, n_D²⁰ 1.376. (2) Not specified. ESTIMATED ERROR: Not specified. 		
	REFERENCES:		

, 9111 911 LIT 1 9 1	ORIGINAL MEASUREMENTS:
<pre>(1) Propanoic acid methyl ester (methyl propionate); C₄H₈O₂; [554-12-1]</pre>	Richon, D.; Viallard, A. Fluid Phase Equilib. <u>1985</u> , 21, 279-93.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

SOURCE AND PURITY OF MATERIALS:

 BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Richon, D. *Thesis*, University de Clermont-Ferrand, <u>1974</u>.

COMPONENTS: (1) Propanoic acid methyl ester (methyl propionate); C ₄ H ₈ O ₂ ; [554-12-1]	ORIGINAL MEASUREMENTS: Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 343	Z. Maczynska	

Mutual solubility of propanoic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
((2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	7.80	98.49	0.0170	0.9302
10.0	6.89	98.23	0.0149	0.9190
20.2	6.24	97.46	0.0134	0.8869
30.9	5.71	97.60	0.0122	0.8926
40.3	5.35	97.22	0.0114	0.8773
50.3	5.10	97.19	0.0109	0.8761
60.1	5.05	96.91	0.0108	0.8651
70.2	4.79	96.76	0.0102	0.8593
std. dev	. 0.03	0.01		

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial sample; purity 98%; used as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above. REFERENCES:</pre>		

<pre>COMPONENTS: (1) Hypochlorous acid 1,1-dimethylethyl ester (tert-butyl hypochlorite); C₄H₉ClO; [507-40-4] (2) Water; H₂O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Westwater, J.W.; Audrieth, L.F. Ind. Eng. Chem. <u>1954</u> , 46, 1281-4.
VARIABLES:	PREPARED BY:
T/K = 273 and 293	A. Skrzecz

Mutual solubility of Hypochlorous acid 1,1-dimethylethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0 ^a	0.15	99.86	0.0002	0.9916
20 ^b	0.32	99.73	0.00053	0.9839

AUXTLTARY	TNFORMATION
VOVIDIUVI	THEORYTICH

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Samples of 10-20g size, placed in a glass-stoppered bottle, were titrated and shook manually. The cloud point was assumed to be reached when the cloud persisted for 2 minutes during shaking. The method and data were reported together with the ternary system Hypochlorous acid 1,1-dimethylethyl ester-water-1,1-dimethylethanol (tert-butyl hypochlorite-watertert-butyl alcohol). SOURCE AND PURITY OF MATERIALS:

- (1) Synthesized from 1,1-dimethyl ethanol (tert-butyl alcohol) by the method reported by Teeter, Bachman, Bell and Cowan (ref 1); washed six timed with $Na_2CO_3(aq)$ and water, vacuumdistilled, the middle cut boiling at 31-33°C at 68-70 mm Hg was used without further purification; purity 94.4% by active chlorine analysis; d^{20} 0.9599, n^{20} 1.40354.
- (2) Deionized; $n_{\rm D}^{20}$ 1.33292.

ESTIMATED ERROR:

^a Temp. +0.6°C. ^b Temp. ±0.1°C.

REFERENCES:

 Teeter, H.M.; Bachman, R.C.; Bell, E.W.; Cowan, J.C. Ind. Eng. Chem. <u>1949</u>, 41, 849.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Propanoic acid ethenyl ester (vinyl propionate); C₅H₈O₂; [105-38-4] (2) Water; H₂O; [7732-18-5] 	Tikhonova, N.K.; Timofeev, V.S.; Kozhukhova, N.I.; Serafimov, L.A. Fiz. Khim. Osn. Rektifikatsii <u>1970</u> , 79-88.	
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES:		

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The solubility of propanoic acid ethenyl ester in water at 20°C was reported to be 0.3 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 5.4×10^{-4} .

The solubility of water in propanoic acid ethenyl ester at 20°C was reported to be 0.5 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.027.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Two-phases mixtures were placed in a thermostated apparatus with a mechanical stirrer and mixed. After separation, the samples of both equilibrium phases were analyzed. Water was determined by the Karl Fischer method. No further details were reported in the paper. The data and method were reported together with the ternary system propanoic acid ethenyl ester-water- acetic acid.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified; used as received; b.p. 94.7°C, n_D^{20} 1.4048. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES:	

COMPONENTS:		EVALUATOR:
(1)	2-Propenoic acid ethyl ester (ethyl acrylate); C ₅ H ₈ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[140-88-5]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732-18-5]	Australia
, - <i>i</i>		January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 2-propenoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2-Propenoic acid ethyl ester (1) - Water (2) System

	Reference	T/K	Solubility	Method
Frolov et	al. (ref 1,2)	293	mutual	titration
Dabrowski	(ref 3)	288,298	mutual	synthetic

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-PROPENOIC ACID ETHYL ESTER (1) IN WATER (2)

The available data for the solubility of 2-propenoic acid ethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data of Frolov *et al.* (ref 1,2) and Dabrowski are in good agreement and the average value is Recommended. At other temperatures, only the values of Dabrowski are available and these data must be classified as Tentative pending further studies.

TABLE 2:Recommended (R) and Tentative Solubilitiesof 2-Propenoic acid ethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values (± σ ,	n) ^a
	g(1)/100g sln	g(1)/100g sln	$10^{3}x_{1}$
288	2.27 (ref 3)	2.3	4.2
293	2.02 (ref 1,2), 2.20* (ref 3)	2.11 ± 0.09 (R)	3.86
298	2.13 (ref 3)	2.1	3.9

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

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COMPONENTS:		EVALUATOR:
(1)	2-Propenoic acid ethyl ester (ethyl acrylate); C ₅ H ₈ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[140-88-5]	Murdoch University, Perth, W.A.,
(2)	Water: H.O: [7732-18-5]	Australia
(-)		January, 1989

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2-PROPENOIC ACID ETHYL ESTER (1)

The available data for the solubility of water (2) in 2-propenoic acid ethyl ester (1) are summarized in Table 3. At 293 K, the only temperature where comparison is possible, the data of Frolov *et al*. (ref 1,2) and Dabrowski (ref 3) are only in fair agreement. Consequently, all data must be classified as Tentative pending further studies.

> TABLE 3: Tentative Solubilities of Water (2) in 2-Propenoic acid ethyl ester (1)

T/K	Solubilities		
	Reported values	"Best" values ^a	
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$
288	1.27 (ref 3)	1.3	6.8
293	0.956 (ref 1,2), 1.38 [*] (ref 3)	1.4	7.3
298	1.49 (ref 3)	1.5	7.8

^a Rounded values of ref 3.

REFERENCES

- Frolov, A. F.; Loginova, M. A.; Pantukh, B. I.; Ustavshchikov, B. F. Zh. Fiz. Khim. <u>1966</u>, 40. 100-1.
- Loginova, M. A.; Frolov, A. F.; Pantukh, B. I. Khim. Prom. <u>1966</u>, 42, 674-7.
- 3. Dabrowski, L. Thesis, I. Ch. F. PAN, Warszawa, 1984.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) 2-Propenoic acid ethyl ester (ethyl acrylate); C₅H₈O₂; [140-88-5]</pre>	Frolov, A.F.; Loginova, M.A.; Pantukh, B.I.; Ustavshchikov, B.F. Zh. Fiz. Khim. <u>1966</u> , 40, 100-1.
(2) Water; H ₂ O; [7732-18-5]	Loginova, M.A.; Frolov, A.F.; Pantukh, B.I. Khim. Prom. <u>1966</u> , 42, 674-7.
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz

The solubility of 2-propenoic acid ethyl ester in water at $20^{\circ}C$ was reported to be 2.02 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00370.

The solubility of water in 2-propenoic acid ethyl ester at 20° C was reported to be 0.956 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.00509.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The titration method was used. Both a direct titration of the sample and a reverse titration up to turbidity were made. The data were reported together with the ternary system 2-propenoic acid ethyl ester-water-ethanol.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified; technical grade; vacuum-distilled; purity 99.5%, b.p. 99.5°C, d4^0 0.924, n_D^0 1.4075. (2) Distilled. ESTIMATED ERROR: Not specified. REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) 2-Propenoic acid ethyl ester	Dabrowski, L.	
(ethyl acrylate); C ₅ H ₈ O ₂ ;	Thesis, Inst. Phys. Chem., Pol.	
[140-88-5]	Acad. Sci., warszawa, <u>1984</u> .	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 288 and 298	A. Skrzecz	
Mutual solubility of 2-prope	enoic acid ethyl ester and water	
T/K g(1)/100g sln	X1	
(2)-rich phase (1)-rich p	phase (2)-rich phase (1)-rich phase	
288.15 2.27 98.73	0.0042 0.9333	
298.15 2.13 98.51	0.0039 0.9225	
AUXILIA	RY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The modified Othmer-White-Trueger method was used. The samples of known composition were slowly cool ed to obtain the temperature of turbidity which was a little below the desired temperature. After addition of a small amount of one component the procedure was repeat ed. The solubility at the desired temperature was obtained by an	 (1) ICSO Blachownia Slaska; used as received; contained 0.24% water; n_D²⁵ 1.40449. (2) Twice distilled. 	
interpolation. All measurements were made in a thermostated vessel of 50 cm ³ in the range ±3°C of the needed temperature. Temperatures of the samples were measured with a mercury-in-glass thermometer. A magnetic stirrer was used. The water included in ester was taken into account. The data and method were reported together with the ternary system 2-propenoic acid ethyl ester-water-2-propenoic acid (ethyl acrylate-water-acrylic acid).	ESTIMATED ERROR: Temp. ±0.05°C. Soly. ±0.02 g(1)/100g sln. REFERENCES:	

COMPONENTS:	EVALUATOR:
<pre>(1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C₅H₈O₂; [80-62-6]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H ₂ O; [7732-18-5]	January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 2-methyl-2-propenoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2-Methyl-2-propenoic acid methyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Shanley and Greenspan (ref	1) R.T. ^a	(2) in (1)	unspecified
Schildknecht (ref 2)	273-353	(1) in (2)	unspecified
Frolov (ref 3)	293	mutual	unspecified
Frolov et al. (ref 4)	293	mutual	GLC, analytical
Arutyunyan et al. (ref 5)	303	(1) in (2)	volumetric
Chubarov et al. (ref 6)	293-363	(2) in (1)	unspecified
Fu et al. (ref 7)	298-333	mutual	synthetic ?

^a R.T. - room temperature

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 2-METHYL-2-PROPENOIC ACID METHYL ESTER (1) IN WATER (2)

The available data for the solubility of 2-methyl-2-propenoic acid methyl ester (1) in water (2) are summarized in Table 2. The value reported by Frolov (ref 3) at 293 K has been rejected as it is lower than all other values and it has therefore been excluded from Table 2. The value reported by Shanley and Greenspan (ref 1) at an unspecified temperature has been similarly excluded from Table 2. All other data are in excellent agreement enabling the average "Best" values to be Recommended over a wide temperature range. Selected data are plotted in Figure 1.

COMPONENTS:	EVALUATOR:
<pre>(1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C₅H₈O₂; [80-62-6]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia
(2) Water; H ₂ O; [7732-18-5]	January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (R) and Tentative Solubilities of 2-Methyl-2-propenoic acid methyl ester (1) in Water (2)

T/K	Solubilit	ies	
	Reported values	"Best" values (± σ	n) ^a
	g(1)/100g sln	g(1)/100g sln	$10^{3}x_{1}$
273	1.85 (ref 2)	1.9	3.5
283	1.71 [*] (ref 2)	1.7	3.1
293	1.59 (ref 2), 1.55 (ref 4)	1.57 ± 0.02 (R)	2.86
298	1.54 [*] (ref 2), 1.54 (ref 7)	1.54 (<i>R</i>)	2.80
303	1.50 [*] (ref 2), 1.50 (ref 5) 1.49 [*] (ref 7)	1.50 (R)	2.73
313	1.43 (ref 2), 1.43 [*] (ref 7)	1.43 (R)	2.60
323	1.43 [*] (ref 2), 1.47 [*] (ref 7)	1.45 ± 0.02 (R)	2.64
333	1.49 (ref 2), 1.59 (ref 7)	1.54 ± 0.05 (R)	2.80
343	1.61 [*] (ref 2)	1.6	2.9
353	1.80 (ref 2)	1.8	3.3

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

2. SOLUBILITY OF WATER (2) IN 2-METHYL-2-PROPENOIC ACID METHYL ESTER (1)

The available data for the solubility of water (2) in 2-methyl-2propenoic acid methyl ester (1) are summarized in Table 3. The data of Chubarov *et al.* (ref 6) and Fu *et al.* (ref 7) are in excellent agreement enabling the average "Best" values to be recommended over a wide range of temperature. Selected data are plotted in Figure 2.



COMPC (1)	DNENTS: 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate);	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth. W.A.,
	C ₅ H ₈ O ₂ ; [80-62-6]	Murdoch University, Perth, W.A., Australia
(2)	Water; H ₂ O; [7732-18-5]	January, 1989

CRITICAL EVALUATION: (continued)

T/K		Solubilities	
	Reported values	"Best"	values $(\pm \sigma_n)^a$
	g(2)/100g sln	g(2)/100g	sln 10x ₂
333	2.09 (ref 6), 2.10 (ref	7) 2.10 (R)	1.07
343	2.43 [*] (ref 6)	2.4	1.2
353	2.75 (ref 6)	2.8	1.4
363	3.17 (ref 6)	3.2	1.6

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass solubilities.



COMPONENTS:		EVALUATOR:
(1) (2)	2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C ₅ H ₈ O ₂ ; [80-62-6] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRIT	ICAL EVALUATION: (continued)	
REFE	RENCES	
1.	Shanley, E. S.; Greenspan, F. P. <i>Ind. Eng. Chem.</i> <u>1947</u> , 39, 1536-43.	
2.	Schildknecht, C. E. Vinyl and Related Polymers, J. Wiley, New York, <u>1952</u> , p.185.	
3.	Frolov, A. F. Zh. Fiz. Khim. <u>1965</u> , 39, 2877-83.	
4.	Frolov, A. F.; Yarovikova, M. M.; Ustavshchikov, B. F.; Nikitina, N. S. <i>Izv. Vyssh. Ucheb. Zaved. Khim. Khim. Tekhnol.</i> <u>1965</u> , 8, 570-3.	
5.	Arutyunyan, R. S.; Atanasyan, E. N.; Beileryan, N. M. <i>Kolloid. Zh.</i> <u>1979</u> , 41, 968-72.	
6.	Chubarov, G. A.; Danov, S. M.; Logutov, V. I.; Brovkina, G. V. <i>Zh. Prikl. Khim. <u>1979</u>, 52,</i> 1082-5.	
7.	Fu, J. Y.; Wang, K.; Hu, Y. Hu	a Kung Hsueh Pao <u>1988</u> , 64-76.

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

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<pre>COMPONENTS: (1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C₅H₈O₂; [80-62-6] (2) Water; H₂O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Shanley, E.S.; Greenspan, F.P. <i>Ind. Eng. Chem.</i> <u>1947</u> , <i>39</i> , 1536-43.
VARIABLES:	PREPARED BY:
T/K = room temperature	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of water in 2-methyl-2 room temperature was reported to be 1 mass per cent and mole fraction, x ₂ , 0.99 g(2)/100g sln and 0.053.	2-propenoic acid methyl ester at 1.0 g(2)/100g(1). The corresponding values calculated by the compiler are
AUXILIARY :	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified. No further details were reported in the paper.	(1) Not specified.(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

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COMPO	NENTS:		ORIGINAL MEASUREMENTS:
(1)	2-Prope	enoic acid, 2-methyl-,	Schildknecht, C.E.
	methyl	ester	
	(methyl	methacrylate); C ₅ H ₈ O ₂ ;	J. Wiley, New York, <u>1952</u> , p 185.
	[80-62-	-6]	
(2)	Water;	H ₂ O; [7732-18-5]	
VARIA	BLES:		PREPARED BY:
<i>т/</i> К =	= 273 -	353	A. Skrzecz
EXPERI	IMENTAL	VALUES:	······
Solu	oility c	of 2-methyl-2-propenoic a	cid methyl ester in water
	t/°C	g(1)/100g sln	x ₁ (compiler)
			0.0034
	20	1.59	0.0029
	40	1.35	0.0025
	40 60	1.49	0.0027
	80	1.80	0.0033
		AUXILIARY	INFORMATION
METHO)/APPARA	TUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The "	nethod w	as not specified.	(1) Source not specified
Presu The M	umably d Monomeri	ata were taken from c Acrylic Esters	presumably containing 0.006% hydroquinone.
(ref	1).		(2) Not specified.
			ESTIMATED ERROR:
			Not specified.
			REFERENCES:
			1. The Monomeric Acrylic Esters, booklet, Rohm and Haas Co., <u>1949</u> .

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<pre>COMPONENTS: (1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C₅H₈O₂; [80-62-6] (2) Water; H₂O; [7732-18-5]</pre>	ORIGINAL MEASUREMENTS: Frolov, A.F. Zh. Fiz. Khim. <u>1965</u> , 39, 2877-83.
VARIABLES: T/K = 293	PREPARED BY: A. Skrzecz
EXPERIMENTAL VALUES: The solubility of 2-methyl-2-propenoi 20°C was reported to be 1.39 g(1)/100 tion, x_1 , value calculated by the com The solubility of water in 2-methyl-2 20°C was reported to be 0.73 g(2)/100 tion, x_2 , value calculated by the com	c acid methyl ester in water at g sln. The corresponding mole frac- piler is 0.00253. -propenoic acid methyl ester at g sln. The corresponding mole frac- piler is 0.039.
AUXILIARY I	NFORMATION
METHOD/APPARATUS/PROCEDURE: The method was not specified. The data were reported together with the quaternary system 2-methyl-2-propenoic acid methyl ester-water-2-methyl-2-propenoic acid-methanol (methyl methacrylate- water-methacrylic acid-methanol).	SOURCE AND PURITY OF MATERIALS: (1) Not specified. (2) Not specified. ESTIMATED ERROR: Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl methacrylate); C₅H₈O₂; [80-62-6]</pre>	Frolov, A.F.; Yarovikova, M.M.; Ustavshchikov, B.F.; Nikitina, N.S. Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. <u>1965</u> , 8, 570-3.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of 2-methyl-2-propenoic acid methyl ester in water at 20° C was reported to be 1.55 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00283. The solubility of water in 2-methyl-2-propenoic acid methyl ester at 20° C was reported to be 1.2 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.063.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE: The analytical method was used. The mixture was thermostated in 100 mL flask and stirred for 1/2 h. Then, after separation (more than 20 min), the phases were analyzed. The glc method for water and the ester and the bromide-bromate method for the 2-methyl-2-propenoic acid methyl ester were used. The data were reported together with the ternary system 2-methyl- 2-propenoic acid methyl ester- water-methanol.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, pure grade; distilled; purity 98.52% by bromide-bromate method, b.p. 100°C, d²⁰ 0.940, n²⁰ 1.4150. (2) Not specified. ESTIMATED ERROR: Soly. <±3.0% (relative error). REFERENCES:</pre>	

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ORIGINAL MEASUREMENTS:
Arutyunyan, R.S.; Atanasyan, E.N.; Beileryan, N.M.
Kolloid. Zh. <u>1979</u> , 41, 968-72.
PREPARED BY:
A. Skrzecz
ompiler is 15.02 g(1)/L sln.

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AUXILIARY INFORMATION				
METHOD/APPARATUS/PROCEDURE: The volumetric method of Shaginyan, Aibazyan and Melkonyan (ref 1) was	SOURCE AND PURITY OF MATERIALS: (1) Source not specified; purified.			
used. The volume of insoluble organic phase was measured. No further details were reported in the paper.	(2) Not specified.			
	ESTIMATED ERROR:			
	Soly. <±1% (relative error).			
	REFERENCES:			
	 Shaginyan, A.A.; Aibazyan, O.M.; Melkonyan, L.G. Arm. Khim. Zh. <u>1974</u>, 27, 904. 			

сомро	NENTS:	ORIGINAL MEASUREMENTS:	
(1) 2-Propenoic acid, 2-methyl-,		Chubarov, G.A.; Danov, S.M.;	
methyl ester		Logutov, V.I.; Brovkina, G.V.	
	(methyl methacrylate); C ₅ H ₈ O ₂ ;	Zh. Prikl. Khim. <u>1979</u> , 52, 1082-5.	
	[80-62-6]		
(2)	Water; H ₂ O; [7732-18-5]		
VARIA	BLES:	PREPARED BY:	
Т/К	= 293 - 363	A. Skrzecz	
EXPER	IMENTAL VALUES:		
Solu	bility of water in 2-methyl-2-pro	openoic acid methyl ester	
	t/°C g(2)/100g sln	x ₂ (compiler)	
	20 1.08	0.0572	
	25 1.19	, 0.0627	
	40 1.54	0.0800	
	60 2.09	0.1060	
	80 2.75	0.1358	
	90 3.17	0.1539	
	AUXILIARY	INFORMATION	
METHO	D/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was as described in Praktikum po Fizicheskoi Khimii (ref 1). The data were reported together with the ternary system 2-methyl-2-propenoic acid methyl ester-water-2-propanone (methyl methacrylate-water-acetone).		(1) Source not specified; distilled; b.p. 100.4°C, d_4^{20} 0.936, n_D^{25} 1.4118. (2) Not specified.	
		ESTIMATED ERROR:	
		Not specified.	
		DEFEDENCES.	
		REFERENCES;	
		 Vorob'lev, N.K.(ed.) Praktikum po Fizicheskoi Khimii, Izd. Khimiya, Moskva, <u>1975</u>. 	

COMPONENTS: (1) 2-Propenoic acid, 2-methyl-, methyl ester (methyl meth- acrylate); $C_5H_8O_2$; [80-62-6] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Fu, Jinyan Y.; Wang, Kun; Hu, Ying <i>Hua Kung Hsueh Pao</i> <u>1988</u> , (1), 64-76.
VARIABLES: T/K = 298 - 333 p/kPa = 7 - 42	PREPARED BY: J. Fu

Mutual solubility of 2-methyl-2-propenoic acid methyl ester and water

<i>x</i> ₁		g(1)/100g sln (compiler)			
t/°C	p/kPa	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
25	7.71	0.0028	0.9369	1.536	98.80
35	12.95	0.0026	0.9259	1.428	98.58
45	21.00	0.0026	0.9139	1.428	98.33
55	33.16	0.0028	0.9006	1.536	98.05
60	41.26	0.0029	0.8934	1.590	97.90

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Mutual solubilities were determined by a static method using a liquid solution, vapor pressure measuring apparatus having a sample cell, a mercury manometer, a degassing ves- sel, and a high vacuum manifold as described in (ref 1). The solutions (in a 50 ml vessel) were degassed with liquid N ₂ and transferred into the sample cell. The free space was about 24 ml (giving a negligible error, by calculation). Paradioxy- benzene was added to prevent poly- merization of (1). Thus, (1) could be kept for 40 days with a vapor pressure change less than 0.1 kPa at 60°C.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; 99.8-99.9% wt. pure; n_D²⁵ 1.3265, b.p. 337.8K. (2) Deionized and distilled. (2) Deionized and distilled. (2) Deionized and distilled. (2) Deionized and distilled. (3) Deionized and distilled. (3) Deionized and distilled. (4) Provide the second state of the se</pre>

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СОМРС	NENTS:		
(1)	Butanoic	acid,	4-chlor

 Butanoic acid, 4-chloro-, methyl ester (methyl 4-chloro- butyrate); C₅H₉ClO₂; [3153-37-5] Water; H₂O; [7732-18-5] 	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, 56-70.
VARIABLES:	PREPARED BY:
T/K = 273 - 363	2. Maczynska

ORIGINAL MEASUREMENTS:

EXPERIMENTAL VALUES:

Mutual solubility of 4-chlorobutanoic acid methyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
 0	1.32	99.30	0.00176	0.9493
9.4	1.18	[.] 99.17	0.00157	0.9403
19.6	1.14	99.07	0.00152	0.9335
30.9	1.07	98.93	0.00142	0.9242
39.6	1.18	98.93	0.00157	0.9242
50.0	1.26	98.50	0.00168	0.8965
60.6	1.31	98.21	0.00175	0.8786
70.0	1.36	97.73	0.00181	0.8503
80.1	1.66	97.67	0.00222	0.8468
90.3	1.68	96.98	0.00225	0.8090
std. dev	7. 0.01	0.03		<u>,</u>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The analytical method was used. (1) Source not specified, commer-Component (1) was equilibrated cial sample; purity 98%; used with component (2) at a given as received. temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a (2) Not specified. weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring ESTIMATED ERROR: by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio Accuracy of method 0.1 wt% or less, (Chromosorb 101 packing and a HP for solubility, see above. 3390 A recorder-integrator), A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. **REFERENCES:**

СОМРО	DNENTS:	EVALUATOR:
(1)	Acetic acid 1-methylethyl ester (isopropyl acetate);	G.T. Hefter, School of Mathematical and Physical Sciences,
	C ₅ H ₁₀ O ₂ ; [108-21-4]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 1-methylethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quanti</u> <u>Acetic acid 1-methy</u>	<u>tative Sol</u> lethyl est	lubility Studies cer (1) - Water (<u>of the</u> 2) System
Reference	T/K	Solubility	Method
Fuehner (ref 1)	293	(1) in (2)	titration
Doolittle (ref 2)	293	mutual	unspecified
Hlavaty and Linek (ref 3)	298	mutual	titration
Skrzecz (ref 4)	291-357	mutual	synthetic, Karl Fischer
Stephenson and Stuart (ref 5)	273-348	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID 1-METHYLETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 1-methylethyl ester (1) in water (2) are summarized in Table 2 with the following exclusions. The datum of Doolittle (ref 2) is rejected because the purity of the ester was low; the reported solubility is also rather lower than other determinations (ref 1,5). The approximate value of Hlavaty and Linek (ref 3) is also rejected because it is significantly lower than other studies (ref 4,5).

The remaining data, mainly due to Skrzecz (ref 4) and Stephenson and Stuart (ref 5), are in excellent agreement enabling the averaged "Best" Values to be Recommended over a wide temperature range. Selected data are plotted in Figure 1.
COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid 1-methylethyl ester (isopropyl acetate);	G.T. Hefter, School of Mathematical and Physical Sciences.
	$C_5H_{10}O_2$; [108-21-4]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

TABLE 2:	Recommended	(R) and	Tentative	Solubilities
of Acetic	acid 1-methy	lethyl	ester (1)	in Water (2)

T/K	Solubilit	ies
	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(1)/100g sln	$g(1)/100g \ sln$ $10^3 x_1$
273	4.08 (ref 5)	4.1 7.5
283	3.40 [*] (ref 5)	3.4 6.2
293	3.09 (ref 1), 2.78 [*] (ref 5)	2.9 ± 0.2 5.2
298	2.67 [*] (ref 4), 2.59 [*] (ref 5)	2.63 ± 0.04 (R) 4.74
303	2.52 [*] (ref 4), 2.42 [*] (ref 5)	2.47 ± 0.05 (R) 4.44
313	2.30 [*] (ref 4), 2.19 [*] (ref 5)	2.25 ± 0.06 (R) 4.04
323	2.17 [*] (ref 4), 2.06 [*] (ref 5)	2.12 ± 0.06 (R) 3.80
333	2.13 [*] (ref 4), 1.94 [*] (ref 5)	2.04 ± 0.10 (R) 3.67
343	2.15 [*] (ref 4), 1.84 [*] (ref 5)	2.0 ± 0.2 3.6
353	2.21 [*] (ref 4), 1.75 [*] (ref 5)	2.0 ± 0.2 3.6

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 1-METHYLETHYL ESTER (1)

All the available solubility data for water (2) in acetic acid 1-methylethyl ester (1) are summarized in Table 3 with the following exceptions. The datum of Doolittle (ref 2) is rejected because of the low ester purity; the reported solubility, also much higher than other determinations (ref 4,5). The approximate value of Hlavaty and Linek (ref 3) is also rejected as it is much higher than other data (ref 4,5).

The remaining data, due to Skrzecz (ref 4) and Stephenson and Stuart (ref 5) are in excellent agreement at $T \leq 313$ but differ increasingly at higher temperatures. The data are plotted in Figure 2.

(continued next page)



СОМРО	NENTS:	EVALUATOR:
(1)	Acetic acid 1-methylethyl ester (<i>isopropyl acetate</i>); C ₅ H ₁₀ O ₂ ; [108-21-4]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

T/K	Solubilit	ies	
	Reported values	"Best" values (± σ_n) ^a
	g(2)/100g sln	g(2)/100g sln	10 <i>x</i> 2
313	2.32 [*] (ref 4), 2.05 [*] (ref 5)	2.2 ± 0.1 (R)	1.13
323	2.71 [*] (ref 4), 2.23 (ref 5)	2.5 ± 0.2	1.3
333	3.15 [*] (ref 4), 2.37 [*] (ref 5)	2.8 ± 0.4	1.4
343	3.64 [*] (ref 4), 2.46 [*] (ref 5)	3.1 ± 0.6	1.5
353	4.17 [*] (ref 4), 2.55 [*] (ref 5)	3.4 ± 0.8	1.7

In Table 3, σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.



COMPO	DNENTS:	EVALUATOR:
(1)	Acetic acid 1-methylethyl ester (<i>isopropyl acetate</i>); C ₅ H ₁₀ O ₂ ; [108-21-4] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989
CRIT	ICAL EVALUATION: (continued)	
REFE	RENCES	
1.	Fuehner, H. Ber. Dtsch. Chem. Ge	s. <u>1924</u> , 57, 510-5.
2.	Doolittle, A. K. Ind. Eng. Chem. <u>1935</u> , 27, 1169-79.	
3.	Hlavaty, K.; Linek, J. <i>Collect. Czech. Chem. Commun.</i> <u>1973</u> , 38, 374-8.	
4.	Skrzecz, A. Pol. J. Chem. <u>1981</u> , 55, 1177-80; see also Skrzecz, A. Thesis, I. Ch. F. PAN, Warszawa, <u>1979</u> .	
5.	Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.	
ACKNO	ACKNOWLEDGEMENT	
	The Evaluator thanks Dr. Brian Clare for the graphics.	

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Acetic acid 1-methylethyl ester (isopropyl acetate); 	Fuehner, H.
C ₅ H ₁₀ O ₂ ; [108-21-4]	<i>Ber. Disch. Chem. Ges.</i> <u>1924</u> , 57, 510-5.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
EXPERIMENTAL VALUES: The solubility of acetic acid 1-methy ported to be 3.40 vol%, 3.09 g(1)/100 corresponding mole fraction, x ₁ , valu 0.00559.	ylethyl ester in water at 20°C was re- Og sln and 0.303 mol(1)/L sln. The De calculated by the compiler is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used. The ester was added from a pipette to a flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remain- ed transparent.	(1) Source not specified, commer- cial product.(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.3 g(1)/100g sln (compiler).

REFERENCES:

СОМРС	DNENTS:	ORIGINAL MEASUREMENTS:
(1)	Acetic acid 1-methylethyl ester (<i>isopropyl acetate</i>); C-H ₁₀ O ₂ : [108-21-4]	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.
(2)	Water; H ₂ O; [7732-18-5]	
VARIA	BLES:	PREPARED BY:
T/K	= 293	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of acetic acid 1-methylethyl ester in water at 20°C was reported to be 2.58 g(1)/100g sln^a and 2.78 g(1)/100g sln^b. The corresponding mole fraction, x_1 , values calculated by the compiler are 0.00465^a and 0.00502^b respectively.

The solubility of water in acetic acid 1-methylethyl ester at 20° C was reported to be 2.86 g(2)/100g sln^a and 5.58 g(2)/100g sln^b. The corresponding mole fraction, x_2 , values calculated by the compiler are 0.143^a and 0.251^b respectively.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	 (1) Source not specified. ^a Commercial product; purity 95%, b.p. range 84-94°C, d²⁰ 0.870. ^b Commercial product; purity 85%, b.p. range 82-90°C, d²⁰ 0.857. (2) Not specified.
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid 1-methylethyl	Hlavaty, K.; Linek, J.
ester (isopropyl acetate);	Collect. Czech. Chem. Commun.
$C_5H_{10}O_2$; [108-21-4]	<u>1973</u> , 38, 374-8.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	2. Maczynska
EXPERIMENTAL VALUES: The solubility of acetic acid 1-methylethyl ester in water at 24.6°C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0040. The solubility of water in acetic acid 1-methylethyl ester at 24.6°C was reported to be 2.2 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.113.	
AUXILIARY	INFORMATION
	SOURCE AND DUDTTY OF MATTERTALS.
The titration method was used	(1) Not specified
The measurements were performed	(1) Not specified
a titration vessel which could be thermostated during the titration. Both the vessel and the burette were thermostated to 24.6 ±0.1°C.	(2) Not specified.
The mixture was agitated vigorous- ly by a magnetic stirrer during the	ESTIMATED ERROR:
titration.	Temp. ±0.1°C.
	Sory, better than 10.3 WT%.
	REFERENCES:
	1. Mertl, I. <i>Thesis</i> , Inst. Chem. Process Fundam., Czechoslovak Academy of Sciences, Prague, <u>1969</u> .

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid 1-methylethyl ester (<i>isopropyl acetate</i>); C₅H₁₀O₂; [108-21-4] (2) Water; H₂O; [7732-18-5] 	<pre>Skrzecz, A. Pol. J. Chem. <u>1981</u>, 55, 1177-80. Skrzecz, A. Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u>.</pre>
VARIABLES: T/K = 291 - 357	PREPARED BY: A. Skrzecz

EXPERIMENTAL VALUES:

Mutual solubility of acetic acid 1-methylethyl ester and water

T/K	x	L	g(1)/100g	sln
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
 291.3 ^a	-	0.9210	_	98.510
292.3	-	0.9078	-	98.240
299.5	0.00474	-	2.629	-
304.6	-	0.8921	-	97.911
306.7	0.00436	-	2.422	-
315.3	0.00406	-	2.259	-
326.4	-	0.8587	-	97.179
335.1	-	0.8417	-	96.789
335.5	0.00386	-	2.150	-

a By the Karl Fischer method.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed in a glass tube connected with a thermostat filled completely with distilled water. During the meas-urements the temperature of the bath was changed continuously and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analyti-cal method, The amount of water in the saturated organic phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

- (1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.28 wt% water by the Karl Fischer method.
- (2) Distilled.

ESTIMATED ERROR:

Temp. $\pm (0.2-0.6)^{\circ}C.$ Soly. see above.

REFERENCES:

COMPONENTS:	ORIGI

- (1) Acetic acid 1-methylethyl
 ester (isopropyl acetate);
 C₅H₁₀O₂; [108-21-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skrzecz, A. Pol. J. Chem. <u>1981</u>, 55, 1177-80.

Skrzecz, A.

Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u>.

EXPERIMENTAL VALUES: (continued)

Mutual solubility of acetic acid 1-methylethyl ester and water

T/K	\boldsymbol{x}_1	L	g(1)/100g	sln
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
	<u></u>		<u></u>	<u></u>
348.2	0.00386	-	2.150	-
355.1	-	0.7970	-	95.700
357.1	0.00406	-	2.259	-
357.1	0.00406	-	2.259	-

Author's smoothing equations:

 $x_1 = 6.4295 \times 10^{-3} - 8.23 \times 10^{-5} (T/K - 273.15) + 6.45 \times 10^{-7} (T/K - 273.15)^2$ st. dev. = 4.91 x 10⁻⁵ (2)-rich phase

 $x_2 = 0.076113 + 6.427 \times 10^{-4} (T/K - 273.15) + 1.102 \times 10^{-5} (T/K - 273.15)^2$ st. dev. = 5.56 x 10⁻⁴ (1)-rich phase

CONDONENTEC -			ODICINAL MEACUDENI	
		ORIGINAL MEASUREMENTS:		
(1) Acetic acid 1-methylethyl		Stephenson, R.; S	Stuart, J.	
$C_{-H_{10}O_{2}}$; [108-21-4]		J. Chem. Eng. Dat 56-70.	ta <u>1986</u> , 31,	
(2) Wat	10^{-2} , 1^{-1}	8-51		
			DDEDADED DV.	
VARIABLES	•		PREPARED BI:	
T/K = 27	3 - 348		2. Maczynska	
EXPERIMEN	TAL VALUES:			
Mut	ual solubility o	of acetic acid	1-methylethyl est	er and water
t/°c	g(1)/10	0g sln	x_1 (comp	oiler)
	(2)-rich phase	(1)-rich phas	e (2)-rich phase	(1)-rich phase
0	4.08		0.00745	_
9.0	3.46	98.66	0.00628	0.9285
19.9	2.79	98.42	0.00504	0.9166
29.7	2.44	98.25	0.00439	0.9083
39.8	2.19	97.80	0.00393	0.8869
50.0	2.07	97.77	0.00371	0.8855
62.2	1.92	97.62	0.00344	0.8786
74.6	1.80	97.50	0.00322	0.8731
sta. dev. 0.02 0.01				
		AUXILIARY 1	INFORMATION	
METHOD/AP	PARATUS/PROCEDUR	E:	SOURCE AND PURITY	OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile		 (1) Source not sp cial sample; as received. (2) Not specified 	pecified, commer- purity 99%; used	
organic	layer sample and	measuring	ESTIMATED ERROR:	
gc the (-Mac thermal con 1)/acetonitrile	peak ratio	Acouracy of mothe	d = 1 with $a = 1 a = -$
(Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)		for solubility, s	see above.	
was used water la	was used to determine (2) in the water layer.		REFERENCES:	

COMPONENTS:		EVALUATOR:
(1)	Acetic acid propyl ester	G.T. Hefter, School of Mathematical
	(propyl acetate); C ₅ H ₁₀ O ₂ ;	and Physical Sciences,
	[109-60-4]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732-18-5]	Australia
(2) (addit, n_20 ; $[7,52,10,5]$		January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Fuehner (ref 3)	293	(1) in (2)	titration
Smith and Bonner (ref 4)	293,308	mutual	analytical
Murti <i>et al</i> . (ref 5)	303	mutual	titration
Venkataratnam <i>et al</i> . (ref 6)	303	mutual	titration
Pick et al. (ref 7)	357	mutual	unspecified
Rao and Rao (ref 8)	303	mutual	titration
Schuberth (ref 9)	293,318	mutual	titration, analytical
Smirnova et al. (ref 10)	323-356	mutual	analytical
Rao et al. (ref 11)	308	mutual	titration
Shakhud et al. (ref 12)	293-333	mutual	titration, analytical
Skrzecz (ref 13)	291-363	mutual	synthetic, Karl Fischer
Tewari et al. (ref 14)	298	(1) in (2)	GLC
Richon and Viallard (ref 15)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 16)	273-363	mutual	GLC

TABLE 1: Quantitative Solubility Studies of the Acetic acid propyl ester (1) - Water (2) System

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

(continued next page)

COMPONENTS:		EVALUATOR:
(1)	Acetic acid propyl ester (propyl acetate); C ₅ H ₁₀ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[109-60-4]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia
		January, 1989

1. SOLUBILITY OF ACETIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid propyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The data of Traube (ref 1) and Fuehner (ref 3) at *ca*. 293 K are significantly lower, and those of Pick *et al*. (ref 7) at 357 K and Shakhud *et al*. (ref 12) at T > 298 K significantly higher, than other studies and are therefore rejected. The results of Rao and co-workers (ref 5,6,8) at 303 K have been taken as one datum.

The remaining data are generally in good agreement (Table 2) enabling the averaged "Best" values to be Recommended over a wide range. Selected data are plotted in Figure 1.

TABLE 2:Recommended (R) and Tentative Solubilitiesof Acetic acid propyl ester (1) in Water (2)

1	т/к	Solubilit	ies	
		Reported values	"Best" values $(\pm \sigma_n)^a$	
		g(1)/100g sln	$g(1)/100g \ sln$ $10^3 x_1$	L
:	273	3.35 (ref 2), 3.21 (ref 16)	3.28 ± 0.07 (R) 5.95	
:	283	2.57 (ref 2), 2.75 [*] (ref 16)	2.66 ± 0.09 (R) 4.80	
	293	2.30 (ref 2), 2.2 (ref 4), 2.2 (ref 9), 2.2 (ref 12), 2.26 (ref 16)	2.23 ± 0.04 (R) 4.01	
	298	2.18 [*] (ref 2), 2.2 [*] (ref 12), 2.18 [*] (ref 13), 2.19 (ref 15), 2.10 [*] (ref 16)	2.17 ± 0.04 (R) 3.90	
	303	2.05 (ref 2), 1.8 (ref 5,6,8), 2.06* (ref 13), 1.98 (ref 16)	1.97 ± 0.10 (<i>R</i>) 3.53	
	313	1.81 ^b (ref 9), 1.89 [*] (ref 13), 1.87 (ref 16)	1.86 ± 0.03 (R) 3.33	
	323	1.70 ^b (ref 9), 1.80 (ref 10), 1.80 [*] (ref 13), 1.72 (ref 16)	1.76 ± 0.05 (R) 3.15	
	333	1.63 ^b (ref 9), 1.80 [*] (ref 10), 1.79 [*] (ref 13), 1.64 [*] (ref 16)	1.72 ± 0.08 (R) 3.08	
	343	1.62 ^b (ref 9), 1.82 [*] (ref 13), 1.72 [*] (ref 16)	1.72 ± 0.08 (R) 3.08	
	353	1.86 (ref 10), 1.88 [*] (ref 13), 1.66 (ref 16)	1.80 ± 0.10 3.22	
e	^a Obtain ^b Calcul	ed by averaging where appropriate. ated using the author's original fi	(continued r itting equation. pa	next

COMPONENTS:	EVALUATOR:
(1) Acetic acid propyl ester	G.T. Hefter, School of Mathematical
[109-60-4]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia
	January, 1989

In Table 2, σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.



FIGURE 1. Selected data for the solubility of acetic acid propyl ester (1) in water (2): ref 13 (\bullet); ref 16 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID PROPYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid propyl ester (1) are summarized in Table 3 with the following exceptions. The data of Murti et al. (ref 5) and of Schuberth (ref 9) and Shakhud et al. (ref 12) are, respectively, much lower and higher than other studies and are rejected. The data of Rao and co-workers (ref 6,8) at 303 K have been taken as one value.

The remaining data (Table 3) are generally only in fair agreement enabling only some of the averaged "Best" values to be Recommended. Selected data are plotted in Figure 2.

(continued next page)

COMPONENTS:		EVALUATOR:
(1)	Acetic acid propyl ester (<i>propyl acetate</i>); C ₅ H ₁₀ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[109-60-4]	Murdoch University, Perth, W.A.,
(2)	Water; H ₂ O; [7732-18-5]	Australia
	, , , , , , , , , , , , , , , , , , , ,	January, 1989

TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid propyl ester (1)

<i>т</i> /к	Solubilit	ies	
	Reported values	"Best" values (±c	(n ^a
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$
273	1.16 (ref 16)	1.2	6.4
283	1.37 [*] (ref 16)	1.4	5.9
293	1.7 (ref 4), 1.7 (ref 9), 1.58 [*] (ref 13), 1.59 (ref 16)	1.64 ± 0.06 (R)	7.5
298	1.72 [*] (ref 13), 1.72 [*] (ref 16)	1.72 (<i>R</i>)	9.0
303	1.6 (ref 6,8), 1.87 [*] (ref 13), 1.88 (ref 16)	1.78 ± 0.13	9.3
313	2.21 [*] (ref 13), 2.17 (ref 16)	$2.19 \pm 0.02 (R)$	11.3
323	2.0 (ref 10), 2.59 [*] (ref 13), 2.29 (ref 16)	2.3 ± 0.2	12
333	2.5 [*] (ref 10), 3.01 [*] (ref 13), 2.34 [*] (ref 16)	2.6 ± 0.3	13
343	3.1 [*] (ref 10), 3.48 [*] (ref 13), 2.93 [*] (ref 16)	3.2 ± 0.2	16
353	3.8 (ref 10), 3.98 [*] (ref 13), 3.01 (ref 16)	3.6 ± 0.4	17
363	4.52 [*] (ref 13)	4.5	21

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.

(continued next page)



COMP	ONENTS:	EVALUATOR:	
(1) (2)	Acetic acid propyl ester (<i>propyl acetate</i>); C ₅ H ₁₀ O ₂ ; [109-60-4] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989	
CRIT	ICAL EVALUATION: (continued)		
REFE	RENCES		
7.	Pick, J.; Hala, E.; Fried, V.	Chem. Listy <u>1958</u> , 561-6.	
8.	Rao, J. R.; Rao, C. V. J. Appl. Chem. <u>1959</u> , 9, 69-73.		
9.	Schuberth, H. Abh. Deut. Akad. Wiss. Berlin Kl. Chem. Geol. Biol. <u>1960</u> , 3, 1-82.		
10.	Smirnova, N. A.; Morachevskii, A. G. Zh. Fiz. Khim. <u>1960</u> , 34, 2546- 53; see also Smirnova, N. A.; Morachevskii, A. G.; Storonkin, A. V. Vestn. Leningr. Univ. Ser. Fiz. Khim. <u>1959</u> , 14(22), 70-80.		
11.	Rao, M. V. R.; Rao, K. S.; Rao, 20B, 379-81.	C. V. J. Sci. Ind. Res. <u>1961</u> ,	
12.	Shakhud, Zh. N.; Markusin, N. P. Univ. Ser. Fiz. Khim. <u>1972</u> , (10),	; Storonkin, A. V. Vestn. Leningr. 89-92.	
13.	Skrzecz, A. Pol. J. Chem. <u>1980</u> , Thesis, I. Ch. F. PAN, Warszawa,	54, 1101-4; see also Skrzecz, A. <u>1979</u> .	
14.	Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E. <i>J. Chem. Eng. Data <u>1982</u>, 27,</i> 451-4.		
15.	Richon, D.; Viallard, A. Fluid	Phase Equil. <u>1985</u> , 21, 279-93.	
16.	Stephenson, R.; Stuart, J. J. C	hem. Eng. Data <u>1986</u> , 31, 56-70.	

ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid propyl ester	Traube, J.	
(propyl acetate); C ₅ H ₁₀ O ₂ ;	Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,	
(109-00-4)	2234-310.	
(2) water; n ₂ 0; [//32-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 295	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at 22°C was reported to be 1 part of propyl acetate in 55-65 parts of water. The corresponding mass percent and mole fraction, x_1 , values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.		
AUXILIARY	INFORMATION	
	SOURCE AND DUDTEY OF MATERIALS.	
The method was not specified	(1) Not specified.	
The meened was not specified.	(1) Not specified	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Soly. ±0.15 g(1)/100g sln.	
	REFERENCES:	

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester	Rayman, J.
(propyl acetate); C ₅ H ₁₀ O ₂ ;	Thesis, Budapest, <u>1906</u> .
[109-60-4]	
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 303	G.T. Hefter
EXPERIMENTAL VALUES: Solubility of acetic acid p	ropyl ester in water
t/°C g(1)/100g(2) g(1)/10 (C	$\begin{array}{llllllllllllllllllllllllllllllllllll$
0. 3.47	3.35 0.00608
10. 2.83	2.57 0.00463
20. 2.36	2.30 0.00414
30. 2.09	2.05 0.00368
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved	 Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated.
	(2) Not specified.
ble to minimize the error arising	ESTIMATED ERROR.
from the solubility of (2) in (1).	Not aposified
	Not specified.
	REFERENCES:
	1. Winkler, L. <i>Z. Phys. Chem.</i> <u>1906</u> , 55, 360.
	 Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u>, Vol. 3, 387-98.

	<u>ا</u>	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid propyl ester	Fuehner, H.	
$(propy1 acetate); C_{5}H_{10}O_{2};$	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57. 510-5.	
(2) Notor: H_{0} : $(7722-18-5)$	577 515 51	
(2) water; n_20 ; [732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at 20°C was reported to be 2.10 vol%, 1.89 g(1)/100g sln and 0.185 mol(1)/L sln. The corre- sponding mole fraction, x_1 , value calculated by the compiler is 0.00339.		
AUXILIARY	INFORMATION	
	CONDER AND DIDTEY OF MAMEDIALC.	
meinob/APPARATUS/PROCEDURE:	(1) County of MATERIALS:	
The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remain- ed transparent.	(1) Source not specified, commer- cial product.	
	(2) Not specified.	
	ESTIMATED ERROR.	
	Solv about to $4 \sigma(1) (100 \pi c)$	
	(compiler).	
	REFERENCES:	

.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acetic acid propyl ester	Smith, T.E.; Bonner, R.F.
(<i>propyl acetate</i>); C ₅ H ₁₀ O ₂ ; [109-60-4]	Ind. Eng. Chem. <u>1950</u> , 42, 896-8.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293 - 308	A. Skrzecz
EXPERIMENTAL VALUES: Mutual solubility of acetic a	acid propyl ester and water
t/°C g(1)/100g sln (2)-rich phase (1)-rich phas	x ₁ (compiler) se (2)-rich phase (1)-rich phase
20 $2 \cdot 2^{a}$ $98 \cdot 3^{b}$	0.0040 0.911
35 1.8 ^a 97.8 ^b	0.0032 0.887
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. The mixture was stirred for about 1 h. and then separated and allowed to stand until each layer was visually perfectly clear (1-16 h.). Then.	(1) Source not specified; distil- led; purity 99.2-99.8 wt%, 0.02 wt% water, 0.053 g/100 mL free acid, n _D ²⁰ 1.3850.
the layers were sampled and analyz- ed. Ester analyses were made by saponifying in an excess of 1N al-	(2) Not specified.
coholic KOH and back-titrating the unreacted alkali with 0.5N HaSO	ESTIMATED ERROR:
using phenolphthalein as the indi- cator. Water was determined by ti- tration with the Karl Fischer rea- gent. The data were reported to- gether with the ternary system acetic acid propyl ester-water- 1-propanol.	Soly. about ±0.1 ^a and ±0.05 ^b g(1)/100g sln (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4] (2) Water; H₂O; [7732-18-5] 	Murti, P.S.; Venkataratnam, A.; Rao, C.V. J. Sci. Ind. Res. <u>1954</u> , 13B, 392-6.	
VARIABLES:	PREPARED BY:	
$T/K = 303^{a}$	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at $30^{\circ}C^{a}$ was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_{1} , value cal-		

The solubility of water in acetic acid propyl ester at $30^{\circ}C^{a}$ was reported to be 1.4 g(2)/100g sln. The corresponding mole fraction, x_{2} , value calculated by the compiler is 0.074.

^a Persumably the measurments were made at 30°C; the temperature was not reported in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. Determinations were made either from the production of turbidity or from its disappearance. The data were reported together with the ternary system acetic acid propyl esterwater-acetic acid. No further details were reported in the paper.

culated by the compiler is 0.0032.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House, laboratory reagent grade; distilled; 101.5°C, d 0.8830, n_D³⁰ 1.3802.

(2) Not specified.

ESTIMATED ERROR:

Soly. about ±0.2 g(1)/100g sln and ±0.5 g(2)/100g sln (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4]</pre>	Venkataratnam, A.; Rao, J.R.; Rao, C.V. <i>Chem. Eng. Sci.</i> <u>1957</u> , 7, 102-10.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 303	A. Skrzecz
EXPERIMENTAL VALUES:	ester in water at 30°C was reported

The solubility of acetic acid propyl ester in water at 30° C was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0032.

The solubility of water in acetic acid propyl ester at 30° C was reported to be 1.6 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.084.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system acetic acid propyl ester-water- 2-propanone (propyl acetate-water- acetone).	 British Drug House Ltd., laboratory reagent grade; distilled; b.p. 101.6°C, d³⁰ 0.8773, n³⁰ 1.3800. Distilled; free of CO₂.
	ESTIMATED ERROR:
	Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).
	REFERENCES:
	 Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240.

	•	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid propyl ester	Pick, J.; Hala, E.; Fried,V.	
(propyl acetate); C ₅ H ₁₀ O ₂ ;	Chem. Listy <u>1958</u> , 52, 561-6.	
(2) Water: H_{-0} : $(7732-18-5)$		
VARTABLES:	PREPARED BY:	
T/K = 357	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at 84.0° C was reported to be $x_1 = 0.005$. The corresponding mass per cent value calculated by the compiler is 2.8 g(1)/100g sln. The solubility of water in acetic acid propyl ester at 84.0° C was reported to be $x_2 = 0.219$. The corresponding mass per cent value calculated by the compiler is $4.71 \text{ g}(2)/100\text{ g sln}$.		
Pressure was reported to be 760 mm Hg.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not described. The ternary solubility at the boiling temperature was measured in a modified Washburn ebulliometer (ref 1,2). The temperature was measured with a calibrated Anschutz thermometer. The data were reported together with the ternary system acetic acid propyl ester-water- propanol.	 (1) Source not specified; distilled; b.p. 101.4°C, d²⁰ 0.88827 ±0.00006, n²⁰ 1.3841 ±0.0001. (2) Distilled 	
	ESTIMATED ERROR:	
	Soly. about ±0.9 g(1)/100g sln and ±0.5 g(2)/100g sln (compiler).	
	REFERENCES:	
	 Washburn, E. J. Am. Chem. Soc. <u>1919</u>, 41, 729. Pick, J.; Fried, V.; Hala, E.; Vilim, O. Chem. Listy <u>1955</u>, 49, 1112. 	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4]</pre>	Rao, R.J.; Rao, C.V. J. Appl. Chem. <u>1959</u> , 9, 69-73.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at 30° C was reported to be 1.8 g(1)/100g sln. The corresponding mole fraction, x_1 , value cal- culated by the compiler is 0.0032.		
The solubility of water in acetic acid propyl ester at 30° C was reported to be 1.6 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.084.		

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system acetic acid propyl ester-water- 1-propanol.	 British Drug House; distilled; b.p. 101.6°C, d³⁰ 0.8773, n_D³⁰ 1.3800. Distilled.
	ESTIMATED ERROR:
	Soly. about ±0.2 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).
	REFERENCES:
	1. Rao, R.J.; Rao, C.V. <i>J. Appl.</i> Chem. <u>1957</u> , 7, 435.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Acetic acid propyl ester		Schuberth, H.		
(propyl acetate); C ₅ H ₁₀ O ₂ ;		Abh. Deut. Akad.	Wiss. Berlin, Kl.	
[109-60-4]		Chem. Geol. Bio	<i>1</i> . <u>1960</u> , <i>3</i> , 1-82.	
(2) Wate	er; H ₂ O; [7732-18	8-5]		
VARIABLES	:		PREPARED BY:	
T/K = 293	3 and 318		A. Skrzecz	
EXPERIMENT	TAL VALUES: Mutual solubility	y of acetic a	acid propyl ester an	d water
t/°C	g(1)/100 (2)-rich phase	Og sln (1)-rich pha	x ₁ (comp se (2)-rich phase	iler) (1)-rich phase
20.0	2.2	98.3 97.3	0.0040	0.911
$x_1 = 0$. $x_1 = -1$.4876x10 ⁻⁶ (<i>T/K</i>) ² L2.965x10 ⁻⁶ (<i>T/K</i>)	- 3.3144x10 ² + 60.338x1	<pre>- (T/K) + 5.9219x10 0⁻⁴ (T/K) + 25.594x1</pre>	(2)-rich phase 0 ⁻² (1)-rich phase
$x_1 = 0$ $x_1 = -1$.4876x10 ⁻⁶ (<i>T/K</i>) ² L2.965x10 ⁻⁶ (<i>T/K</i>)	- 3.3144x10 ² + 60.338x1	- (T/K) + 5.9219x10 0 ⁻⁴ (T/K) + 25.594x1	(2)-rich phase 0 ⁻² (1)-rich phase
$x_1 = 0$ $x_1 = -1$.4876x10 ⁻⁶ (<i>T/K</i>) ² L2.965x10 ⁻⁶ (<i>T/K</i>)	- 3.3144x10 ² + 60.338x1 AUXILIARY	- (<i>T/K</i>) + 5.9219x10 0 ⁻⁴ (<i>T/K</i>) + 25.594x1 	(2)-rich phase 0 ⁻² (1)-rich phase
$x_1 = 0.$ $x_1 = -1$ IETHOD/APP	2.965x10 ⁻⁶ (<i>T/K</i>) 2.965x10 ⁻⁶ (<i>T/K</i>) PARATUS/PROCEDURI	- 3.3144x10 ² + 60.338x1 AUXILIARY	<pre>- (T/K) + 5.9219x10 0⁻⁴ (T/K) + 25.594x1 INFORMATION SOURCE AND PURITY (</pre>	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase DF MATERIALS:</pre>
$x_1 = 0.$ $x_1 = -1$ $x_1 = -1$ $x_1 = -1$ $x_1 = -1$	A876x10 ⁻⁶ (T/K) ² L2.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI Ly the titration methods were used od were reported	- 3.3144x10 ² + 60.338x1 AUXILIARY E: and ana- d. The data together	<pre>- (T/K) + 5.9219x10 0⁻⁴ (T/K) + 25.594x1 INFORMATION SOURCE AND PURITY ((1) Synthesized; (distilled; b.) d²⁰ 0.8879, n^D</pre>	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase DF MATERIALS: dried over CuSO₄, 0. 101.6°C, 0 1.3844.</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ IETHOD/APH Presumabl lytical m and methor with the propyl est butyl est butyl ace	A876x10 ⁻⁶ (T/K) ² 2.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI by the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 ² + 60.338x1 AUXILIARY E: and ana- i. The data together acetic acid cacid ate-water-	$(T/K) + 5.9219 \times 10^{-4} (T/K) + 25.594 \times 10$	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ IETHOD/APH Presumabl lytical m and methor with the propyl est butyl est butyl ace	2.965x10 ⁻⁶ (T/K) 2.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURN by the titration methods were used bod were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 ² + 60.338x1 AUXILIARY E: and ana- i. The data together acetic acid ate-water-	INFORMATION SOURCE AND PURITY ((1) Synthesized; o distilled; b. d^{20} 0.8879, n_{D}^{2} (2) Twice distilled	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ IETHOD/APH Presumabl lytical m and method with the propyl est butyl est butyl ace	A876x10 ⁻⁶ (T/K) ² 22.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI by the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta state).	- 3.3144x10 ² + 60.338x1 ² + 60.338x1 AUXILIARY E: and ana- d. The data together acetic acid ate-water-	$(T/K) + 5.9219 \times 10$ $0^{-4} (T/K) + 25.594 \times 1$ INFORMATION SOURCE AND PURITY ((1) Synthesized; (distilled; b.) d^{20} 0.8879, n_D^2 (2) Twice distilled ESTIMATED ERROR: Temp. ±0.01°C. Soly. ±0.05 g(1)/2	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0 DF MATERIALS: dried over CuSO₄, 0 1.3844. ed. 100g sln.</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ IETHOD/APH Presumabl lytical m and methor with the propyl est butyl est butyl ace	A876x10 ⁻⁶ (T/K) ² 2.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI by the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 ² + 60.338x1 AUXILIARY E: and ana- d. The data together acetic acid ate-water-	$(T/K) + 5.9219 \times 10$ $0^{-4} (T/K) + 25.594 \times 1$ INFORMATION SOURCE AND PURITY ((1) Synthesized; of distilled; b.) $d^{20} 0.8879, n_{\rm D}^{20}$ (2) Twice distill(ESTIMATED ERROR: Temp. ±0.01°C. Soly. ±0.05 g(1)/2	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ TETHOD/APH Presumabl lytical m and methor propyl est butyl est butyl ace	A876x10 ⁻⁶ (T/K) ² 12.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI by the titration methods were used bod were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 AUXILIARY AUXILIARY E: and ana- i. The data together acetic acid c acid ate-water-	$(T/K) + 5.9219 \times 10$ $0^{-4} (T/K) + 25.594 \times 1$ INFORMATION SOURCE AND PURITY ((1) Synthesized; (distilled; b.) d ²⁰ 0.8879, n ^D (2) Twice distill(ESTIMATED ERROR: Temp. ±0.01°C. Soly. ±0.05 g(1)/2 REFERENCES:	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
$x_1 = 0$. $x_1 = -1$ $x_1 = -1$ IETHOD/APH Presumabl lytical m and method with the propyl est butyl est butyl ace	A876x10 ⁻⁶ (T/K) ² 12.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI Ly the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta state).	- 3.3144x10 ² + 60.338x1 AUXILIARY E: and ana- d. The data together acetic acid ate-water-	<pre>- (T/K) + 5.9219x10 0⁻⁴ (T/K) + 25.594x1 INFORMATION SOURCE AND PURITY ((1) Synthesized; (distilled; b.) d²⁰ 0.8879, n^D (2) Twice distill(ESTIMATED ERROR: Temp. ±0.01°C. Soly. ±0.05 g(1)/: REFERENCES:</pre>	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
<pre>x₁ = 0. x₁ = -1 x₁ = -1 UETHOD/APH Presumabl lytical m and methor with the propyl est butyl est butyl ace</pre>	A876x10 ⁻⁶ (T/K) ² 12.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI by the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 AUXILIARY E: and ana- d. The data together acetic acid ate-water-	$(T/K) + 5.9219 \times 10$ $0^{-4} (T/K) + 25.594 \times 1$ INFORMATION SOURCE AND PURITY ((1) Synthesized; o distilled; b.) d^{20} 0.8879, n_D^2 (2) Twice distilled ESTIMATED ERROR: Temp. $\pm 0.01^{\circ}$ C. Soly. ± 0.05 g(1)/2 REFERENCES:	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>
<pre>x₁ = 0. x₁ = -1 X₁ = -1 ETHOD/APH Presumabl lytical m and methow with the propyl est butyl est butyl ace</pre>	A876x10 ⁻⁶ (T/K) ² L2.965x10 ⁻⁶ (T/K) PARATUS/PROCEDURI Ly the titration methods were used od were reported ternary system a ster-water-acetic cer (propyl aceta etate).	- 3.3144x10 ² + 60.338x1 AUXILIARY E: and ana- d. The data together acetic acid c acid ate-water-	$(T/K) + 5.9219 \times 10$ $0^{-4} (T/K) + 25.594 \times 1$ INFORMATION SOURCE AND PURITY ((1) Synthesized; (distilled; b., d^{20} 0.8879, n_p^2 (2) Twice distill() ESTIMATED ERROR: Temp. ±0.01°C. Soly. ±0.05 g(1)/2 REFERENCES:	<pre>-2 (2)-rich phase 0⁻² (1)-rich phase 0⁻² (</pre>

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COMPONENTS:		ORIGINAL MEASUREMENTS:				
(1) Acetic acid propyl ester		Smirnova, N.A.; Morachevskii, A.G.				
(propyl acetate); C ₅ H ₁₀ O ₂ ;				<u>.960</u> , 34, 2546-55	•	
[109	9-60-4]		S	mirnova, N.A.; M Storonkin, A.V.	lorachevskii, A.G	•;
(2) Wate	er; H ₂ O; [7732	-18-5]	V	est. Leningrad. <u>1959</u> , 14(22), 7	Univ., Fiz., Khi 0-80.	т.
VADTABLES		······································			· · · · · · · · · · · · · · · · · · ·	
VARIADLES	•		FR	EFARED DI.		
T/K = 323	3 - 356		A	. Skrzecz		
EXPERIMENT	TAL VALUES:					-
1	Mutual solubil	ity of acetic a	acid	propyl ester ar	nd water	
t/°c	g(1)/	100g sln				
	(2)-rich phas	e (1)-rich phas	se	(2)-rich phase	(1)-rich phase	
50	1.80	98.0		0.0032	0.896	
50.45 ^a	1.80	98.0		0.0032	0.896	
65	1.80	97.2		0.0032	0.860	
66.30 ^a	1.80	97.1		0.0032	0.856	
76.50 ^a	1.84	96.5		0.0033	0.828	
80	1.86	96.2		0.0033	0.817	
82.76 ^a	1.86	96.0		0.0033	0.810	
· · · · · · · · · · · · · · · · · · ·		λυντιτλογ	INFO	ΡΜλͲΤΟΝ		<u> </u>
		AUXILIARI .				
METHOD/APP	PARATUS/PROCED	URE:	SOL	JRCE AND PURITY	OF MATERIALS:	
The analytical method was used. The mixture of (1) and (2) was placed into a thermostated flask with a stirrer for 2 h. After separation, the ester was determined by sapon- ification with 0.5N KOH and titra- tion of the excess of KOH.		(1	1) Synthesized a laboratory; b d_4^{20} 0.8884, n_1^{20} 2) Not specified	nd purified in t .p. 101.56°C, 2 ⁰ 1.3844.	he	
			EST	IMATED ERROR:		
			Sc	emp. <±0.5°C. oly. ±0.1% (erro:	r of analysis).	
			REF	FERENCES:		

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	ORIGINAL MEASUREMENTS:	
(1) Acetic acid propyl ester	Rao, M.V.R.; Rao, K.S.; Rao, C.V.	
(propyl acetate); C ₅ H ₁₀ O ₂ ; [109-60-4]	J. Sci. Ind. Res. <u>1961</u> , 20B, 379-81.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 308	Z. Maczynska	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl to be 2.1 g(1)/100g sln. The correspon culated by the compiler is 0.0038. The solubility of water in acetic acid to be 2.0 g(2)/100g sln. The correspon culated by the compiler is 0.104.	ester in water at 35° C was reported onding mole fraction, x_1 , value cal- d propyl ester at 35° C was reported onding mole fraction, x_2 , value cal-	
AUXILIARY	INFORMATION	
AUXILIARY : METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:	
AUXILIARY METHOD/APPARATUS/PROCEDURE: The titration method was used. The data were reported together with the ternary system acetic acid propyl ester-water-formic acid. No further details were reported in the paper.	INFORMATION SOURCE AND PURITY OF MATERIALS: (1) BDH, laboratory reagent grade; used as received. (2) Not specified.	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4]</pre>	Shakhud, Zh.N.; Markuzin, N.P.; Storonkin, A.V. Vestn. Leningrad. Univ., Fiz., Khim. 1972, (10), 89-92.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293 - 333	A. Skrzecz	
FYDEDIMENTAL VALUES.	1	
Mutual solubility of acetic	acid propyl ester and water	
$t/^{\circ}$ C x_1	q(1)/100q sln (compiler)	
(2)-rich phase (1)-rich phase	se (2)-rich phase (1)-rich phase	
20 0.004 0.886	2.2 97.8	
40 0.004 0.860	2.2 97.2	
60 0.004 0.838	2.2 96.7	
AUXILIARY		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The analytical and titration methods as described by Shakhud, Markuzin and Storonkin (ref 1) were used. The two-phase mixture was stirred in a thermostated flask for 1 h. and then separated. The analysis of ester was made by sa- ponification with 0.4N KOH in eth-	 (1) Synthesized; three times distilled; d₄²⁰ 0.8879, n_D²⁰ 1.3845. (2) Twice distilled; n_D²⁰ 1.3332. 	
anol and then with titration using 0.1N HCl. The solubility of water in ester was established by the ti- tration method in a flask with a mercury valve.	ESTIMATED ERROR: Temp. ±0.02°C. Soly. ±1% (max. dev.).	
	REFERENCES: 1. Shakhud, Zh.N.; Markuzin, N.P.; Storonkin, A.V. Vestn. Lenin- grad. Univ., Fiz., Khim. <u>1972</u> , (10), 85.	

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СОМРО	NENTS:	ORIGINAL MEASUREMENTS:	
(1)	Acetic acid propyl ester (<i>propyl acetate</i>); C ₅ H ₁₀ O ₂ ; [109-60-4] Water; H ₂ O; [7732-18-5]	Skrzecz, A. Pol. J. Chem. <u>1980</u> , 54, 1101-4. Skrzecz, A. Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u> .	
VARIA	BLES:	PREPARED BY:	
T/K = 291 - 363		A. Skrzecz	
EXPER	IMENTAL VALUES: Mutual solubility of acetic a	cid propyl ester and water	
Ψ/	K X.	a(1)/100a slp	

1/1	<u>^1</u>		g(1)/100g 511	
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
291.3	_	0.9253 ^a	~	98.596
294.0	-	0.9093	-	98.271
300.2	0.00382	-	2.128	-
307.9	0.00351	-	1.958	-
310.3	-	0.8902	-	97.871
311.5	0.00344	-	1.919	-
314.2	0.00333	-	1.859	-
322.4	0.00324	-	1.809	-
331.3	-	0.8539	-	97.070
336.4	0.00324	-	1.809	-
345.6	0.00328	-	1.831	-
345.9	-	0.8269	-	96.439
351.6	0.00333	-	1.859	-

^a By the Karl Fischer method.

(continued next page)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic-phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

SOURCE AND PURITY OF MATERIALS:

(1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.15 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp. $\pm (0.2-0.6)^{\circ}C$. Soly. see above.

REFERENCES:

COMPONENT	s:		ORIGINAL MEASUREME	ENTS:	
(1) Ace	tic acid propyl	ester	Skrzecz, A.		
(pr	opyl acetate); (C ₅ H ₁₀ O ₂ ;	Pol. J. Chem. <u>19</u>	<u>80</u> , 54, 1101-4.	
(2) Wat	9-60-4	0-51	Skrzecz, A.		
(2) Wal	er; n ₂ 0; [//32-1	.6-5]	Thesis, Inst. Ph Acad. Sci., War	ys. Chem., Pol. szawa, <u>1979</u> .	
EXPERIMEN	TAL VALUES: (CO	ontinued)	·	<u> </u>	
	Mutual solubilit	y of acetic a	ncid propyl ester an	nd water	
т/к	2	⁴ 1	g(1)/100	lg sin	
	(2)-rich phase	(1)-rich phas	se (2)-rich phase	(1)-rich phase	
355.6	0.00340	-	1.897	-	
357.8	0.00344	-	1.919	-	
361.5	0.00351	-	1,958	-	

Author's smoothing equations:

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362.7

 $\begin{aligned} x_2 &= 0.071291 + 7.085 \times 10^{-4} (T/K - 273.15) + 9.57 \times 10^{-6} (T/K - 273.15)^2 \\ &\text{st. dev.} = 1.21 \times 10^{-3} & (1) \text{-rich phase} \\ x_1 &= 5.0250 \times 10^{-3} - 5.97 \times 10^{-5} (T/K - 273.15) + 4.85 \times 10^{-7} (T/K - 273.15)^2 \\ &\text{st. dev.} = 3.96 \times 10^{-5} & (2) \text{-rich phase} \end{aligned}$

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95.480

0.7884

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4] (2) Water; H₂O; [7732-18-5] 	Tewari, Y.B.; Miller, M.M.; Wasik,S.P.; Martire, D.E. <i>J. Chem. Eng. Data</i> <u>1982</u> , 27, 451-4.	
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid propyl ester in water at 25°C was reported to be 0.200 mol(1)/L sln.		

The corresponding value on a mass/volume basis calculated by the compiler is 20.4 g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique. SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; purity >99% by glc.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C. Soly. ±1.0%.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4]</pre>	Richon, D.; Viallard, A. <i>Fluid Phase Equilib</i> . <u>1985</u> , 21, 279-93.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	

EXPERIMENTAL VALUES:

The solubility of acetic acid propyl ester in water at 298.1K was reported to be 0.0219 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1 , values calculated by the compiler are 2.19 g(1)/100g sln and 0.00393.

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE: The refractometric method was used. The Phoenix model 1-2000T differen- tial refractometer from Texas Instruments was used and the solu- bility was determined from a char- acteristic calibration curve as described in the thesis of Richon (ref 1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Soly. about ±0.02 g(1)/100g sln (compiler). REFERENCES: 1. Richon, D. Thesis, University de Clermont-Ferrand, 1974.</pre>		

2	0	0

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid propyl ester (propyl acetate); C₅H₁₀O₂; [109-60-4]</pre>	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, 56-70.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 363	Z. Maczynska	
EXPERIMENTAL VALUES: Mutual solubility of acetic acid propyl ester and water		

t/°C	g(1)/10)0g sln	x_1 (comp	oiler)
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase
0	3.21	98.84	0.00581	0.9376
9.5	2.78	98.64	0.00503	0.9275
20.0	2.26	. 98.41	0.00406	0.9161
30.0	1.98	98.12	0.00355	0.9020
40.0	1.87	97.83	0.00335	0.8883
50.0	1.72	97.71	0.00308	0.8827
60.1	1.64	97.66	0.00293	0.8804
70.5	1.72	97.05	0.00308	0.8530
80.0	1.66	96.99	0.00297	0.8504
90.2	1.35	-	0.00241	-
std. dev	v. 0.02	0.04		······

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

REFERENCES:

COMPO	NENTS:	EVALUATOR:
(1)	Butanoic acid methyl ester (methyl butyrate); C ₅ H ₁₀ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[623-42-7]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia	
	January, 1989	

CRITICAL EVALUATION:

Quantitative solubility data for the butanoic acid methyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Butanoic acid methyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Hemptinne (ref 2)	298	(1) in (2)	analytical
Fuehner (ref 3)	294	(1) in (2)	titration
Stephenson and Stuart (ref 4)	273-364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF BUTANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid methyl ester (1) in water (2) are summarized in Table 2 with the exception of the datum of Hemptinne (ref 2) which is reported in w/v units and hence is excluded from this Evaluation.

At ca. 294 K, the only temperature where comparison is possible, the independent studies (ref 1,3,4) are in reasonable agreement suggesting that the data of Stephenson and Stuart (ref 4) at other temperatures should also be reliable. However, pending further studies, the data of Stephenson and Stuart must be considered Tentative.

TABLE 2:Tentative SolubilitiesButanoic acid methyl ester (1) in Water (2)

T/K	Sol	ubilities	
	Reported values	"Best" value	s ^a
	g(1)/100g sln	g(1)/100g sln	$10^{3}x_{1}$
273	2.62 (ref 4)	2.6	4.7

(continued next page)

СОМРО	NENTS:	EVALUATOR:
(1)	Butanoic acid methyl ester (methyl butyrate); C ₅ H ₁₀ O ₂ ;	G.T. Hefter, School of Mathematical and Physical Sciences,
	[623-42-7]	Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia	
	January, 1989	

T/K	Solubilities		
	Reported values	"Best" values ^a	
	g(1)/100g sln	g(1)/100g sln	$10^{3}x_{1}$
283	2.21 [*] (ref 4)	2.2	4.0
293	1.65 ^b (ref 1), 1.56 ^c (ref 3), 1.86 [*] (ref 4)	1.9	3.3
298	1.76 [*] (ref 4)	1.8	3.0
303	1.67 [*] (ref 4)	1.7	2.8
313	1.53 [*] (ref 4)	1.5	2.6
323	1.44 (ref 4)	1.4	2.5
333	1.42 [*] (ref 4)	1.4	2.5
343	1.42 [*] (ref 4)	1.4	2.5
353	1.41 [*] (ref 4)	1.4	2.5
363	1.27 [*] (ref 4)	1.3	2.3

^a Rounded values from ref 4, see text.

^b 295 K, not included in "Best" value at 293 K.

c 294 K, not included in "Best" value at 293 K.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID METHYL ESTER (1)

The only data available for the solubility of water (2) in butanoic acid methyl ester (1) are those due to Stephenson and Stuart (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental solubilities.

REFERENCES

1. Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u>, 17, 2294-316.

2. Hemptinne, A. Z. Phys. Chem. <u>1894</u>, 13, 561-9.

3. Fuehner, H. Ber. Dtsch. Chem. Ges. <u>1924</u>, 57, 510-5.

4. Stephenson, R.; Stuart, J. J. Chem. Eng. Data 1986, 31, 56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Butanoic acid methyl ester (methyl butyrate); C₅H₁₀O₂; [623-42-7]</pre>	Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u> , 17, 2294-316.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 295	A. Skrzecz

EXPERIMENTAL VALUES:

The solubility of butanoic acid methyl ester in water at $22^{\circ}C$ was reported to be 1 part of methyl butyrate in 55-65 parts of water. The corresponding mass percent and mole fraction, x_1 , values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Not specified.
	(2) Not specified.
	ESTIMATED ERROR:
	Soly. ± 0.15 g(1)/100g sln.
	REFERENCES:
COMPONENTS:	ORIGINAL MEASUREMENTS:
--	---
(1) Butanoic acid methyl ester	Hemptinne, A.
(methyl butyrate); C ₅ H ₁₀ O ₂ ; [623-42-7]	Z. Phys. Chem. <u>1894</u> , 13, 561-9.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

reported in the paper.

The analytical method was used. The mixture of water with excess

ester was heated for some time in a

water bath and the ester phase was filtered. A sample of known volume was then transferred to a smaller flask, heated with the known amount of baryta until complete saponification was obtained and then titrated. No further details were SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butanoic acid methyl ester	Fuehner, H.
(methyl butyrate); C ₅ H ₁₀ O ₂ ; [623-42-7]	Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 294	A. Skrzecz
to be 1.792 vol%, 1.559 g(1)/100g sln sponding mole fraction, x_1 , value cal	and 0.1528 mol(1)/L sln. The corre- culated by the compiler is 0.002786.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The titration method was used. The ester was added from a pipette to the flask with a constant amount of water (50, 100 or 1000 mL) so long as, on shaking, the mixture remained transparent.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer cial product. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Butanoic acid methyl ester		Stephenson, R.; Stuart, J.		
(methyl butyrate); C ₅ H ₁₀ O ₂ ; [623-42-7]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.		
(2) Water; H ₂ O; [7732-18-5]		18-5]		
ARIABLES	5:		PREPARED BY:	,
T/K = 27	73 - 364		Z. Maczynska	
t/°C	g(1)/10	00g sln	x ₁ (comp	iler)
t/°C	g(1)/10 (2)-rich phase	00g sln (1)-rich phase	x ₁ (comp (2)-rich phase	iler) (1)-rich phase
t/°C 	g(1)/10 (2)-rich phase 2.62	00g sln (1)-rich phase 99.16	x ₁ (comp (2)-rich phase 	iler) (1)-rich phase 0.9542
t/°C 0 9.4	g(1)/10 (2)-rich phase 2.62 2.24	00g sln (1)-rich phase 99.16 99.03	x ₁ (comp (2)-rich phase 0.00472 0.00402	iler) (1)-rich phase 0.9542 0.9474
t/°C 9.4 19.7	g(1)/10 (2)-rich phase 2.62 2.24 1.87	00g sln (1)-rich phase 99.16 99.03 98.86	x ₁ (comp (2)-rich phase 0.00472 0.00402 0.00335	iler) (1)-rich phase 0.9542 0.9474 0.9386
t/°C 0 9.4 19.7 29.7	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68	00g sln (1)-rich phase 99.16 99.03 (98.86 98.73	x ₁ (comp (2)-rich phase 0.00472 0.00402 0.00335 0.00300	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320
t/°C 0 9.4 19.7 29.7 39.5	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68 1.54	00g sln (1)-rich phase 99.16 99.03 98.86 98.73 98.55	x_1 (comp. (2)-rich phase 0.00472 0.00402 0.00335 0.00300 0.00275	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320 0.9230
t/°C 0 9.4 19.7 29.7 39.5 50.0	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68 1.54 1.44	00g sln (1)-rich phase 99.16 99.03 98.86 98.73 98.55 98.50	x ₁ (comp (2)-rich phase 0.00472 0.00402 0.00335 0.00300 0.00275 0.00257	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320 0.9230 0.9205
t/°C 0 9.4 19.7 29.7 39.5 50.0 60.3	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68 1.54 1.44 1.45	00g sln (1)-rich phase 99.16 99.03 98.86 98.73 98.55 98.55 98.50 98.25	x ₁ (comp (2)-rich phase 0.00472 0.00402 0.00335 0.00300 0.00275 0.00257 0.00259	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320 0.9230 0.9205 0.9083
t/°C 0 9.4 19.7 29.7 39.5 50.0 60.3 70.3	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68 1.54 1.44 1.45 1.42	00g sln (1)-rich phase 99.16 99.03 98.86 98.73 98.55 98.50 98.25 98.25 98.34	x_1 (comp (2)-rich phase 0.00472 0.00402 0.00335 0.00300 0.00275 0.00257 0.00259 0.00253	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320 0.9230 0.9205 0.9083 0.9127
t/°C 0 9.4 19.7 29.7 39.5 50.0 60.3 70.3 80.1	g(1)/10 (2)-rich phase 2.62 2.24 1.87 1.68 1.54 1.44 1.45 1.42 1.41	00g sln (1)-rich phase 99.16 99.03 98.86 98.73 98.55 98.50 98.25 98.25 98.34 97.98	x ₁ (comp (2)-rich phase 0.00472 0.00402 0.00335 0.00300 0.00275 0.00257 0.00259 0.00253 0.00252	iler) (1)-rich phase 0.9542 0.9474 0.9386 0.9320 0.9230 0.9205 0.9083 0.9127 0.8953

AUXILIARY INFORMATION

0.02

METHOD/APPARATUS/PROCEDURE:

0.01

std. dev.

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

 Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Formin and butul actor	Stophongon D. Stuppt J
(i) Formate (buty) formate): C-H-2O-:	Stephenson, K., Stuart, S.
[592-84-7]	J. Chem. Eng. Data <u>1986</u> , 31, 56-70.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 273 - 364	Z. Maczynska
EXPERIMENTAL VALUES:	
Solubility of water in formic ac	id butyl ester
t/°C g(1)/100g sln	x ₁ (compiler)
0 99.20	0,9563
9.5 98.95	0.9432
20.2 98.86	0.9386
30.8 98.96	0.9438
40.0 98.79	0.9350
50.2 98.63	0.9270
60.5 98.45	0.9180
70.3 98.46	0.9185
80.1 98.34	0.9126
90.6 98.07	0.8996
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propagol) to the	 (1) Source not specified, commer- cial sample; purity 97%; used as received. (2) Not specified.
organic layer sample and measuring	ESTIMATED ERROR:
gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP	Accuracy of method 0.1 wt% or less,
3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol)	for solubility, see above.
was used to determine (2) in the water layer.	REFERENCES:

COMPC	DNENTS:	EVALUATOR:
(1)	Formic acid 2-methylpropyl	G.T. Hefter, School of Mathematical
	<pre>ester (isobutyl formate);</pre>	and Physical Sciences,
	C ₅ H ₁₀ O ₂ ; [542-55-2]	Murdoch University, Perth, W.A.,
(2)	Water: H ₂ O: [7732-18-5]	Australia
(-)		January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the formic acid 2-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Formic acid 2-methylpropyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Stephenson and Stuart (ref 2)	273-353	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

As can be seen from Table 1 the only comparison possible is for the solubility of (1) in (2) at 295 K. The reported values of 1 (ref 1) and 0.90 (ref 2) g(1)/100g sln are in good agreement suggesting that the values of Stephenson and Stuart (ref 2) are probably reliable. However, in the absence of confirmatory studies, all of these data (ref 2) must be regarded as Tentative. The interested user is referred to the relevant Data Sheet for the experimental solubilities of Stephenson and Stuart.

- 1. Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u>, 17, 2294-2316.
- 2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

	209	
COMPONENTS: (1) Formic acid 2-methylpropyl ester (<i>isobutyl</i> formate); C ₅ H ₁₀ O ₂ ; [542-55-2]	ORIGINAL MEASUREMENTS: Traube, J. Ber. Dtsch. Chem. Ges. <u>1884</u> , 17, 2294-316.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 295	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of formic acid 2-methylpropyl ester in water at 22°C was reported to be 1 part of isobutyl formate in 99 parts of water. The cor- responding mass percent and mole fraction, x_1 , values calculated by the compiler are 1 g(1)/100g sln and 0.0002.		
	ΙΝΕΟΡΜΑΨΙΟΝ	
method/APPAKATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	 Not specified. Not specified. 	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

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2	1	Δ
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COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Formic acid 2-methylpropyl ester (<i>isobutyl formate</i>); C₅H₁₀O₂; [542-55-2] (2) Water; H₂O; [7732-18-5] 	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , <i>31</i> , 56-70.
VARIABLES: T/K = 273 - 353	PREPARED BY: Z. Maczynska
EXPERIMENTAL VALUES:	l

Mutual solubility of formic acid 2-methylpropyl ester and water

t∕°C	g(1)/10	0g sln	x_1 (comp	iler)
((2)-rich phase	(1)-rich phase	(2)~rich phase	(1)-rich phase
0	1.14		0.00159	
9.8	1.11	99.29	0.00155	0.9509
20.8	0.93	99.14	0.00130	0.9410
30.8	0.82	98.95	0.00114	0.9288
39.8	0.76	98.98	0.00106	0.9307
50.3	0.79	98.79	0.00110	0.9187
60.4	0.78	98.65	0.00109	0.9100
70.3	-	98.61	-	0.9075
80.2	-	98.33	-	0.8907
std. dev	7. 0.01	0.01	······································	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 96%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENTS:	EVALUATOR:
 Propanoic acid ethyl ester (ethyl propionate); C₅H₁₀O₂; 	G.T. Hefter, School of Mathematical and Physical Sciences,
(2) Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

<u>TABLE 1: Quantitative Solubility Studies of the</u> <u>Propanoic acid ethyl ester (1) - Water (2) System</u>

Reference	T/K	Solubility	Method
Traube (ref 1)	295	(1) in (2)	unspecified
Rayman (ref 2)	273-303	(1) in (2)	volumetric
Doolittle (ref 3)	293	mutual	unspecified
Rao and Rao (ref 4)	301,303	mutual	titration
Rao and Rao (ref 5)	303	mutual	titration
Venkataratnam et al. (ref 6)	303	mutual	titration
Rao and Rao (ref 7)	303	mutual	titration?
Bomshtein et al. (ref 8)	293-353	mutual	titration
Tewari et al. (ref 9)	298	(1) in (2)	GLC
Richon and Viallard (ref 10)	298	(1) in (2)	refractometric
Stephenson and Stuart (ref 11)	273 - 364	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID ETHYL ESTER (1) IN WATER (2)

The available data for the solubility of propanoic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exceptions. The data of Traube (ref 1), Bomshtein *et al.* (ref 8, at T < 313 K) and Richon and Viallard (ref 10) have been rejected as they are considerably lower (> $3\sigma_n$) than other reported values (ref 2,3,11). The datum of Venkataratnam *et al.* (ref 6) at 303 K has also been rejected as it is much higher than other values at this temperature (ref 2,4,5,7,11).

COMPONENTS:	EVALUATOR:
<pre>(1) Propanoic acid ethyl ester (ethyl propionate); C₅H₁₀O₂; [105-37-3]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A.,
(2) Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION: (continued)

At higher temperatures, the data of Bomshtein *et al.* (ref 8) and Stephenson and Stuart (ref 11) are in serious disagreement, showing an opposite trend in solubility with temperature. It should be noted that in general ester solubilities in water decrease with temperature up to *ca.* 333 K, i.e., opposite to the trend reported by Bomshtein *et al.* (ref 8). However, although the data of Stephenson and Stuart (ref 10) have been preferred in deriving the "Best" values, in the absence of independent studies, it is not possible at this stage to reject either data set. Further studies of this system are clearly warranted. Selected data are plotted in Figure 1.

TABLE 2:Recommended (R) and Tentative Solubilitiesof Propanoic acid ethyl ester (1) in Water (2)

T/K	Solubilit	ies
i	Reported values	"Best" values $(\pm \sigma_n)^a$
	g(1)/100g sln	$g(1)/100g \ sln$ $10^3 x_1$
273	3.41 (ref 2), 3.26 (ref 11)	3.34 ± 0.08 (R) 6.0
283	2.78 (ref 2), 2.58 [*] (ref 11)	2.68 ± 0.10 (R) 4.8
293	2.32 (ref 2), 1.92 (ref 3), 2.21* (ref 11)	2.2 ± 0.2 4.0
298	2.17 [*] (ref 2), 2.06 [*] (ref 11)	2.12 ± 0.06 (R) 3.81
303	2.02 (ref 2), 2.01 (ref 4), 2.2 (ref 5), 2.2 (ref 7), 1.92* (ref 11)	2.07 ± 0.11 (R) 3.72
313	2.12 (ref 8), 1.74 [*] (ref 11)	1.7 ^b 3.0
323	2.28 (ref 8), 1.66 (ref 11)	1.7 ^b 3.0
333	2.50 (ref 8), 1.61 [*] (ref 11)	1.6 ^b 2.9
343	2.88 (ref 8), 1.58 [*] (ref 11)	1.6 ^b 2.9
353	3.63 (ref 8), 1.59 [*] (ref 11)	1.6 ^b 2.9

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

^b Rounded value of ref 11; see text.



FIGURE 1. Selected data for the solubility of propanoic acid ethyl ester (1) in water (2): ref 8 (\bullet); ref 11 (0). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in propanoic acid ethyl ester (1) are summarized in Table 3 except for the data at 303 K of Rao and Rao (ref 7) which appear to be self-contradictory and are rejected.

The remaining data are in general in reasonable agreement and the solubility values of Bomshtein *et al.* (ref 8) and Stephenson and Stuart (ref 11), although somewhat divergent, at least show the same trend with temperature (*cf.* the water-rich phase above). Selected data are plotted in Figure 2. In the absence of confirmatory studies it is not possible, at this stage, to prefer either data set.

COMPONENTS:	EVALUATO

(1) Propanoic acid ethyl ester (ethyl propionate); C₅H₁₀O₂; [105-37-3]

(2) Water; H₂O; [7732-18-5]

DR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989

CRITICAL EVALUATION: (continued)

<u>TABLE 3: Recommended (R) and Tentative Solubilities</u> of Water (2) in Propanoic acid ethyl ester (1)

T/K	Solubilit	ies	
values (±σ	Reported values n) ^a		"Best"
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$
273	0.89 (ref 10)	0.9	4.9
283	1.05 [*] (ref 10)	1.1	5.9
293	1.22 (ref 2), 1.40 (ref 7), 1.24 (ref 10)	1.28 ± 0.08 (R)	6.9
298	1.55 [*] (ref 7), 1.38 [*] (ref 10)	1.47 ± 0.09 (R)	7.8
303	2.00 (ref 3), 1.4 (ref 4), 1.8 (ref 5), 1.70 (ref 7), 1.51* (ref 10)	1.7 ± 0.2	8.9
313	2.10 (ref 7), 1.71 [*] (ref 10)	1.9 ± 0.2	9.9
323	2.50 (ref 7), 1.86 (ref 10)	2.2 ± 0.3	11
333	3.00 (ref 7), 1.92 [*] (ref 10)	2.5 ± 0.5	13
343	3.50 (ref 7), 1.98 [*] (ref 10)	2.7 ± 0.8	14
353	4.00 (ref 7), 2.19 [*] (ref 10)	3 ± 1	15
363	2.38 (ref 10)	-	

a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass % solubilities.



COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid ethyl ester	Traube, J.	
(ethyl propionate); $C_5H_{10}O_2$;	Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,	
(105-57-5)	2294-310.	
WARIABLES:	PREPARED BY:	
17K = 295	A. SKIZECZ	
EXPERIMENTAL VALUES: The solubility of propanoic acid ethyl ester in water at 22°C was reported to be 1 part of ethyl propionate in 55-65 parts of water. The correspond- ing mass percent and mole fraction, x_1 , values calculated by the compiler are 1.65 g(1)/100g sln and 0.0030.		
AUXILIARY 1	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The method was not specified.	(1) Not specified.	
	(2) Not specified.	
	ESTIMATED ERROR:	
	Soly. ±0.15 g(1)/100g sln.	
	REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid ethyl ester	Rayman, J.	
(ethyl propionate); C ₅ H ₁₀ O ₂ ;	Thesis, Budapest, <u>1906</u> .	
[105-37-3]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 273 - 303	G.T. Hefter	
EXPERIMENTAL VALUES:		
Solubility of propanoic acid	ethyl ester in water	
$t/^{\circ}C$ q(1)/100q(2) q(1)/100q solution x_1		
(cc	ompiler) (compiler)	
0. 3.54	3.44 0.00619	
10. 2.86	2.78 0.00502	
20. 2.38	2.32 0.00417	
30. 2.06	2.02 0.00363	
AUXILIARY	INFORMATION	
	SOURCE AND DUDTTY OF MATERIALS.	
METHOD/APPARATUS/PROCEDURE: The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an appara- tus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved	 (1) Kahlbaum or Merck; washed with salt water; dried over CaCl₂ or CuSO₄; purity not stated. (2) Not specified. 	
ble to minimize the error arising from the solubility of (2) in (1).	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	
	1. Winkler, L. <i>Z. Phys. Chem.</i> <u>1906</u> , 55, 360.	
	 Hill, A.E. International Criti- cal Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u>, Vol. 3, 387-98. 	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid ethyl ester	Doolittle, A.K.
(i) Propanoic acta echyl ester (ethyl propionate); $C_{s}H_{10}O_{2}$;	Tod End Cham 1025 27 11(0-70
[105-37-3]	Ind. End. Chem. <u>1935</u> , 27, 1169-79.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 293	A. Skrzecz
The solubility of propanoic acid ethy	r^{1} ester in water at 20° C was reported
to be 1.92 $g(1)/100g$ sln. The corresp	ponding mole fraction, x_1 , value cal-
culated by the compiler is 0.00344.	, 1,
The solubility of water in propanoic	acid ethyl ester at 20°C was reported
to be 1.22 g(2)/100g sin. The corresp culated by the compiler is 0.0654	bonding mole fraction, x_2 , value cal-
Caracea by the compiler is 0.0034.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified.
	commercial product; purity 96%, b.p. range 90-118°C, d_4^{20} 0.891.
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	net operation.
	DEFEDENCES
	NDI DRENCEO.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propanoic acid ethyl ester (ethyl propionate); $C_5H_{10}O_2$; [105-37-3]	Rao, G.J.R.; Rao, C.V. <i>J. Sci. Ind. Res.</i> <u>1955</u> , 14B, 444-8.
(2) water; H_20 ; [7/32-18-5]	
VARIABLES:	PREPARED BY:
T/K = 301 and 303	Z. Maczynska

The solubility of propanoic acid ethyl ester in water at 28 and 30° C was reported to be 2.01 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00361.

The solubility of water in propanoic acid ethyl ester at 28 and 30° C was reported to be 2.00 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.104.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The titration method was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-propionic acid. No further details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Naarden; b.p. 99.1°C, d³⁰ 0.8792; used as received. (2) Distilled and boiled; free from CO₂. ESTIMATED ERROR: Temp. ±0.1°C.</pre>	
	REFERENCES:	

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid ethyl ester	Rao, J.R.; Rao, C.V.	
(ethyl propionate); C ₅ H ₁₀ O ₂ ;	J. Appl. Chem. <u>1957</u> , 7, 435-9.	
[105-37-3]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid ethyl ester in water at 30° C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0040. The solubility of water in propanoic acid ethyl ester at 30° C was reported to be 1.4 g(2)/100g sln. The corresponding mole fraction, x_2 , value calcu- lated by the compiler is 0.074.		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The data were reported together with the ternary system propanoic	(1) Naarden, reagent grade; b.p. 99.1 ^o C, d ³⁰ 0.8790, n _D ³⁰ 1.3812.	
acid ethyl ester-water-methanol.	(2) Distilled; free from CO ₂ .	
	ESTIMATED ERROR:	
	Temp. ±0.02°C.	
	REFERENCES:	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
<pre>(1) Propanoic acid ethyl ester (ethyl propionate); C₅H₁₀O₂; [105-37-3]</pre>		Venkataratnam, A.; Rao, J.R.; Rao, C.V. Chem. Eng. Sci. <u>1957</u> , 7, 102-10.	
(2) Water; H ₂ O;	; [7732-18-5]		
VARIABLES:		PREPARED BY:	
T/K = 303		A. Skrzecz	

The solubility of propanoic acid ethyl ester in water at 30° C was reported to be 2.7 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.049.

The solubility of water in propanoic acid ethyl ester at 30° C was reported to be 1.8 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.094.

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system propanoic acid ethyl ester-water-2- propanone (ethylpropionate-water- acetone). No further details were reported in the paper.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Naarden, analytical grade; used as received; b.p. 99.1°C, d³⁰ 0.8790, n³⁰ 1.3812. (2) Distilled; free of CO₂. ESTIMATED ERROR: Not specified.</pre>	
	REFERENCES: 1. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u> , 33, 1240.	

n	2	n
2	2	۷

	1	
COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Propanoic acid ethyl ester	Rao, R.J.; Rao, C.V.	
(ethyl propionate); C ₅ H ₁₀ O ₂ ;	J. Appl. Chem. <u>1959</u> , 9, 69-73.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid ethyl ester in water at 30° C was reported to be 2.2 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0040. The solubility of water in propanoic acid ethyl ester at 30° C was reported to be 1.0 g(2)/100g sln and 98.6 g(1)/100g sln ^a . The corresponding mole fraction, x_2 , values calculated by the compiler are 0.054 and 0.074 ^a .		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURTTY OF MATERIALS.	
Presumably the titration method	(1) Naardon analytical grade.	
described by Rao and Rao (ref 1)	b.p. 99.1°C, d ³⁰ 0.8790,	
together with the ternary system	$n_{\bar{D}}^{-1.3812}$	
propanoic acid ethyl ester-water- 1-propanol.	(2) Distilled.	
	ESTIMATED ERROR:	
	Not specified	
	Not specified.	
	REFERENCES:	
	1. Rao, R.J.; Rao, C.V. <i>J. Appl.</i> Chem. <u>1957</u> , 7, 435.	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Propanoic acid ethyl ester (ethyl propionate); C₅H₁₀O₂; [105-37-3]</pre>	Bomshtein, A.L.; Trofimov, A.N.; Serafimov, L.A. Zh. Prikl. Khim. <u>1978</u> , 51, 1280-2.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293 - 353	A. Skrzecz	

Mutual solubility of propanoic acid ethyl ester and water

t/°C	x _] (2)-rich phase	(1)-rich phase	g(1)/100g sl (2)-rich phase	n (compiler) (1)-rich phase
20	0.0011	0.9255	0.62	98.60
30	0.0029	0.9107	1.62	98.30
40	0.0038	0.8916	2.12	97.90
50	0.0041	0.8731	2.28	97.50
60	0.0045	0.8509	2.50	97.00
70	0.0052	0.8295	2.88	96.50
80	0.0066	0.8090	3.63	96.00

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The titration method was used at constant temperature. No further details were reported in the paper. (1) Source not specified; distil- led; without impurities by glc, b.p. 99.1°C, n _D ²⁰ 1.383. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:			
<pre>METHOD/APPARATUS/PROCEDURE: The titration method was used at constant temperature. No further details were reported in the paper.</pre> SOURCE AND PURITY OF MATERIALS: (1) Source not specified; distil- led; without impurities by glc, b.p. 99.1°C, n _D ²⁰ 1.383. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:	AUXILIARY INFORMATION		
	METHOD/APPARATUS/PROCEDURE: The titration method was used at constant temperature. No further details were reported in the paper.	SOURCE AND PURITY OF MATERIALS: (1) Source not specified; distil- led; without impurities by glc, b.p. 99.1°C, n_D^{20} 1.383. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
 (1) Propanoic acid ethyl ester (<i>ethyl propionate</i>); C₅H₁₀O₂; [105-37-3] (2) Water; H₂O; [7732-18-5] 	Richon, D.; Viallard, A. <i>Fluid Phase Equilib</i> . <u>1985</u> , <i>21</i> , 279-93.	
VARIABLES:	PREPARED BY:	
T/K = 298	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of propanoic acid ethyl ester in water at 298.1 K was re- ported to be 0.0172 mol(1)/100g(2). The corresponding mass per cent and mole fraction, x_1 , values calculated by the compiler are 1.726 g(1)/100g sln and 0.00309.		

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE: The refractometric method was used. The Phoenix model 1-2000T differ- ential refractometer from Texas Instruments was used and the solu- bility was determined from a char- acteristic calibration curve as described in the thesis of Richon (ref 1).	<pre>SOURCE AND PURITY OF MATERIALS: (1) BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible. (2) Distilled. ESTIMATED ERROR: Not specified.</pre>	
	REFERENCES: 1. Richon, D. <i>Thesis</i> , University de Clermont-Ferrand, <u>1974</u> .	

			· · · · · · · · · · · · · · · · · · ·	
COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Propanoic acid ethyl ester		Stephenson, R.; Stuart, J.		
(ethyl propionate); C ₅ H ₁₀ O ₂ ; [105-37-3]		J. Chem. Eng. Data <u>1986</u> , 31, 56-70.		
(2) Wat	er; H ₂ O; [7732-1	.8-5]		
VARIABLES	:		PREPARED BY:	
T/K = 27	3 - 364		7 Maczynska	
EXPERIMENTAL VALUES: Mutual solubility of propanoic		c acid ethyl ester ar	nd water	
±/°C	g(1)/10)0g sln	x. (compi	ler)
	(2)-rich phase	(1)-rich phas	se (2)-rich phase ((1)-rich phase
0	3.26	99.11	0.00591	0.9516
9.7	2.59	98.96	0.00467	0.9438
19.5	2.23	98.76	0.00401	0.9335
29.7	1.93	98.50	0.00346	0.9205
39.5	1.75	98.30	0.00313	0.9107
50.0	1.66	98.14	0.00297	0.9030
60.1	1.61	98.08	0.00288	0.9001
70.2	1.58	98.02	0.00282	0.8972
80.3	1.59	97.80	0.00284	0.8869
90.5		97.61	-	0.8781
std. dev. 0.01 0.02				
		AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY O	F MATERIALS:	
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.		 (1) Source not special sample; pas received. (2) Not specified. 	cified, commer- urity 97%; used	
		ESTIMATED ERROR:		
		Accuracy of method for solubility, se	0.1 wt% or less, e above.	
		REFERENCES:		
]

COMPONENTS: (1) Propanoic acid, 2-methly-, methyl ester (methyl isobutyrate); C ₅ H ₁₀ O ₂ ;	ORIGINAL MEASUREMENTS: Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31,	
[547-63-7] (2) Water; H ₂ O; [7732-18-5]	56-70.	
VARIABLES:	PREPARED BY:	
T/K = 273 - 353	Z. Maczynska	
EXPERIMENTAL VALUES: Mutual solubility of 2-methylpropanoic acid methyl ester and water		
t/°C g(1)/100g sln (2)-rich phase (1)-rich phas	x ₁ (compiler) e (2)-rich phase (1)-rich phase	

	*			
0	2.68	98.97	0.00483	0.9442
9.1	2.23	98.79	0.00401	0.9350
18.9	1.96	98.70	0.00351	0.9305
29.5	1.69	98.52	0.00302	0.9215
39.9	1.52	98.38	0.00271	0.9146
49.8	1.46	98.21	0.00260	0.9063
60.4	1.38	97.75	0.00246	0.8845
70.5	1.40	97.93	0.00250	0.8930
80.3	1.32	97.85	0.00235	0.8892
std. dev.	0.01	0.02		

	- ,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each	 Source not specified, commer- cial sample; purity 99%; used as received.
layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the	(2) Not specified.
organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP	ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for solubility, see above.
A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the	
water layer.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid 2-methoxyethyl	Alvaroz I P · Noila I I	
ester	Alvalez, J.K., Mella, J.J.	
(2-methoxyethyl acetate);	An. Quim. <u>1978</u> , 74, 326-32.	
C ₅ H ₁₀ O ₃ ; [110-49-6]		
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	Z. Maczynska	
The solubility of acetic acid 2-methoxyethyl ester in water at 25°C was reported to be 45.5 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.1129. The solubility of water in acetic acid 2-methoxyethyl ester at 25°C was reported to be 46.4 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.850.		
· · · · · · · · · · · · · · · · · · ·		
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Presumably the titration method was used. The data were reported together with the ternary system 2-methoxyethyl acetate-water- phenol. No further details were reported in the paper.	(1) Source not specified, commer- cial product; used as received; $d_4^{18.1}$ 1.0051, n_D^{20} 1.4048. (2) Twice distilled over KMnO ₄ .	
	ESTIMATED ERROR:	
	Not specified.	
	REFERENCES:	

COMPONENTS:		EVALUATOR:
(1)	Carbonic acid diethyl ester (<i>diethyl carbonate</i>); C ₅ H ₁₀ O ₃ ;	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University Porth W A
(2)	Water; H ₂ O; [7732-18-5]	Australia January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the carbonic acid diethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Carbonic acid diethyl ester (1) - Water (2) System

Reference	T/K	Solubility	Method
Doolittle (ref 1)	293	mutual	unspecified
Stephenson and Stuart (ref 2)	273-363	mutual	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF CARBONIC ACID DIETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of carbonic acid diethyl ester (1) in water (2) are summarized in Table 2. At 293 K, the only temperature where comparison is possible, the data (ref 1,2) are in excellent agreement and the average "Best" value is Recommended. At other temperatures only the data of Stephenson and Stuart (ref 2) are available and, pending further studies, these must be regarded as Tentative.

TABLE 2:Recommended (R) and Tentative Solubilitiesof Carbonic acid diethyl ester (1) in Water (2)

T/K	Solubilities		
	Reported values	"Best" values (:	±σ _n) ^a
	g(1)/100g sln	g(1)/100g sln	10 ³ x ₁
273	2.49 (ref 2)	2.5	3.9
283	2.14 [*] (ref 2)	2.1	3.3
293	1.88 (ref 1), 1.90 [*] (ref 2)	$1.89 \pm 0.01 (R)^{b}$	2.93
298	1.77 [*] (ref 2)	1.8	2.6

a Rounded values of ref 2 unless otherwise indicated.

^b Average value.

COMPONENTS:		EVALUATOR:	
(1)	Carbonic acid diethyl ester (<i>diethyl carbonate</i>); C ₅ H ₁₀ O ₃ ; [105-58-8] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989	
CRITICAL EVALUATION: (continued)			
T/K	T/K Solubilities		

- /	001401110	100	
	Reported values	"Best" values (± σ	n) ^a
	g(1)/100g sln	g(1)/100g sln	10 ³ x ₁
303	1.67 (ref 2)	1.7	2.5
313	1.58 (ref 2)	1.6	2.4
323	1.53 (ref 2)	1.5	2.3
333	1.53 [*] (ref 2)	1.5	2.3
343	1.6 [*] (ref 2)	1.6	2.4
353	1.6 [*] (ref 2)	1.6	2.4
363	1.6 [*] (ref 2)	1.6	2.4

^a Rounded values of ref 2 unless otherwise indicated.

In Table 2, σ_n has no statistical significance; mole fraction solubility (x_1) has same status and (relative) percentage uncertainty as mass% solubility.

2. SOLUBILITY OF WATER (2) IN CARBONIC ACID DIETHYL ESTER (1)

As for the solubility of carbonic acid diethyl ester (1) in water (2) the only comparable data available for the solubility of (2) in (1) are at 293 K. However, unlike the H_2O -rich phase the datum of 2.60 g(2)/100 g sln of Doolittle (ref 1) is in poor agreement with the interpolated value of 0.86 g(2)/100 g sln of Stephenson and Stuart (ref 2). In the absence of confirmatory studies it is not possible to decide between these data although it may be noted that the data of Doolittle often differ significantly from reliable values in other systems.

The interested user is referred to the Data Sheet for the experimental solubilities of Stephenson and Stuart for water in carbonic acid diethyl ester.

- 1. Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79.
- 2. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Carbonic acid diethyl ester (diethyl carbonate); C ₅ H ₁₀ O ₃ ;	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.	
(2) Water; H_2O ; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 293	A. Skrzecz	
EXPERIMENTAL VALUES:		

The solubility of carbonic acid diethyl ester in water at 20° C was reported to be 1.88 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00291.

The solubility of water in carbonic acid diethyl ester at 20° C was reported to be 2.60 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1490.

METHOD/APPARATUS/PROCEDURE: The method was not specified. (1) Source not specified, commercial product; purity 91%, b.p. range 87-127°C, d²⁰ 0.957. (2) Not specified. ESTIMATED ERROR: Not specified. REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Ca	Carbonic acid diethyl ester		Stephenson, R.; Stuart, J.	
(đ. [1	iethyl carbonate) 05-58-8]	; C ₅ H ₁₀ O ₃ ;	J. Chem. Eng. Dat 56~70.	a <u>1986</u> , 31,
(2) Wa	ter; H ₂ O; [7732-1	.8-5]		
VARIABLES:			PREPARED BY:	
T/K = 273 - 363		Z. Maczynska		
EXPERIME	NTAL VALUES: Mutual solubility	y of carbonic a	acid diethyl ester	and water
t/°C g(1)/100g sln		x ₁ (compiler)		
	(2)-rich phase	(1)-rich phase	e (2)-rich phase	(1)-rich phase
0	2.49	99.35	0.00388	0.9589
9,9	2.15	99.28	0.00334	0.9546
20.1	1.90	`99.11	0.00294	0.9444
30.0	1.67	98.94	0.00258	0.9343

AUXILIARY INFORMATION

98.88

98.68

98.38

98.27

97.63

97.22

0.01

METHOD/APPARATUS/PROCEDURE:

1.58

1.53

1.54

1.63

1.69

1.63

0.02

40.0

50.0

60.2

70.1

80.1

90.3

std. dev.

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

 Source not specified, commercial sample; purity 99%; used as received.

(2) Not specified.

0.00244

0.00236

0.00238

0.00252

0.00261

0.00252

0.9309

0.9193

0.9025

0.8965

0.8627

0.8421

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Butenedioic acid dimethyl ester (dimethyl maleate); $C_6H_8O_4$; [624-48-6] (2) Water; H_2O ; [7732-18-5]	Stephenson, R.; Stuart, J. <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, 56-70.
VARIABLES: T/K = 273 - 364	PREPARED BY: Z. Maczynska

Mutual solubility of 2-butenedioic acid dimethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)		
	(2)-rich phase	(1)-rich phase	(2)-rich phase	(1)-rich phase	
·	7.7	97.90	0.0103	0.8535	
9.6	7.3	97.46	0.0097	0.8275	
19.8	7.6	96.82	0.0102	0.7919	
29.7	7.8	96.24	0.0105	0.7619	
39.5	8.1	95.50	0.0109	0.7262	
50.0	8.7	94.50	0.0118	0.6823	
59.9	8.9	93.57	0.0121	0.6453	
69.8	9.6	92.40	0.0131	0.6031	
80.1	10.4	90.92	0.0143	0.5559	
90.5	10.9	89.62	0.0151	0.5190	
std. de	v. 0.2	0.03			

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENT		ORIGINAL MEASUREMENTS: Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F.		
(1) 1-N (1-	<pre>Methyl-2-propen-1-ol acetate -methylallyl acetate);</pre>			
C ₆ H	I ₁₀ 0 ₂ ; [6737-11-7]	Ind. Eng. Chem. <u>1945</u> , 37, 890-4.		
(2) Wat	cer; H ₂ 0; [7732-18-5]			
VARIABLES	5:	PREPARED BY:		
T/K = 29	99 - 348	A. Skrzecz		
EXPERIMEN Mut	NTAL VALUES: Cual solubility of 1-Methyl-2	-propen-1-ol acetate and water		
t/°C	g(1)/100g sln	x ₁ (compiler)		
	(2)-rich phase (1)-rich phase	se (2)-rich phase (1)-rich phase		
26	1.32 99.0	0.0021 0.940		
50	0.8 98.9	0.0013 0.934		
75	2.0 98.1	0.0032 0.891		
METHOD/AI	PPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Presumably the titration method reported by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system 1-Methyl-2-propen- 1-ol acetate-water-1,2-butanediol (1-methylallyl acetate-water-		 (1) Synthesized from methyl vinyl carbinol; washed with water, dried with CaCl₂, distilled; b.p. range 112-113°C. (2) Not specified. 		
butylene	glycol).			
		ESTIMATED ERROR:		
		Not specified.		
		REFERENCES:		
		1. Othmer, D.F.; White, R.E.; Trueger,E. Ind. Eng. Chem. <u>1941</u> , 33, 1240.		

			235
COMPONENTS:		ORIGINAL MEASUREME	NTS:
(1) Butanoic acid,	3-oxo-, ethyl	Pai, M.U.; Sane,	A.G.
ester (ethyl a $C_{c}H_{10}O_{2}$; [141-9	cetoacetate); 97-9]	Indian J. Technol	. <u>1966</u> , <i>4</i> , 373-5.
(2) Water; H ₂ O; [7	732-18-5]		
VARIABLES:		PREPARED BY:	
<i>T</i> /K = 273 and 303		A. Skrzecz	
EXPERIMENTAL VALUES: Mutual solubil	ity of 3-oxobutanc	bic acid ethyl ester	and water
t/°C g((2)-rich p	1)/100g sln hase (1)-rich phas	x ₁ (comp se (2)-rich phase	iler) (1)-rich phase
0 12.15	93.55	0.01879	0,6675
30 10.04	92.02	0.01521	0.6148
	AUXILIARY I	INFORMATION	
METHOD/APPARATUS/PRO	CEDURE:	SOURCE AND PURITY	OF MATERIALS:
METHOD/APPARATUS/PROCEDURE: The turbidity method described by Othmer, White and Trueger (ref 1) was used. Mutual solubilities were determined in a 25 mL glass stop- pered flask placed in a thermostat. The data were reported together with the ternary system 3-oxo- butanoic acid ethyl ester-water- acetic acid ethyl ester (ethyl acetoacetate-water-ethyl acetate).		 (1) Merc CP grade at 10 ±1 mm Ho cut at 67 ±0.1 purity 99.9%, d²⁰ 1.025. (2) Twice distillo ESTIMATED ERROR: Temp. ±0.1°C. 	; distilled g and the middle 5°C was used; b.p. 180.9°C, ed.
		REFERENCES:	
		1. Othmer, D.F.; W Trueger,E. Inc <u>1941</u> , 33, 1240	White, R.E.; d. Eng. Chem.

COMPC	DNENTS:	ORIGINAL MEASUREMENTS:
(1)	Ethanedioic acid diethyl ester	Stephenson, R.; Stuart, J.
	(diethyl oxalate); C ₆ H ₁₀ O ₄ ;	J. Chem. Eng. Data 1986. 31.
	[95-92-1]	56-70.

(2) Water; H₂O; [7732-18-5]

VARIABLES:

T/K = 273 - 364

Z. Maczynska

PREPARED BY:

EXPERIMENTAL VALUES:

Mutual solubility of ethanedioic acid diethyl ester and water

t/°C	g(1)/100g sln		x_1 (compiler)		
	(2)-rich phase	(1)-rich phase 99.40 99.23	(2)-rich phase	(1)-rich phase 0.9533 0.9408	
	5.47		0,00708		
9.5			0.00571		
19.7	3.82	`98.92	0.00487	0.9186	
30.9 3.71 39.8 3.17 49.7 2.74	3.71	98.80 98.65 98.30	0.00473	0.9103 0.9001 0.8770	
	3.17		0.00402 0.00346		
	2.74				
60.0	-	97.92	-	0.8530	
70.2	-	97.48	-	0.8266 0.7821	
80.4	-	96.68	-		
90.7	-	96.12	-	0.7533	
std. de	v. 0.09	0.03			

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. Component (1) was equilibrated with component (2) at a given temperature in a thermostat. Each layer was sampled with a syringe; (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity gc the (1)/acetonitrile peak ratio (Chromosorb 101 packing and a HP 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer.

SOURCE AND PURITY OF MATERIALS:

- Source not specified, commercial sample; purity 99%; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Accuracy of method 0.1 wt% or less, for solubility, see above.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1,1-Ethanediol diacetate (ethylidene diacetate); C₆H₁₀O₄; [542-10-9] Water; H₂O; [7732-18-5] 	Smith, J.C. <i>J. Phys. Chem.</i> <u>1942</u> , 46, 229-32.
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska
EXPERIMENTAL VALUES:	

The solubility of 1,1-ethanediol diacetate in water at $25^{\circ}C$ was reported to be 5 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.006.

The solubility of water in 1,1-ethanediol diacetate at $25^{\circ}C$ was reported to be 5 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.3.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Presumably the titration method was	(1) Not specified.		
ported together with the ternary system 1,1-ethanediol diacetate- water-acetic acid.	(2) Not specified.		
	ESTIMATED ERROR:		
	Not specified.		
	REFERENCES:		

СОМРС	DNENTS:	EVALUATOR:
(1)	1,2-Ethanediol diacetate	G.T. Hefter, School of Mathematical
	(ethylene glycol diacetate);	and Physical Sciences,
	C ₆ H ₁₀ O ₄ ; [111-55-7]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732-18-5]	Australia
(2)		January, 1989

CRITICAL EVALUATION:

Quantitative solubility data for the 1,2-ethanediol diacetate (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1:	Quant	itative	Solubi	lity	Studies	of the
1,2-Ethan	ediol	diaceta	te (1)	- Wa	ter (2)	System

Reference	T/K	Solubility	Method
Doolittle (ref 1)	. 293	mutual	unspecified
Othmer et al. (ref 2)	298	mutual	unspecified
Kraus et al. (ref 3)	298	mutual	analytical
	250	ind Cut I	unarycrear

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF 1,2-ETHANEDIOL DIACETATE (1) IN WATER (2)

All the available data for the solubility of 1,2-ethanediol diacetate (1) in water (2) are summarized in Table 2. As can be seen, the data are in only fair agreement with the value of Doolittle looking to be high. However, pending further studies, none of these data can be rejected at this stage.

TABLE 2:	<u> Tentative</u> So	<u>olubilities</u>	
of 1,2-Ethanediol	diacetate	(1) in Water (2)	

T/K	Solubilities			
	Reported values	"Best" values (±σ	n) ^a	
	g(1)/100g sln	g(1)/100g sln	$10^2 x_1$	
293	21.3 (ref 1)	21 ^b	3.2	
298	17.8 ^c (ref 2), 16 (ref 3)	17 ± 1	2.5	

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass % solubilities.

^b But see text.

с 297.7 K.

COMPONENTS:		EVALUATOR:		
(1)	1,2-Ethanediol diacetate	G.T. Hefter, School of Mathematical		
	(ethylene glycol diacetate);	and Physical Sciences,		
	C ₆ H ₁₀ O ₄ ; [111-55-7]	Murdoch University, Perth, W.A.,		
(2)	Water; H ₂ O; [7732-18-5]	Australia		
		January, 1989		

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 1,2-ETHANEDIOL DIACETATE (1)

All the available data for the solubility of water (2) in 1,2ethanediol diacetate (1) are summarized in Table 3. The data of Othmer *et al.* (ref 2) and Kraus *et al.* (ref 3) at *ca.* 298 K are in fair agreement but the value of Doolittle (ref 1) is very much higher. However, in the absence of confirmatory studies no Critical Evaluation is possible.

> TABLE 3: Tentative Solubilities of Water (2) in 1,2-Ethanediol diacetate (1)

T/K	Solubilities			
	Reported values	"Best" values (± σ	n) ^a	
	g(2)/100g sln	g(2)/100g sln	x ₂	
293	21.2 (ref 1)	21 ^b	0.68	
298	10.0 ^c (ref 2), 7.65 (ref 3)	9 ± 1	0.45	

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_2) have the same status and (relative) percentage uncertainties as the mass solubilities.

^b But see text.

с 297.7 К.

REFERENCES

1. Doolittle, A. K. Ind. Eng. Chem. 1935, 27, 1169-79.

 Othmer, D. F.; White, R. E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240-8.

 Kraus, K. A.; Rardon, R. J.; Baldwin, W. H. J. Am. Chem. Soc. <u>1964</u>, 86, 2571-6.
COMPONENTS:	ORIGINAL MEASUREMENTS:			
<pre>(1) 1,2-Ethanediol diacetate (ethylene glycol diacetate); C₆H₁₀O₄; [111-55-7]</pre>	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.			
(2) Water; H ₂ O; [7732-18-5]				
VARIABLES:	PREPARED BY:			
T/K = 293	A. Skrzecz			
EXPERIMENTAL VALUES: The solubility of 1,2-ethanediol diacetate in water at 20°C was reported to be 21.3 g(1)/100g sln. The corresponding mole fraction, x_1 , value cal-				

The solubility of water in 1,2-ethanediol diacetate at 20°C was reported to be 21.2 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.686.

culated by the compiler is 0.0323.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	<pre>(1) Source not specified, commercial product; purity 99%, b.p. range 184-191°C, d₄²⁰ 1.107.</pre>
	(2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:		
<pre>(1) 1,2-Ethanediol diacetate (ethylene glycol diacetate); C₆H₁₀O₄; [111-55-7]</pre>	Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u> , 33, 1240-8.		
(2) Water; H ₂ O; [7732-18-5]			
VARIABLES:	PREPARED BY:		
T/K = 298	A. Skrzecz		

The solubility of 1,2-ethanediol diacetate in water at 24.5°C was reported to be 17.8 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.0260.

The solubility of water in 1,2-ethanediol diacetate at 24.5°C was reported to be 10.0 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.474.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Nothing was specified in the paper. (1) Not specified. (2) Not specified. ESTIMATED ERROR: Temp. ±0.5°C (mean of reported range). REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 1,2-Ethanediol diacetate (ethylene glycol diacetate); 	Kraus, K.A.; Raridon, R.J.; Baldwin, W.H.
C ₆ H ₁₀ O ₄ ; [111-55-7]	J. Am. Chem. Soc. <u>1964</u> , 86, 2571-6.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	2. Maczynska
The solubility of 1,2-ethanediol diad to be 16 g(1)/100g sln. The correspon culated by the compiler is 0.023. The solubility of water in 1,2-ethane to be 7.65 g(2)/100g sln. The corresp culated by the compiler is 0.402.	cetate in water at 25°C was reported inding mole fraction, x_1 , value cal- ediol diacetate at 25°C was reported ponding mole fraction, x_2 , value cal-
AUXILIARY	INFORMATION
	COUDCE AND DUDTERY OF NAMEDIALCO
The analytical methods were used. The mutual solubilities of (1) and (2) were determined by shaking mixtures in stoppered tubes in a constant temperature bath. The (1)-rich phases were analyzed for water by the use of Karl Fischer titrations. The (2)-rich phases were analyzed for acetate by a semimicro adaptation of the stand- ard saponification technique whereby back titration of excess alkali is performed on a boiling solution to minimize carbonate error, and in a flask under a reflux condenser to minimize loss of acetic acid.	<pre>(1) Obtained by distillation under reduced pressure of commercial- ly available material; fraction of unacetylated hydroxyl groups was less than 0.03. (2) Not specified. ESTIMATED ERROR: Soly. ±5 g(1)/100g sln and ±1 g(2)/100g sln (precision). REFERENCES:</pre>
	KEFERENCES:

COMPONENTS:	EVALUATOR:				
 (1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4] (2) Water: H₂O: [7732-18-5] 	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia				
(1)		January, 1989			
CRITICAL EVALUATION:					
Quantitative solubility data for	the a	cetic acid buty]	. ester (1) - water		
(2) system have been reported in	the p	ublications list	ed in Table 1.		
<u>TABLE 1: Quantita</u> <u>Acetic acid butyl</u>	tive S ester	olubility Studie (1) - Water (2)	<u>s of the</u> System		
Reference	T/K	Solubility	Method		
Bridgman (ref 1) 2	83-303	(2) in (1)	synthetic		
Park and Hopkins (ref 2)	298	(1) in (2)	unspecified		
Park and Hofmann (ref 3)	298	mutual	unspecified		
Doolittle (ref 4)	293	mutual	unspecified		
Othmer et al. (ref 5)	297	mutual	unspecified		
Othmer et al. (ref 6)	ef 6) 323 mutual synthetic				
Donahue and Bartell (ref 7)	298	mutual	interferometric, Karl Fischer		
Rao and Rao (ref 8)	303	mutual	titration		
Bushmakin and Lutugina (ref 9)	364	mutual	analytical		
Schuberth and Leibnitz (ref 10)	318	mutual	titration, analytical		
Schuberth (ref 11) 3	18-342	mutual	titration, Karl Fischer		
Rao and Rao (ref 12)	303	mutual	titration		
Schuberth (ref 13) 2	93,318	mutual	titration, analytical		
Rao et al. (ref 14)	308	mutual	titration		
Narasimhan (ref 15)	303	mutual	titration, refractometric		
Hirata and Hirose (ref 16) 3	03-364	mutual	titration		
Ramanarao <i>et al</i> . (ref 17)	303	mutual	turbidometric		
Blank and Popova (ref 18)	303	(2) in (1)	titration		
Krupatkin and Glagoleva (ref 19)	298	mutual	titration		
Pop et al. (ref 20)	293	mutual	titration		
Bergovykh <i>et al</i> . (ref 21)	364	mutual	unspecified		
Iguchi and Fuse (ref 22)	298	mutual	titration		
Krupatkin and Shcherbakova (ref 23)	298	mutual	titration		
· /			(continued next page)		

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COMPONENTS:		EVALUATOR:			
 Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4] Water; H₂O; [7732-18-5] 		G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989			
CRITICAL EVALUATION: (continue	d)				
Reference	T/K	Solubility	Method		
Utkin et al. (ref 24) 298		mutual	titration		
Andreeva et al. (ref 25) 363		mutual	titration		
Skrzecz (ref 26) 291-362		mutual	synthetic, Karl Fischer		
Tewari et al. (ref 27)	298	(1) in (2)	GLC		
Cho et al. (ref 28) 364		mutual	titration		
Ouyang et al. (ref 29) 323		mutual	GLC		
Richon and Viallard (ref 30) 298		mutual	calorimetric, refractometric		
Stephenson and Stuart (ref 31)	273-364	mutual	GLC		

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid butyl ester (1) in water (2) are summarized in Table 2 with the following exceptions.

The data of Park and Hofmann (ref 3), Iguchi and Fuse (ref 22), and Richon and Viallard (ref 30) at 298 K, and of Bergovykh et al. (ref 21), Hirata and Hirose (ref 16), and Andreeva et al. (ref 25) at ca. 364 K are all much higher than other values and are rejected. Similarly, the data of Doolittle (ref 4), Bushmakin and Lutugina (ref 9), Narasimhan et al. (ref 15) and Ouyang et al. (ref 29) are much lower than other studies and are also rejected. The data of Park and Hopkins (ref 2) and Tewari et al. (ref 27) reported in v/v and w/v units are also excluded from consideration and the various data of Rao and co-workers (ref 8,12) at 303 K and of Schuberth (ref 10,11,13) at 318 K are not regarded as independent determinations for the purpose of this Evaluation.

At lower temperatures the plethora of remaining data are in reasonable agreement although the σ_n values are too large for most of the averaged "Best" values to be Recommended. Outside the range 293-323 K most of the data are due to Skrzecz (ref 26) and to Stephenson and Stuart (ref 31). These two studies diverge somewhat at higher temperatures. Selected data are plotted in Figure 1.

сомро	NENTS:	EVALUATOR:
(1)	Acetic acid butyl ester	G.T. Hefter, School of Mathematical
	(butyl acetate); C ₆ H ₁₂ O ₂ ;	and Physical Sciences,
	[123-86-4]	Murdoch University, Perth, W.A.,
(2)	Water: H ₂ O; [7732-18-5]	Australia
(-)		January, 1989

CRITICAL EVALUATION: (continued)

TABLE 2:Recommended (R) and Tentative Solubilitiesof Acetic acid butyl ester (1) in Water (2)

T/K	Solubilities					
	Reported values	"Best" values $(\pm \sigma_n)^a$				
	g(1)/100g sln	$g(1)/100g \ sln$ $10^3 x_1$				
273	0.96 (ref 31)	0.96 1.50				
283	0.75 [*] (ref 31)	0.75 1.17				
293	0.7 (ref 13), 0.712 (ref 20), 0.64* (ref 26), 0.62* (ref 31)	0.67 ± 0.04 1.04				
298	0.68 ^b (ref 5), 0.638 (ref 7), 0.73 (ref 19), 0.76 (ref 23), 0.8 (ref 24), 0.61 [*] (ref 26), 0.57 [*] (ref 31)	0.68 ± 0.08 1.06				
303	0.9 (ref 8,12), 0.70 (ref 16), 0.94 (ref 17), 0.58 [*] (ref 26), 0.53 [*] (ref 31)	0.73 ± 0.17 1.13				
313	0.60 (ref 10,11,13), 0.6 (ref 24), 0.55* (ref 26), 0.50* (ref 31)	0.55 ± 0.04 0.85				
323	0.69 (ref 6), 0.57 ^c (ref 11), 0.54 [*] (ref 26), 0.50 [*] (ref 31)	0.58 ± 0.07 0.90				
333	0.54 ^c (ref 11), 0.55 [*] (ref 26), 0.50 [*] (ref 31)	0.53 ± 0.02 (R) 0.83				
343	0.53 ^c (ref 11), 0.58 [*] (ref 26), 0.49 [*] (ref 31)	0.53 ± 0.04 0.83				
353	0.65 [*] (ref 26), 0.48 [*] (ref 31)	0.57 ± 0.09 0.89				
363	0.73 [*] (ref 26), 0.83 ^d (ref 28), 0.47 [*] (ref 31)	0.7 ± 0.2 1.1				

^a Obtained by averaging where appropriate; σ_n has no statistical significance. Mole fraction solubilities (x_1) have the same status and (relative) percentage uncertainties as the mass solubilities.

^b 297 К.

^c Calculated from the original author's fitting equation.

d 364.2 K.

(continued next page)

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FIGURE 1. Selected data for the solubility of acetic acid butyl ester (1) in water (2): ref 10, 11, 13 (X); ref 26 (\bullet); ref 31 (O). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID BUTYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid butyl ester (1) are summarized in Table 3 with the following exceptions.

The data of Park and Hofmann (ref 3), Doolittle (ref 4), Othmer et al. (ref 6), Hirata and Hirose (ref 16), Ramanarao et al. (ref 17), Krupatkin and Glagoleva (ref 19), at various temperatures (Table 1) are higher than other studies and are rejected. Similarly, the data of Pop et al. (ref 20) and Richon and Viallard (ref 30) are lower than all other studies and are also rejected.

As for the water-rich phase, the numerous independent studies at lower temperatures are in reasonable agreement, although none of the averaged "Best" values have been Recommended because of the high spread of the experimental solubilities. At higher temperatures (T > 323 K) the data,

(continued next page)

COMPONENTS	:	EVALUATOR:			
(1) Acet (but [123 (2) Wate	ic acid butyl ester yl acetate); C ₆ H ₁₂ O ₂ ; -86-4] r; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989			
CRITICAL E	VALUATION: (continued)				
mainly due to Schuberth (ref 11), Skrzecz (ref 26), and Stephenson and Stuart (ref 31) are in poor agreement. Further studies are clearly warranted. Selected data are plotted in Figure 2.					
	<u>TABLE 3: Tentat</u> of Water (2) in Acetic	<u>ive Solubilities</u> : acid butyl ester (1)			
т/к	Sol	ubilities			
	Reported values	"Best" values (±	o _n) ^a		
	g(2)/100g sln	g(2)/100g sln	$10^2 x_2$		
273	0.78 (ref 31)	0.8	5		
283	1.21 [*] (ref 1), 0.85 [*] (ref 3)	1) 1.0 ± 0.2	6		
293	1.36 [*] (ref 1), 1.2 (ref 13) 1.04 [*] (ref 26), 0.99 [*] (ref 2	, 1.15 ± 0.15 31)	7.0		
298	1.46 [*] (ref 1), 1.2 ^b (ref 5) 1.23 (ref 7), 1.07 (ref 22) 1.46 (ref 23), 1.3 (ref 24) 1.08 [*] (ref 26), 1.12 [*] (ref 26)	, 1.24 ± 0.15 , , 31)	7.5		
303	1.56 [*] (ref 1), 1.1 (ref 8,1 1.45 (ref 15), 1.13 (ref 16 1.04 (ref 18), 1.13 [*] (ref 2 1.24 [*] (ref 31)	2), 1.24 ± 0.18), 5),	7.5		
313	1.5 (ref 24), 1.28 [*] (ref 26 1.35 (ref 31)), 1.38 ± 0.09	8.3		
318	1.69 ^c (ref 10,11,13), 1.38 [*] (ref 26), 1.37 [*] (ref 3	1.48 ± 0.15 31)	8.8		
323	1.82 ^d (ref 11), 1.49 [*] (ref 2 1.91 (ref 29), 1.37 [*] (ref 3	26), 1.65 ± 0.22 1)	9.8		
333	2.07 ^d (ref 11), 1.76 [*] (ref 2 1.38 [*] (ref 31)	26), 1.7 ± 0.3	10		
343	2.36 ^d (ref 11), 2.08 [*] (ref 2 1.37 [*] (ref 31)	26), 1.9 ± 0.4	11		
353	2.47* (ref 26), 1.44* (ref 3	31) 2.0 ± 0.5	12		
363	2.60 ^e (ref 9), 4.19 ^e (ref 21) 2.91 (ref 26), 3.55 ^e (ref 28 1.55 [*] (ref 31)	, 3.0 ± 0.9 3),	17		

(relative) percentage uncertainties as the mass % solubilities.

^b 297 K.

° 317.6 K.



COMP	ONENTS:	EVALUATOR:		
(1)	Acetic acid butyl ester (<i>butyl acetate</i>); C ₆ H ₁₂ O ₂ ; [123-86-4] Water; H ₂ O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia January, 1989		
CRIT	ICAL EVALUATION: (continued)			
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12.	Rao, J. R.; Rao, C. V. J. Appl.	Chem. <u>1959</u> , 9, 69-73.		
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22.	Iguchi, A.; Fuse, K. Kagaku Kog	aku <u>1971</u> , 35, 1035-7.		
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29.	Ouyang, F.; Wang, G.; Gao, W.	Hua Kung Hsueh Pao <u>1985</u> , 110 - 8.		
		(continued next page)		

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СОМРО	NENTS:	EVALUATOR:
(1)	Acetic acid butyl ester	G.T. Hefter, School of Mathematical
	(butyl acetate); C ₆ H ₁₂ O ₂ ;	and Physical Sciences,
	[123-86-4]	Murdoch University, Perth, W.A.,
(2)	Water: H_O: [7732-18-5]	Australia
(2)		January, 1989

CRITICAL EVALUATION: (continued)

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ACKNOWLEDGEMENT

The Evaluator thanks Dr. Brian Clare for the graphics.

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COMPONENTS:		01	RIGINAL M	EASURE	IENTS:		
(1) Acetic acid butyl ester			Bridgman, J.A.				
(butyl	acetate); C ₆ H ₁₂ O ₂ ;		Ind. End.	Chem.	<u>1928</u> ,	20,	184-7.
[123-8	6-4]						
(2) Water;	H ₂ O; [7732-18-5]						
VARIABLES:		PI	REPARED B	Y:			
T/K = 283 -	303	:	2. Maczyn	ska			
EXPERIMENTAL	EXPERIMENTAL VALUES:						
So	lubility of water in ac	etic	acid buty	yl ester	:		
t/°C	q(2)/100q(1) q(2)/10	Q sln	X	 5	_	
	(compi	ler)	(con	 npiler)		
						<u> </u>	
9.5	1.202	1.1	88 63	0.	0719		
21.0	1.375	1.3	56	0.	0814		
29.5	1.549	1.5	25	0.	0908		
	AUXILIAR	RY INF	ORMATION	_			
METHOD/APPARA	ATUS/PROCEDURE:	so	URCE AND	PURITY	OF MA	reri <i>i</i>	ALS:
The synthet	ic method similar to		1) Sourc	e not s	pecifi	ed; d	distil-
was used. A	glass tube of about	'	boile	b.p. ra d for s	nge 12 ome ti	4-120 me in	n open
100 mL capad filled with	city with a stopcock wa weighed (1) and (2). B	s v	flask	before	used.		-
shaking the	tube after it had been		2) Not s	pecifie	d.		
solved compl	letely in the ester,						
after which a 2-liter be	the tube was placed in eaker filled with water	ES	TIMATED	ERROR:			
and equipped	d with an agitator. By	. n	emp. ±0.	25 ⁰ C (a	uthor).		
it was possi	ible to determine, with	<u>-</u> 8	Soly. abo	ut ±0.3	g(2)/	100g	sln
in about 0.5 which water	5°C, the temperature at was precipitated from		(00	whriei)	•		
the solution	n, as shown by the	-					
clear again	when the temperature	RI	FERENCES	:			
was slightly	/ increased.	1	. Grosch <u>1911</u> ,	uff, E. 17, 348	<i>Z.E</i> :	lektr	cochem.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4]</pre>	Park, J.G.; Hopkins, M.B. Ind. Eng. Chem. <u>1930</u> , 22, 826-30.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	A. Skrzecz

The solubility of acetic acid butyl ester in water at $25^{\circ}C$ was reported to be 0.7 mL(1)/100mL(2).

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	 (1) Source not specified, commer- cial samples; used as received. (2) Not specified.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<pre>(1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4]</pre>	Park, J.G.; Hofmann, H.E. Ind. Eng. Chem. <u>1932</u> , 24 132-4.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 298	Z. Maczynska	
EXPERIMENTAL VALUES:		
the solubility of acetic acid butyl ester in water at 25°C was reported to be 2.3 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu-		
lated by the compiler is 0.0036.		

The solubility of water in acetic acid butyl ester at $25^{\circ}C$ was reported to be 2.4 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.137.

	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	Nothing was specified in the paper.	(1) Not specified.
		(2) Not specified.
		ESTIMATED ERROR:
		Soly. about $\pm 1.7 \text{ g}(1)/100 \text{g sln}$ and $\pm 1.4 \text{ g}(2)/100 \text{g sln}$ (compiler).
		REFERENCES:
f		

COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) Acetic acid (butyl acet [123-86-4]	butyl ester ate); C ₆ H ₁₂ O ₂ ;	Doolittle, A.K. Ind. End. Chem. <u>1935</u> , 27, 1169-79.
(2) Water; H ₂ O;	[7732-18-5]	
VARIABLES:		PREPARED BY:
T/K = 293		A. Skrzecz

The solubility of acetic acid butyl ester in water at 20°C was reported to be 0.43 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 6.7 x 10^{-4} .

The solubility of water in acetic acid butyl ester at 25°C was reported to be 1.86 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.109.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was not specified.	(1) Source not specified, commercial product; purity 90%, b.p. range 119-127°C, d ₄ ²⁰ 0.876.
	(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.2 g(1)/100g sln and ±0.9 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4] (2) Water; H₂O; [7732-18-5] 	Carbide and Carbon Chemicals Corporation, Solvent Chart. Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u> , 33, 1240-8,
VARIABLES: T/K = 297	1513. PREPARED BY: A. Skrzecz

The solubility of acetic acid butyl ester in water at 24°C was reported to be 0.68 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00106.

The solubility of water in acetic acid butyl ester at $24^{\circ}C$ was reported to be 1.2 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.073.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing was specified in the paper.	(1) Not specified.
	(2) Not specified.
	ESTIMATED ERROR:
	Soly. about ±0.06 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler).
	REFERENCES:

COMPONENTS

СОМРО	NENTS:	ORIGINAL MEASUREMENTS:
(1)	Acetic acid butyl ester (<i>butyl acetate</i>); C ₆ H ₁₂ O ₂ ; [123-86-4]	Othmer, D.F.; Bergen, W.S.; Shlechter, N.; Bruins, P.F. Ind. Eng. Chem. <u>1945</u> , 37, 890-4.
(2)	Water; H ₂ O; [7732-18-5]	
VARIA	BLES:	PREPARED BY:
Т/К	= 323	A. Skrzecz

The solubility of acetic acid butyl ester in water at 50° C was reported to be 0.69 g(1)/100g sln. The corresponding mole fraction, x_1 , value calculated by the compiler is 0.00108.

The solubility of water in acetic acid butyl ester at 50° C was reported to be 3.19 g(2)/100g sln. The corresponding mole fraction, x_2 , value calculated by the compiler is 0.1752.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was not described. Presumably the indirect or synthetic method reported by Othmer, White and Trueger (ref 1) was used. The solution was kept at the desired temperature using a constant temperature water bath. The data and method were reported together with the ternary system acetic acid butyl ester-water-2,3-butanediol (butyl acetate- water-2,3-butylene glycol).

SOURCE AND PURITY OF MATERIALS:

- Source not specified; carefully fractionated from commercial material; b.p. range 1°C.
- (2) Not specified.

ESTIMATED ERROR:

REFERENCES:

 Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4]</pre>	Donahue, D.J.; Bartell, F.E. J. Phys. Chem. <u>1952</u> , 56, 480-4.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES:	PREPARED BY:
T/K = 298	Z. Maczynska

The solubility of acetic acid butyl ester in water at $25^{\circ}C$ was reported to be $x_1 = 0.000995$. The corresponding mass per cent value calculated by the compiler is 0.638 g(1)/100 sln.

The solubility of water in acetic acid butyl ester at $25^{\circ}C$ was reported to be $x_2 = 0.0745$. The corresponding mass per cent value calculated by the compiler is 1.233 g(2)/100g sln.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The analytical method was used. Samples of (1) with (2) were placed in glass stoppered flasks and were shaken intermittently for at least three days in a water bath held at 25°C.The (1)-rich phases were ana- lyzed for (2) content by the Karl Fischer method and the (2)-rich phases were analyzed using inter- ferometery.	<pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; best reagent grade; purified by fractional distillation and treatment with silica gel; purity not specified. (2) Purified. ESTIMATED ERROR: Temp. ±0.1°C (authors). Soly. about ±0.03 g(1)/100g sln and ±0.2 g(2)/100g sln (compiler). REFERENCES:</pre>

200

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid butyl ester	Rao, J.R.; Rao, C.V.	
(butyl acetate); $C_6H_{12}O_2$;	J. Appl. Chem. <u>1957</u> , 7, 435-9.	
[123-00-4]		
(2) water; h ₂ 0; [//32-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid butyl ester in water at 30° C was reported to be 0.9 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0014. The solubility of water in acetic acid butyl ester at 30° C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2 , value calcu- lated by the compiler is 0.067.		
The fitzetion method was weed my	SOURCE AND PURITY OF MATERIALS:	
The titration method was used. The data were reported together with the ternary system acetic acid butyl ester-water-methanol.	(1) British brug house Ltd., reagent grade; b.p. 126.0°C, d^{30} 0.8710, n_D^{30} 1.3916. (2) Distilled; free from CO ₂ .	
	ESTIMATED ERROR:	
	Temp. $\pm 0.02^{\circ}$ C (authors). Soly. about ± 0.3 g(1)/100g sln and ± 0.05 g(2)/100g sln (compiler).	
	REFERENCES:	

ORIGINAL MEASUREMENTS: Bushmakin, I.N.; Lutugina, N.V. Vestn. Leningrad. Univ., Fiz., Khim. <u>1958</u> , (10), 75-83.	
Bushmakin, I.N.; Lutugina, N.V. Vestn. Leningrad. Univ., Fiz., Khim. <u>1958</u> , (10), 75-83.	
Vestn. Leningrad. Univ., Fiz., Khim. <u>1958</u> , (10), 75-83.	
PREPARED BY:	
A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid butyl ester in water at 91.04°C ^a was report ed to be $x_1 = 0.001$. The corresponding mass per cent value calculated by the compiler is 0.6 g(1)/100g sln. The solubility of water in acetic acid butyl ester at 91.04°C ^a was report ed to be $x_2 = 0.147$. The corresponding mass per cent value calculated by the compiler is 2.60 g(2)/100g sln. ^a Boiling temperature of the two-phase mixture at 760 mm Hg.	
INFORMATION	
SOURCE AND PURITY OF MATERIALS:	
 (1) Synthesized; several times distilled; b.p. 125.2°C, n_D²⁰ 1.3942. (2) Distilled. 	
ESTIMATED ERROR: Temp. ±0.1 ^o C, pressure ±0.1 mm Hg (authors). Soly. about ±0.2 g(1)/100g sln and ±0.4 g(2)/100g sln (compiler).	

OPICINAL MEASUREMENTS.	
Cristian MLABORIMENTS.	
Schuberth, H.; Leibhitz, E.	
J. Prakt. Chem. <u>1958</u> , 6, 31-45.	
PREPARED BY:	
A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid butyl ester in water at 44.4°C was reported to be 0.60 g(1)/100g sln with a corresponding mole fraction, x_1 , value of 0.0009. The solubility of water in acetic acid butyl ester at 44.4°C was reported to be 1.7 g(2)/100g sln with a corresponding mole fraction, x_2 , value of 0.100. The measurments were made at 760 mm Hg.	
INFORMATION	
SOURCE AND PURITY OF MATERIALS:	
 (1) Buna-Werke Merseburg, technical grade; dried over CuSO₄, twice distilled; without impurities by IR spectroscopy method, 0.03% water by the K. Fischer method, b.p. 126.1°C, d²⁰ 0.882, n_D²⁰ 1.3941. (2) Twice distilled; n_D^{44.4} 0.9904. ESTIMATED ERROR: Temp. ±0.05°C. Soly. ±0.0001 mole fraction. 	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Acetic acid butyl ester (butyl acetate); C₆H₁₂O₂; [123-86-4]</pre>	Schuberth, H. <i>J. Prakt. Chem.</i> <u>1958</u> , 6, 266-88.
(2) Water; H ₂ O; [7732-18-5]	
VARIABLES: T/K = 318	PREPARED BY: A. Skrzecz

The solubility of acetic acid butyl ester in water at 317.6 K was reported to be $x_1 = 0.0009$. The corresponding mass per cent value calculated by the compiler is 0.6 g(1)/100g sln.

The solubility of water in acetic acid butyl ester at 317.6 K was reported to be $x_2 = 0.0999$. The corresponding mass per cent value calculated by the compiler is 1.692 g(2)/100g sln.

Saturation lines in the range 317.6-341.7 K were described by equations: $x_2 = 5.21 \times 10^{-6} (T/K)^2 - 2.077 \times 10^{-3} (T/K) + 0.2340$ (1)-rich phase $x_2 = -8.6 \times 10^{-8} (T/K)^2 + 6.06 \times 10^{-5} (T/K) + 0.98851$ (2)-rich phase

AUXTLTARY	TNFORMATION
VOVIDIULI	THE OLGIULT TON

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method was used, as described by Schuberth and Leibnitz (ref 1). Water was analyzed by the Karl Fischer titration method and butyl acetate by saponification and titration up to neutralization.	 Source not specified, technical grade; dried, twice distilled; b.p. 126.1°C, d²⁰ 0.8815, n²⁰_D 1.3941, IR in agreement with literature. Twice distilled.
	ESTIMATED ERROR:
	Soly. about ±0.05 g(1)/100g sln and ±0.3 g(2)/100g sln (compiler).
	REFERENCES:
	 Schuberth, H.; Leibnitz, E. J. Prakt. Chem. <u>1958</u>, 6, 31.

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COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Acetic acid butyl ester	Rao, R.J.; Rao, C.V.	
(butyl acetate); C ₆ H ₁₂ O ₂ ; [123-86-4]	J. Appl. Chem. <u>1959</u> , 9, 69-73.	
(2) Water; H ₂ O; [7732-18-5]		
VARIABLES:	PREPARED BY:	
T/K = 303	A. Skrzecz	
EXPERIMENTAL VALUES: The solubility of acetic acid butyl ester in water at 30° C was reported to be 0.9 g(1)/100g sln. The corresponding mole fraction, x_1 , value calcu- lated by the compiler is 0.0014. The solubility of water in acetic acid butyl ester at 30° C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction, x_2 , value calcu- lated by the compiler is 0.067.		
AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	

Presumably the titration method described by Rao and Rao (ref 1) was used. The data were reported together with the ternary system acetic acid butyl ester-water-1-propanol.

SOURCE AND PURITY OF MATERIALS:

(1) British Drug House Ltd., analytical grade; b.p. 126.0°C, d^{30} 0.8710, n_D^{30} 1.3916.

(2) Distilled.

ESTIMATED ERROR:

Soly. about ±0.3 g(1)/100g sln and ±0.05 g(2)/100g sln (compiler).

REFERENCES:

1. Rao, R.J.; Rao, C.V. J. Appl. Chem. <u>1957</u>, 7, 435.

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| COMPONENTS:                                                                                                                                                                                                                           | ORIGINAL MEASUREMENTS:                                                                                                                                                                                                                   |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| (1) Acetic acid butyl ester                                                                                                                                                                                                           | Schuberth, H.                                                                                                                                                                                                                            |
| (butyl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[123-86-4]                                                                                                                                                        | Abh. Deut. Akad. Wiss. Berlin, Kl.<br>Chem. Geol. Biol. <u>1960</u> , 3, 1-82.                                                                                                                                                           |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                              |                                                                                                                                                                                                                                          |
| VARIABLES:                                                                                                                                                                                                                            | PREPARED BY:                                                                                                                                                                                                                             |
| T/K = 293 and 318                                                                                                                                                                                                                     | A. Skrzecz                                                                                                                                                                                                                               |
| EXPERIMENTAL VALUES:<br>Mutual solubility of acetic ad                                                                                                                                                                                | cid butyl ester and water                                                                                                                                                                                                                |
| t/°C g(1)/100g sln<br>(2)-rich phase (1)-rich phas                                                                                                                                                                                    | x <sub>1</sub> (compiler)<br>se (2)-rich phase (1)-rich phase                                                                                                                                                                            |
| 20.0 0.7 98.8                                                                                                                                                                                                                         | 0.0011 0.927                                                                                                                                                                                                                             |
| 44.4 0.59 98.3                                                                                                                                                                                                                        | 0.00092 0.900                                                                                                                                                                                                                            |
|                                                                                                                                                                                                                                       |                                                                                                                                                                                                                                          |
| AUXILIARY INFORMATION                                                                                                                                                                                                                 |                                                                                                                                                                                                                                          |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                           | SOURCE AND PURITY OF MATERIALS:                                                                                                                                                                                                          |
| Presumably the titration and ana-<br>lytical methods were used. The data<br>and method were reported with the<br>ternary system acetic acid butyl<br>ester-water-acetic acid propyl<br>ester (butyl acetate-water-propyl<br>acetate). | <ol> <li>Buna-Werke Merseburg, technical product; washed with H<sub>2</sub>O, dried over CuSO<sub>4</sub>, twice distilled; b.p. 126.2°C, d<sup>20</sup> 0.8818, n<sub>D</sub><sup>20</sup> 1.3941.</li> <li>Twice distilled.</li> </ol> |
|                                                                                                                                                                                                                                       | ESTIMATED ERROR:                                                                                                                                                                                                                         |
|                                                                                                                                                                                                                                       | Temp. ±0.01°C.                                                                                                                                                                                                                           |
|                                                                                                                                                                                                                                       | Soly. 10.05 g(1)/100g Sin.                                                                                                                                                                                                               |

| 2 | 6 | 4 |
|---|---|---|
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| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                               | ORIGINAL MEASUREMENTS:                                                                                                      |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|--|
| (1) Acetic acid butyl ester                                                                                                                                                                                                                                                                                                                                                                                                               | Rao, M.V.R.; Rao, K.S.; Rao, C.V.                                                                                           |  |
| (butyl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[123-86-4]                                                                                                                                                                                                                                                                                                                                                            | J. Sci. Ind. Res. <u>1961</u> , 20B,<br>379-81.                                                                             |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                                                                             |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                                | PREPARED BY:                                                                                                                |  |
| T/K = 308                                                                                                                                                                                                                                                                                                                                                                                                                                 | Z. Maczynska                                                                                                                |  |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid butyl ester in water at $35^{\circ}$ C was reported to<br>be 0.9 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calcu-<br>lated by the compiler is 0.0014.<br>The solubility of water in acetic acid butyl ester at $35^{\circ}$ C was reported to<br>be 2.0 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calcu-<br>lated by the compiler is 0.116. |                                                                                                                             |  |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                 | INFORMATION                                                                                                                 |  |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                                                                                                                                                                                                                               | SOURCE AND PURITY OF MATERIALS:                                                                                             |  |
| The titration method was used. The<br>data were reported together with<br>the ternary system acetic acid<br>butyl ester- water-formic acid. No<br>further details were reported in<br>the paper.                                                                                                                                                                                                                                          | <ul> <li>(1) Source not specified,<br/>technical grade;<br/>distilled; b.p. 126.5°C.</li> <li>(2) Not specified.</li> </ul> |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                           | ESTIMATED ERROR:<br>Soly. about ±0.3 g(1)/100g sln and<br>±0.9 g(2)/100g sln<br>(compiler).                                 |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                           | REFERENCES:                                                                                                                 |  |

| COMPONENTS:                                                                                                      | ORIGINAL MEASUREMENTS:                                                                             |
|------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|
| <pre>(1) Acetic acid butyl ester   (butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;   [123-86-4]</pre> | Narasimhan, K.S.; Reddy, C.C.;<br>Chari, K.S.<br><i>J. Chem. Eng. Data</i> <u>1962</u> , 7, 340-3. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                         |                                                                                                    |
| VARIABLES:                                                                                                       | PREPARED BY:                                                                                       |
| T/K = 303                                                                                                        | A. Skrzecz                                                                                         |
|                                                                                                                  |                                                                                                    |

The solubility of acetic acid butyl ester in water at  $30^{\circ}$ C was reported to be 0.29 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is  $4.5 \times 10^{-4}$ .

The solubility of water in acetic acid butyl ester at  $30^{\circ}$ C was reported to be 1.45 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.0866.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The titration and the analytical methods were used as reported for the ternary system butyl acetatewater-phenol. In the titration procedure, a known weight of mixture was taken in 100mL stoppered conical flask and kept in a thermostat for 1/2 h. which was found to be sufficient for equilibrium. Then, the selected component was added dropwise until a permanent turbidity appeared in the solution. In the analytical method, the mixture was stirred for 1 h. in a thermostated equilibrium apparatus. After separation the refractive indexes of both layers were measured and the corresponding compositions were obtained graphically from a previously drawn plot relating the refractive index and composition.

SOURCE AND PURITY OF MATERIALS:

- (1) Source not specified; commercial grade; twice-distilled; purity 98.25-98.56%, b.p. range  $124-126^{\circ}C$ ,  $d_{20}^{30}$  0.8714,  $n_{D}^{25}$  1.3890.
- (2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C. Soly. ±0.03 g(1)/100g sln.

**REFERENCES:** 

| 66                                                                                                                                                                                                                         |                                                                                                                                                                                                                 |                                                                                                                                                                    |                                                                                                                                                                          |                                                                                                                                                                                               |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| COMPONENTS:<br>(1) Acetic acid butyl ester<br>(butyl acetate); $C_6H_{12}O_2$ ;<br>[123-86-4]<br>(2) Water; $H_2O$ ; [7732-18-5]<br>VARIABLES:<br>T/K = 303 - 364<br>EXPERIMENTAL VALUES:<br>Mutual solubility of acetic a |                                                                                                                                                                                                                 |                                                                                                                                                                    | ORIGINAL MEASURE<br>Hirata, M.; Hir<br>Kagaku Kogaku<br>PREPARED BY:<br>A. Skrzecz                                                                                       | MENTS:<br>ose, Y.<br><u>1963</u> , 27(6), 407-14.                                                                                                                                             |
| $t/^{\circ}C$<br>(<br>30.0<br>90.7 <sup>a</sup><br>91.0 <sup>a</sup><br>91.3 <sup>a</sup><br>a Boil<br>the<br>The relat<br>were repo                                                                                       | g(1)/10<br>2)-rich phase<br>0.70 <sup>b</sup><br>-<br>1.61 <sup>d</sup><br>-<br>ing temperatur<br>pressure was r<br>ive densities<br>rted to be $d_4^{30}$                                                      | og sln<br>(1)-rich phas<br>98.87 <sup>c</sup><br>92.91 <sup>e</sup><br>-<br>93.2 <sup>e</sup><br>Te at atmosphe<br>not specified)<br>of the water-<br>0.9954 and d | $x_1$ (consection)<br>$x_1$ (consection)<br>$x_1$ (consection)<br>0.00109<br>-<br>0.00253<br>-<br>-<br>-<br>-<br>-<br>-<br>-<br>-                                        | mpiler)<br>e (1)-rich phase<br>0.9314<br>0.6702<br>-<br>0.6801<br>value of<br>e ester-rich phase<br>lively.                                                                                   |
|                                                                                                                                                                                                                            | <u>,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,</u>                                                                                                                                                                    | AUXILIARY 3                                                                                                                                                        | INFORMATION                                                                                                                                                              |                                                                                                                                                                                               |
| 1ETHOD/APPA<br>The titrat<br>Othmer (re<br>The mixtur<br>3-4 h. and<br>The temper<br>was used a<br>second com<br>tions to t<br>four-necke<br>ture of th.<br>measured a                                                     | RATUS/PROCEDUR<br>ion method as<br>f 1) was used<br>e was thermost<br>shaken each 1<br>ature titratic<br>t the boiling<br>ponent was add<br>he mixture pla<br>d flask and th<br>e boiling liqu<br>s proposed by | E:<br>proposed by<br>at 30°C.<br>ated for<br>5 min.<br>n method<br>point. The<br>led in por-<br>ced in a<br>le tempera-<br>id was<br>Ogawa                         | SOURCE AND PURITY<br>(1) Source not a<br>cial grade;<br>$d_4^{25}$ 0.8750,<br>(2) Not specific<br>$n_D^{25}$ 1.3325.<br>ESTIMATED ERROR:<br>Soly. about ±0.2<br>and ±4.6 | Y OF MATERIALS:<br>specified, commer-<br>used as received;<br>$n_D^{25}$ 1.3920.<br>ed; $d_4^{25}$ 0.9971,<br>1 <sup>b</sup> , ±0.05 <sup>c</sup> , ±0.8 <sup>d</sup><br>$a_4^{(1)}/100g$ sln |

## **REFERENCES:**

literature values because of

superheating. The method and data were reported together with the ternary system acetic acid butyl ester-water-acetic acid.

- 1. Othmer, D.F. et al. Ind. Eng. Chem. <u>1941</u>, 33, 1240.
- 2. Ogawa, S. Kagaku Kikai Gijyutsu 1954, (6), 22.

| COMPONENTS:                                                                                                      | ORIGINAL MEASUREMENTS:                                                                    |
|------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| <pre>(1) Acetic acid butyl ester   (butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;   [123-86-4]</pre> | Ramanarao, M.V.; Husain, A.;<br>Chari, K.S.<br>Indian J. Technol. <u>1964</u> , 2, 252-4. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                         |                                                                                           |
| VARIABLES:                                                                                                       | PREPARED BY:                                                                              |
| T/K = 303                                                                                                        | A. Skrzecz                                                                                |

The solubility of acetic acid butyl ester in water at  $30^{\circ}$ C was reported to be 0.9368 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.0014645.

The solubility of water in acetic acid butyl ester at  $30^{\circ}$ C was reported to be 1.8110 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.10629.

#### METHOD/APPARATUS/PROCEDURE:

The turbidity end point method described by Narasimhan, Reddy and Chari (ref 1) was used. Only the method for the ternary system was described. A known weight of mixture was placed into a 100 mL stoppered conical flask and kept in a thermostat for 1/2 h. which was found to be sufficient for equilibrium. Then, the selected component was added dropwise until a permanent turbidity appeared in the solution. SOURCE AND PURITY OF MATERIALS:

- Source not specified; twice distilled; b.p. 126.0°C.
- (2) Distilled.

## ESTIMATED ERROR:

#### **REFERENCES:**

 Narasimhan, K.S.; Reddy, C.C.; Chari, K.S. J. Chem. Eng. Data 1962, 7, 340.

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | ORIGINAL MEASUREMENTS:                                                                                                                                                                                                                                                                                                                                                                                     |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre>(1) Acetic acid butyl ester   (butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;   [123-86-4]</pre>                                                                                                                                                                                                                                                                                                                                                                                                             | Blank, M.G.; Popova, T.V.<br><i>Ukr. Khim. Zh. <u>1970</u>, 36,</i> 563-6.                                                                                                                                                                                                                                                                                                                                 |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                            |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | PREPARED BY:                                                                                                                                                                                                                                                                                                                                                                                               |
| T/K = 303                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | A. Skrzecz                                                                                                                                                                                                                                                                                                                                                                                                 |
| T/K = 303       A. Skrzecz         EXPERIMENTAL VALUES:       The solubility of water in acetic acid butyl ester at 30°C was report be $x_2 = 0.0637$ . The corresponding mass per cent value calculated by t compiler is 1.044 g(2)/100g sln.                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                            |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                |
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used.<br>The titrations were made from<br>burettes protected from moisture.<br>The volume proportions of (1)<br>and (2) were measured. The same<br>amounts of components were weighed<br>separately and the composition of<br>the solution was calculated.<br>Experiments were repeated several<br>times. The data were reported<br>together with the ternary system<br>acetic acid butyl ester-water-<br>ethanol. No further details were<br>reported in the paper. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified; washed with NaCl and Na<sub>2</sub>CO<sub>3</sub> solutions, dried with MgSO<sub>4</sub>, fractionated; b.p. 126.1°C, d<sup>20</sup><sub>4</sub> 0.8815, n<sup>20</sup><sub>0</sub> 1.3941. (2) Distilled three times (second distillation with KMnO<sub>4</sub> and KOH). ESTIMATED ERROR: Soly. &lt;±0.1 g(2)/100g sln. REFERENCES:</pre> |

| COMPONENTS:                                                                                                                                                                             | ORIGINAL MEASUREMENTS:                                                                |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| <ul> <li>(1) Acetic acid butyl ester</li> <li>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> <li>[123-86-4]</li> <li>(2) Water: H<sub>2</sub>O: [7732-18-5]</li> </ul> | Krupatkin, I.L.; Glagoleva, M.F.<br><i>Zh. Obshch. Khim.</i> <u>1970</u> , 40, 17-21. |
| VARIABLES:<br>T/K = 298                                                                                                                                                                 | PREPARED BY:<br>Z. Maczynska                                                          |

The solubility of acetic acid butyl ester in water at  $25^{\circ}$ C was reported to be 0.73 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.00114.

The solubility of water in acetic acid butyl ester at  $25^{\circ}C$  was reported to be 1.92 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.112.

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                 |                                                                                                                                                                         |  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used. The<br>data were reported together with<br>the ternary system acetic acid<br>butyl ester-water-2-furancarbonal<br>(butyl acetate- water-furfural). No<br>further details were reported in<br>the paper. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified,    analytical reagent;    b.p. 125°C, d<sup>15</sup> 0.8800. (2) Twice distilled. ESTIMATED ERROR:</pre> |  |
|                                                                                                                                                                                                                                                                       | Soly. about ±0.1 g(1)/100g sln and<br>±0.9 g(2)/100g sln<br>(compiler).<br>REFERENCES:                                                                                  |  |

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|                                                                                                                                                                                                                                                                                                                                                                                                                             | ······                                                                   |  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|--|
| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                 | ORIGINAL MEASUREMENTS:                                                   |  |
| (1) Acetic acid butyl ester                                                                                                                                                                                                                                                                                                                                                                                                 | Pop. A.; Weiss, G.; Cormos, L.                                           |  |
| (butyl acetate); $C_6H_{12}O_2$ ;                                                                                                                                                                                                                                                                                                                                                                                           | Stud. Univ. Babes-Bolyai, Ser.                                           |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             | chem. $1970$ , $15(2)$ , $77-82$ .                                       |  |
| (2) water; $H_20$ ; [7/32-18-5]                                                                                                                                                                                                                                                                                                                                                                                             |                                                                          |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                  | PREPARED BY:                                                             |  |
| T/K = 293                                                                                                                                                                                                                                                                                                                                                                                                                   | Z. Maczynska                                                             |  |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid butyl ester in water at 20°C was reported to<br>be 0.712 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calcu-<br>lated by the compiler is 0.00111.<br>The solubility of water in acetic acid butyl ester at 20°C was reported to<br>be 0.750 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calcu-<br>lated by the compiler is 0.0465. |                                                                          |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                          |  |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                   | INFORMATION                                                              |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                          |  |
| The titration method was used. The data were reported together with                                                                                                                                                                                                                                                                                                                                                         | <ul> <li>(1) Source not specified;</li> <li>99% purity.</li> </ul>       |  |
| the ternary system acetic acid<br>butyl ester-water-2-hydroxybenzoic<br>acid (butyl acetate-water-salicylic<br>acid). No further details were re-<br>ported in the paper.                                                                                                                                                                                                                                                   | (2) Distilled.                                                           |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             | ESTIMATED ERROR:                                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             | Soly. about ±0.07 g(1)/100g sln<br>and ±0.2 g(2)/100g sln<br>(compiler). |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                             | REFERENCES:                                                              |  |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ORIGINAL MEASUREMENTS:                                                                       |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------|--|
| <pre>(1) Acetic acid butyl ester<br/>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;<br/>[123-86-4]</pre>                                                                                                                                                                                                                                                                                                                                                                                                                                                          | Beregovykh, V.V.; Timofeev, V.S.;<br>Luk'yanova, R.N.; Yakushchev, V.<br>M.; Serafimov, L.A. |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | Uch. Zap., Mosk. Inst. Tonkoi Khim.<br>Tekhnol. <u>1971</u> , 1(3), 31-8.                    |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | PREPARED BY:                                                                                 |  |
| T/K = 364                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | A. Skrzecz                                                                                   |  |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid butyl ester in water at $91.04^{\circ}C^{a}$ was report-<br>ed to be $x_{1} = 0.017$ . The corresponding mass per cent value calculated by<br>the compiler is $10.0 \text{ g(1)}/100 \text{ g sln}$ .<br>The solubility of water in acetic acid butyl ester at $91.04^{\circ}C^{a}$ was report-<br>ed to be $x_{2} = 0.220$ . The corresponding mass per cent value calculated by<br>the compiler is $4.19 \text{ g(2)}/100 \text{ g sln}$ .<br><sup>a</sup> Boiling temperature of the two-phase mixture at 760 mm Hg. |                                                                                              |  |
| AUXILIARY J                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | INFORMATION                                                                                  |  |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | SOURCE AND PURITY OF MATERIALS:                                                              |  |
| The method was not specified.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | (1) Not specified.                                                                           |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | (2) Not specified.                                                                           |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | ESTIMATED ERROR:                                                                             |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Soly. about ±9.2 g(1)/100g sln and<br>±1.2 g(2)/100g sln<br>(compiler).                      |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | REFERENCES:                                                                                  |  |

| COMPONENTS:                                                                    | ORIGINAL MEASUREMENTS:                     |
|--------------------------------------------------------------------------------|--------------------------------------------|
| (1) Acetic acid butyl ester                                                    | Iguchi, A.; Fuse, K.                       |
| (buty1 acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[123-86-4] | Kagaku Kogaku <u>1971</u> , 35(9), 1035-7. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                       |                                            |
| VARIABLES:                                                                     | PREPARED BY:                               |
| T/K = 298                                                                      | A. Skrzecz                                 |

The solubility of acetic acid butyl ester in water at  $25^{\circ}$ C was reported to be 0.96 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.00150.

The solubility of water in acetic acid butyl ester at  $25^{\circ}$ C was reported to be 1.07 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.0652.

| AUXILIARY | INFORMATION |
|-----------|-------------|
|           | T A         |

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The samples were titrated with the second component to obtain turbidity. The method and data were reported together with the ternary system acetic acid butyl ester-wateracetic acid. No further details were reported in the paper. SOURCE AND PURITY OF MATERIALS:

 Source not specified, commercial grade of high purity, used as received.

(2) Not specified.

ESTIMATED ERROR:

```
Temp. ±0.1°C.
Soly. about ±0.3 g(1)/100g sln and
±0.05 g(2)/100g sln
(compiler).
```

**REFERENCES:** 

| COMPONENTS:                                                                                                     | ORIGINAL MEASUREMENTS:                                                            |
|-----------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| <pre>(1) Acetic acid butyl ester   (butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;  [123-86-4]</pre> | Krupatkin, I.L.; Shcherbakova, T.A.<br>Zh. Prikl. Khim. <u>1971</u> , 44, 307-11. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                        |                                                                                   |
| VARIABLES:                                                                                                      | PREPARED BY:                                                                      |
| T/K = 298                                                                                                       | A. Skrzecz                                                                        |

The solubility of acetic acid butyl ester in water at  $25^{\circ}$ C was reported to be 0.76 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.00119.

The solubility of water in acetic acid butyl ester at  $25^{\circ}C$  was reported to be 1.46 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.0872.

| AUXILIARY INFORMATION                                                                                                                                                                                                                          |                                                                                                                                                                                                      |  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used. The<br>amount of water in pure ester was<br>taken into account. The data were<br>reported together with the ternary<br>system acetic acid butyl ester-<br>water-phosphoric acid. | <ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Source not specified,<br/>analytical grade;<br/>b.p. range 125-126°C,<br/>d<sup>15</sup> 0.880-0.890.</li> <li>(2) Twice distilled.</li> </ul> |  |
|                                                                                                                                                                                                                                                | ESTIMATED ERROR:<br>Temp. ±0.1 <sup>o</sup> C (authors).<br>Soly. about ±0.15 g(1)/100g sln<br>and ±0.4 g(2)/100g sln<br>(compiler).<br>REFERENCES:                                                  |  |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                 | ORIGINAL MEASUREMENTS:                                                                                                                                                                                                                                                                                             |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre>(1) Acetic acid butyl ester<br/>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;<br/>[123-86-4]</pre>                                                                                                                                                                                                                                                                                                                        | Utkin, G.K.; Zamyatina, V.K.;<br>Andronnikov, N.V.; Golikov, L.V.<br>Gidroliz. Lesokhim. Prom. <u>1971</u> ,                                                                                                                                                                                                       |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                                    | 24(8), 9-10.                                                                                                                                                                                                                                                                                                       |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                                  | PREPARED BY:                                                                                                                                                                                                                                                                                                       |
| T/K = 298 and 313                                                                                                                                                                                                                                                                                                                                                                                                                           | A. Skrzecz                                                                                                                                                                                                                                                                                                         |
| EXPERIMENTAL VALUES:<br>Mutual solubility of acetic                                                                                                                                                                                                                                                                                                                                                                                         | acid butyl ester and water                                                                                                                                                                                                                                                                                         |
| t/°C g(1)/100g sln<br>(2)-rich phase (1)-rich phas                                                                                                                                                                                                                                                                                                                                                                                          | x <sub>1</sub> (compiler)<br>Se (2)-rich phase (1)-rich phase                                                                                                                                                                                                                                                      |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$                                                                                                                                                                                                                                                                                                                                                                                       | 0.0012 0.922<br>0.0009 0.911                                                                                                                                                                                                                                                                                       |
|                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                                                    |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                   | INFORMATION                                                                                                                                                                                                                                                                                                        |
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used. A<br>one-phase mixture was titrated and<br>mixed in a thermostated apparatus<br>with a reflux condenser for 1 h.<br>until an opalescence appeared. Only<br>the measurements for the ternary<br>systems were described. The data<br>were reported together with the<br>ternary system acetic acid butyl<br>ester-water-propanoic acid (butyl<br>acetate-water-propionic acid). | <ul> <li>SOURCE AND PURITY OF MATERIALS:</li> <li>(1) Source not specified, pure for analysis; distilled, fraction boiling at 125-126°C was used; purity 99.3-99.5%, dry residue 0.001%, without ashes, d<sup>20</sup> 0.875.</li> <li>(2) Distilled; without CO<sub>2</sub>.</li> <li>ESTIMATED ERROR:</li> </ul> |
|                                                                                                                                                                                                                                                                                                                                                                                                                                             | Soly. about ±0.2 <sup>a</sup> , ±0.05 <sup>b</sup> and<br>±0.3 <sup>c</sup> g(1)/100g sln<br>(compiler).<br>REFERENCES:                                                                                                                                                                                            |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                           | ORIGINAL MEASUREMENTS:                                                                                                                       |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|--|
| (1) Acetic acid butyl ester                                                                                                                                                                                                                                                                                                                           | Andreeva, N.G.; Komarova, L.F.;                                                                                                              |  |
| (butyl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;                                                                                                                                                                                                                                                                                      | Zh. Prikl. Khim. 1978. 51. 2031-6.                                                                                                           |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                              |                                                                                                                                              |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                            | PREPARED BY:                                                                                                                                 |  |
| T/K = 363                                                                                                                                                                                                                                                                                                                                             | A. Skrzecz                                                                                                                                   |  |
|                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                              |  |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid butyl ester in water at its boiling tempera-<br>ture at atmospheric pressure $(90.2^{\circ}C)^{a}$ was reported to be $x_{1} = 0.017$ . The<br>corresponding mass per cent value calculated by the compiler is<br>10.0 g(1)/100g sln.                                                           |                                                                                                                                              |  |
| The solubility of water in acetic acid butyl ester at its boiling tempera-<br>ture at atmospheric pressure $(90.2^{\circ}C)^{a}$ was reported to be $x_{2} = 0.022$ . The<br>corresponding mass per cent value calculated by the compiler is<br>0.35 g(2)/100g sln.                                                                                   |                                                                                                                                              |  |
| <sup>a</sup> Numerical value of the boiling temperature at atmospheric pressure<br>was not reported in the paper. The value 90.2°C was adopted<br>from Horsley (ref 1).                                                                                                                                                                               |                                                                                                                                              |  |
|                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                              |  |
|                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                              |  |
| METHOD/APPARATUS/PROCEDURE:<br>The titration method of Mozzhukhin,<br>Tyurikov and Mitropolskaya (ref 2)<br>was used. The data were reported<br>together with the ternary system<br>acetic acid butyl ester-water-<br>acetic acid 3-methyl-1-butanol<br>(butyl acetate-water-isopentyl<br>acetate). No further details were<br>reported in the paper. | SOURCE AND PURITY OF MATERIALS:                                                                                                              |  |
|                                                                                                                                                                                                                                                                                                                                                       | (1) Not specified.                                                                                                                           |  |
|                                                                                                                                                                                                                                                                                                                                                       | (2) Not specified.                                                                                                                           |  |
|                                                                                                                                                                                                                                                                                                                                                       | ESTIMATED ERROR:                                                                                                                             |  |
|                                                                                                                                                                                                                                                                                                                                                       | Soly. about ±9 g(1)/100g sln and<br>±2.7 g(2)/100g sln<br>(compiler).                                                                        |  |
|                                                                                                                                                                                                                                                                                                                                                       | REFERENCES:                                                                                                                                  |  |
|                                                                                                                                                                                                                                                                                                                                                       | 1. Horsley, L.E. Azeotrpic Data<br>III, Advances in Chemistry<br>Series 116, American Chemical<br>Society, Washington, <u>1973</u> .         |  |
|                                                                                                                                                                                                                                                                                                                                                       | <ol> <li>Mozzhukhin, A.S.; Tyurikov,<br/>I.D.; Mitropolskaya, V.A. in<br/>Fiz. Khim. Osn. Rektifikatsii,<br/>Moskva, <u>1970</u>.</li> </ol> |  |
|                                                                                                                                                                                                                                                                                                                                                       |                                                                                                                                              |  |
| COMPONENTS:                                                                                                                                                                   | ORIGINAL MEASUREMENTS:                                                                                                                       |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| <ul> <li>(1) Acetic acid butyl ester<br/>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;<br/>[123-86-4]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul> | <pre>Skrzecz, A. Pol. J. Chem. <u>1980</u>, 54, 1101-4. Skrzecz, A. Thesis, Inst. Phys. Chem., Pol. Acad. Sci., Warszawa, <u>1979</u>.</pre> |
| VARIABLES:<br>T/K = 291 - 362                                                                                                                                                 | PREPARED BY:<br>A. Skrzecz                                                                                                                   |

Mutual solubility of acetic acid butyl ester and water

| T/K   | <i>x</i> <sub>1</sub> |                      | g(1)/100g sln  |                |
|-------|-----------------------|----------------------|----------------|----------------|
|       | (2)-rich phase        | (1)-rich phase       | (2)-rich phase | (1)-rich phase |
| 290.8 |                       | .0.9388 <sup>a</sup> |                | 98.999         |
| 292.1 | 0.00101               | -                    | 0.648          | -              |
| 305.0 | -                     | 0.9269               | -              | 98.792         |
| 310.3 | 0.00088               | -                    | 0.565          | -              |
| 326.9 | -                     | 0.9072               | -              | 98.438         |
| 337.1 | -                     | 0.8922               | -              | 98.161         |
| 341.8 | 0.00088               | -                    | 0.565          | -              |
| 349.0 | -                     | 0.8658               | -              | 97.652         |
| 352.2 | 0.00101               | -                    | 0.648          | -              |
| 361.9 | -                     | 0.8412               | _              | 97.156         |

<sup>a</sup> By the Karl Fischer method.

```
Author's smoothing equations:
```

| $x_1$ | = | $1.3088 \times 10^{-3} - 1.90 \times 10^{-5} (T/K)$ | $-273.15) + 1.90 \times 10^{-7} (T/K - 273.15)^2$      |
|-------|---|-----------------------------------------------------|--------------------------------------------------------|
|       |   | st. dev. = $3.01 \times 10^{-5}$                    | (2)-rich phase                                         |
| x2    | = | $0.059761 - 1.010 \times 10^{-4} (T/K -$            | $273.15$ ) + $1.378 \times 10^{-5}$ $(T/K - 273.15)^2$ |
|       |   | st. dev. = $2.70 \times 10^{-3}$                    | (1)-rich phase                                         |

AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew and the analytical method were used. An ampoule with the solution of fixed concentration was placed into a glass tube connected with a thermostat filled completely with distilled water. The temperature of the bath was changed continuously during the measurements and the appearance and disappearance of turbidity within the ampoule was observed visually. For the analytical method, The amount of water in the saturated organic-phase was determined using a Karl Fischer titration procedure. The amount of water in the pure ester was taken into account.

#### SOURCE AND PURITY OF MATERIALS:

(1) POCH Gliwice, pure grade; distilled; purity 99.99% by glc, 0.19 wt% water by the Karl Fischer method.

(2) Distilled.

ESTIMATED ERROR:

Temp.  $\pm (0.2-0.6)^{\circ}C$ . Soly. see above.

**REFERENCES:** 

| COMPONENTS:                                                                                                                                                                             | ORIGINAL MEASUREMENTS:                                                                                            |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <ul> <li>(1) Acetic acid butyl ester</li> <li>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> <li>[123-86-4]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul> | Tewari, Y.B.; Miller, M.M.;<br>Wasik,S.P.; Martire, D.E.<br><i>J. Chem. Eng. Data</i> <u>1982</u> , 27,<br>451-4. |
| VARIABLES:<br>T/K = 298                                                                                                                                                                 | PREPARED BY:<br>A. Skrzecz                                                                                        |

The solubility of acetic acid butyl ester in water at  $25^{\circ}C$  was reported to be 0.0577 mol(1)/L sln. The corresponding value on a mass/volume basis calculated by the compiler is 6.70 g(1)/L sln.

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## METHOD/APPARATUS/PROCEDURE:

The analytical method was used. The aqueous phase was generated by pumping water into the inlet of a coated generator column which was thermostated, either by using a minipump or by means of a water reservoir using compressed air at 5 psi. The aqueous solution was extracted by the use of a known amount of immiscible-with-water solution and then analyzed by a gas chromatographic technique.

- (1) Source not specified; purity >99% by glc.
- (2) Not specified.

ESTIMATED ERROR:

Temp. ±0.1°C. Soly. ±1.0%.

REFERENCES:

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278
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| <b></b>                                                             |                                                 |  |
|---------------------------------------------------------------------|-------------------------------------------------|--|
| COMPONENTS:                                                         | ORIGINAL MEASUREMENTS:                          |  |
| (1) Acetic acid butyl ester                                         | Cho, TH.; Ochi, K.; Kojima, K.                  |  |
| (butyl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;    | Fluid Phase Equilib. <u>1983</u> , 11,          |  |
| [123-86-4]                                                          | 137-52.                                         |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                            |                                                 |  |
| VARIABLES:                                                          | PREPARED BY:                                    |  |
| T/K = 364                                                           | A. Skrzecz                                      |  |
|                                                                     |                                                 |  |
| EXPERIMENTAL VALUES:                                                |                                                 |  |
| The solubility of acetic acid butyl $($                             | ester in water at 363.89 K <sup>-</sup> was re- |  |
| by the compiler is $0.83 \text{ g(1)}/100\text{ g sl}$              | n.                                              |  |
| 2] CHC COMPTER 12 0100 9(1)/1009 21                                 |                                                 |  |
| The solubility of water in acetic ac                                | id butyl ester at 363.89 K <sup>a</sup> was re- |  |
| ported to be $x_2 = 0.1918$ . The corresp                           | oonding mass per cent value calculated          |  |
| by the compiler is 3.550 g(2)/100g s                                | ln.                                             |  |
| a Boiling townorsture at 101 22 kpc                                 |                                                 |  |
| boiling cemperature at 101.32 KPc                                   |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
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|                                                                     |                                                 |  |
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|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
| AUXILIARY                                                           | INFORMATION                                     |  |
| METHOD/APPARATUS/PROCEDURE:                                         | SOURCE AND PURITY OF MATERIALS:                 |  |
| The titration method was used.                                      | (1) Wako Pure Chem. Ind. Ltd.,                  |  |
| The liquid-liquid equilibrium at                                    | special grade; used as receiv-                  |  |
| directly in a modified ebulliometer                                 | ea; 99.99 wt% by giC,<br>b.p. 126.11°C.         |  |
| with a boiling flask of about<br>600 mL charge. The bubble-point of | (2) Not specified.                              |  |
| the homogenous solution was measur-                                 |                                                 |  |
| added until a cloudiness appeared.                                  | ESTIMATED EPROP.                                |  |
|                                                                     | Detinated Entor.                                |  |
|                                                                     | Temp. ±0.01°C.                                  |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     | REFERENCES:                                     |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |
|                                                                     |                                                 |  |

| COMPONENTS               | :                                                                                                               | ORIGINAL MEASUREMENTS:                                                            |
|--------------------------|-----------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| (1) Acet<br>(but<br>[123 | tic acid butyl ester<br>(yl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>(-86-4]                | Ouyang, F.; Wang, G.; Gao, W.<br>Hua Kung Hsueh Pao <u>1985</u> , (1),<br>110-18. |
| (2) Wate                 | er; H <sub>2</sub> O; [7732-18-5]                                                                               |                                                                                   |
| VARIABLES:               |                                                                                                                 | PREPARED BY:                                                                      |
| T/K = 323                | i de la companya de l | J. Fu                                                                             |

The proportion of acetic acid butyl ester in the water-rich phase at equilibrium at  $50^{\circ}$ C was reported to be 0.15 g(1)/100 g sln. The corresponding mole fraction solubility,  $x_1$ , is 0.0002.

The proportion of water in the acetic acid butyl ester-rich phase at equilibrium at  $50^{\circ}$ C was reported to be 1.91 g(2)/100g sln. The corresponding mole fraction solubility,  $x_2$ , is 0.1115.

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                             |  |  |  |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|--|
| METHOD/APPARATUS/PROCEDURE:<br>An analytical method was used. Sam-<br>ple mixtures in an equilibrium cell<br>immersed in a constant temperature<br>water bath were stirred with a mag-<br>netic agitator to be emulsified.<br>Then, the mixture was settled for<br>4 h. and samples withdrawn from the<br>upper and lower layers were analyz-<br>ed by gas chromatograph. | SOURCE AND PURITY OF MATERIALS:<br>(1) Analytical pure reagent.<br>(2) Twice distilled; b.p. 100.00°C.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |  |  |  |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ORIGINAL MEASUREMENTS:                                                                                                                                                                                                                                                                               |  |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| (1) Acetic acid butyl ester                                                                                                                                                                                                                                                                                                                                                                                                                                   | Richon, D.: Viallard, A.                                                                                                                                                                                                                                                                             |  |
| (butyl acetate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;                                                                                                                                                                                                                                                                                                                                                                                              | Fluid Phage Equilib 1995 21                                                                                                                                                                                                                                                                          |  |
| [123-86-4]                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 279–93.                                                                                                                                                                                                                                                                                              |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                                                                                                                                                                                      |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                                                    | PREPARED BY:                                                                                                                                                                                                                                                                                         |  |
| T/K = 298                                                                                                                                                                                                                                                                                                                                                                                                                                                     | A. Skrzecz                                                                                                                                                                                                                                                                                           |  |
| EXPERIMENTAL VALUES:<br>Mutual solubility of acetic                                                                                                                                                                                                                                                                                                                                                                                                           | acid butyl ester and water                                                                                                                                                                                                                                                                           |  |
| $\frac{1}{T/K} \mod (1) / x_1$                                                                                                                                                                                                                                                                                                                                                                                                                                | g(1)/100g sln (compiler)                                                                                                                                                                                                                                                                             |  |
| 100g(2) (2)-rich ph. (2)                                                                                                                                                                                                                                                                                                                                                                                                                                      | L)-rich ph. (2)-rich ph. (1)-rich ph.                                                                                                                                                                                                                                                                |  |
| $298.1^{a}$ - $9.95 \times 10^{-4}$                                                                                                                                                                                                                                                                                                                                                                                                                           | 0.928 0.638 <sup>d</sup> 98.81 <sup>e</sup>                                                                                                                                                                                                                                                          |  |
| 298.1 <sup>b</sup> 0.00570 10.26 x 10 <sup>-4 c</sup>                                                                                                                                                                                                                                                                                                                                                                                                         | - 0.658 <sup>d</sup> -                                                                                                                                                                                                                                                                               |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                      |  |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                                     | INFORMATION                                                                                                                                                                                                                                                                                          |  |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                                                                                                                                                                                                                                                   | SOURCE AND PURITY OF MATERIALS:                                                                                                                                                                                                                                                                      |  |
| The calorimetric and differential<br>refractometric methods were used.<br>The calorimetric method was de-<br>scribed by Richon (ref 1) and by<br>Richon and Villard (ref 2). For<br>the refractometric measurements,<br>a Phoenix model 1-2000T differen-<br>tial refractometer from Texas In-<br>struments was used, and the solu-<br>bility was determined from a char-<br>acteristic calibration curve as<br>described in the thesis of Richon<br>(ref 1). | <ul> <li>(1) Fluka (puriss); purified by<br/>preparation gas chromatographic<br/>method; purity &gt;99.5%, water<br/>content was negligible.</li> <li>(2) Distilled.</li> <li>ESTIMATED ERROR:</li> <li>Soly. about ±0.05<sup>d</sup> and ±0.15<sup>e</sup><br/>g(1)/100g sln (compiler).</li> </ul> |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                               | REFERENCES:                                                                                                                                                                                                                                                                                          |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 1. Richon, D. <i>Thesis</i> , University<br>de Clermont-Ferrand, <u>1974</u> .                                                                                                                                                                                                                       |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 2. Richon, D.; Villard, A. <i>Can. J.</i><br><i>Chem.</i> <u>1976</u> , 54, 2584.                                                                                                                                                                                                                    |  |

| COMPONENTS:                                                                                                                                                                  | ORIGINAL MEASUREMENTS:                                                              |  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|--|
| <ul> <li>(1) Acetic acid butyl ester</li> <li>(butyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> <li>[123-86-4]</li> <li>(2) Water: H-O: [7732-18-5]</li> </ul> | Stephenson, R.; Stuart, J.<br><i>J. Chem. Eng. Data</i> <u>1986</u> , 31,<br>56-70. |  |
| VARIABLES:<br>T/K = 273 - 364                                                                                                                                                | PREPARED BY:<br>Z. Maczynska                                                        |  |

Mutual solubility of acetic acid butyl ester and water

| t/°C | g(1)/100g sln  |                | x <sub>1</sub> (compiler) |                |
|------|----------------|----------------|---------------------------|----------------|
|      | (2)-rich phase | (1)-rich phase | (2)-rich phase            | (1)-rich phase |
| 0    | 0.96           | 99.22          | 0.00150                   | 0.9518         |
| 9.1  | 0.76           | 99.16          | 0.00119                   | 0.9482         |
| 19.7 | 0.64           | 99.02          | 0.00100                   | 0.9400         |
| 30.3 | 0.52           | 98.75          | 0.00081                   | 0.9245         |
| 39.6 | 0.50           | 98.65          | 0.00078                   | 0.9189         |
| 50.0 | 0.50           | 98.72          | 0.00078                   | 0.9228         |
| 60.2 | 0.50           | 98.62          | 0.00078                   | 0.9172         |
| 70.2 | 0.47           | 98.63          | 0.00073                   | 0.9178         |
| 80.1 | 0.48           | 98.56          | 0.00075                   | 0.9139         |
| 90.5 | 0.48           | 98.45          | 0.00075                   | 0.9078         |

| std. | dev. | 0.01 | 0.02 |
|------|------|------|------|
| Duu. | ac   | 0.01 | 0.00 |

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                    |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                                                                                                    |
| <pre>METHOD/APPARATUS/PROCEDURE:<br/>The analytical method was used.<br/>Component (1) was equilibrated<br/>with component (2) at a given<br/>temperature in a thermostat. Each<br/>layer was sampled with a syringe;<br/>(1) was determined by adding a<br/>weighed amount of acetonitrile<br/>(or sometimes propanol) to the<br/>organic layer sample and measuring<br/>by a Gow-Mac thermal conductivity<br/>gc the (1)/acetonitrile peak ratio<br/>(Chromosorb 101 packing and a HP<br/>3390 A recorder-integrator).<br/>A similar procedure but a higher<br/>boiling material (e.g. 1-hexanol)<br/>was used to determine (2) in the<br/>water layer.</pre> SOURCE AND PURITY OF MATERIALS:<br>(1) Source not specified, commer-<br>cial sample; purity 99%; used<br>as received.<br>(2) Not specified.<br>(2) Not specified.<br>(3) Source not specified.<br>(2) Not specified.<br>(3) Source not specified.<br>(2) Not specified.<br>(2) Not specified.<br>(3) Source not specified.<br>(2) Not specified.<br>(3) Source not specified.<br>(4) Source not specified.<br>(5) Source not specified.<br>(5) Source not specified.<br>(5) Source not specified.<br>(6) Source not specified.<br>(6) Source not specified.<br>(7) Source not specified.<br>(7) Source not specified.<br>(7) Source not specified.<br>(8) Source not specified.<br>(7) Source not specified.<br>(8) Source not specified.<br>(8) Source not specified.<br>(8) Source not specified.<br>(8) Source not specified.<br>(9) Sourc | METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used.<br>Component (1) was equilibrated<br>with component (2) at a given<br>temperature in a thermostat. Each<br>layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile<br>(or sometimes propanol) to the<br>organic layer sample and measuring<br>by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher<br>boiling material (e.g. 1-hexanol)<br>was used to determine (2) in the<br>water layer. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer-<br/>cial sample; purity 99%; used<br/>as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less,<br/>for solubility, see above. REFERENCES:</pre> |

| 2 | o | 2 |
|---|---|---|
| Z | o | Z |

| COMPONENTS:                         |                                                         | ORIGINAL MEASUREMENTS:        |                                                   |                                        |
|-------------------------------------|---------------------------------------------------------|-------------------------------|---------------------------------------------------|----------------------------------------|
| (1) Acet                            | ic acid 1,1-dim                                         | ethyl ethyl                   | Stephenson, R.; Stuart, J.                        |                                        |
| este                                | er (tert-butyl a                                        | cetate);                      | J. Chem. Eng. Dat                                 | a <u>1986</u> , 31,                    |
| C <sub>6</sub> H <sub>1</sub>       | 2 <sup>0</sup> 2; [540-88-5]                            |                               | 56-70.                                            |                                        |
| (2) Wate                            | er; H <sub>2</sub> O; [7732-1                           | 8-5]                          |                                                   |                                        |
| VARIABLES:                          |                                                         |                               | PREPARED BY:                                      |                                        |
| T/K = 273 - 361                     |                                                         | Z. Maczynska                  |                                                   |                                        |
| EXPERIMENTAL VALUES:                |                                                         | 1                             |                                                   |                                        |
| Mutual                              | solubility of a                                         | cetic acid 1,                 | 1-dimethyl ethyl es                               | ster and water                         |
| t/°C                                | g(1)/10                                                 | 0g sln                        | $x_1$ (comp                                       | iler)                                  |
|                                     | (2)-rich phase                                          | (1)-rich phas                 | e (2)-rich phase                                  | (1)-rich phase                         |
| 0                                   | 1.170                                                   | 99.17                         | 0.001832                                          | 0.9488                                 |
| 9.2                                 | 1.000                                                   | 99.03                         | 0.001564                                          | 0.9406                                 |
| 19.2                                | 0.803                                                   | 98.87                         | 0.001253                                          | 0.9313                                 |
| 29.6                                | 0.703                                                   | 98.70                         | 0.001096                                          | 0.9217                                 |
| 40.0                                | 0.620                                                   | 98.68                         | 0.000966                                          | 0.9206                                 |
| 50.0                                | 0.573                                                   | 98.65                         | 0.000893                                          | 0.9189                                 |
| 60.5                                | 0.526                                                   | 98.53                         | 0.000819                                          | 0.9122                                 |
| 70.5                                | 0.538                                                   | 98.29                         | 0.000838                                          | 0.8991                                 |
| 80.5                                | 0.499                                                   | 98.31                         | 0.000777                                          | 0.9002                                 |
| 88.0                                | -                                                       | 98.34                         | -                                                 | 0.9018                                 |
| std. de                             | ev. 0.004                                               | 0.02                          | • • • • • • • • • • • • • • • • • • •             | ······································ |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         | AUXILIARY                     | INFORMATION                                       | ·····                                  |
| METHODIAD                           | ADATIIS / DDOCEDII                                      | ۲۰                            | SOURCE AND DURTTY                                 | OF MARFDIALS.                          |
|                                     | ANATOS/FROCEDOR                                         |                               | SOURCE AND PURITY OF MATERIALS:                   |                                        |
| Component<br>with comp              | cical method wa<br>(1) was equili<br>ponent (2) at a    | s used.<br>brated<br>given    | (1) Source not sp<br>cial sample;<br>as received. | eclifed, commer-<br>purity 99%; used   |
| layer was<br>(1) was d<br>weighed a | s sampled with a<br>letermined by ac<br>mount of acetor | syringe;<br>ding a<br>ditrile | (2) Not specified                                 |                                        |
| (or somet                           | imes propanol)                                          | to the                        |                                                   |                                        |
| by a Gow-                           | Mac thermal cor                                         | ductivity                     | ESTIMATED ERROR:                                  |                                        |
| gc the (1)/acetonitrile peak ratio  |                                                         | Accuracy of metho             | d 0.1 wt% or less,                                |                                        |
| 3390 A re                           | corder-integrat                                         | or).                          | for solubility, s                                 | ee above.                              |
| A similar<br>boiling m              | procedure but<br>aterial (e.g. 1                        | a higher<br>-hexanol)         |                                                   |                                        |
| was used                            | to determine (2                                         | ) in the                      | l                                                 | ···· -                                 |
| water lay                           | er.                                                     |                               | REFERENCES:                                       |                                        |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         |                               |                                                   |                                        |
|                                     |                                                         |                               |                                                   |                                        |

| COMPONENTS: |                                                            | EVALUATOR:                          |
|-------------|------------------------------------------------------------|-------------------------------------|
| (1)         | Acetic acid 1-methylpropyl                                 | G.T. Hefter, School of Mathematical |
|             | ester (sec-buty1 acetate);                                 | and Physical Sciences,              |
|             | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [105-46-4] | Murdoch University, Perth, W.A.,    |
| (2)         | Water: $H_{2}0$ : [7732-18-5]                              | Australia                           |
| (-)         |                                                            | Januarv. 1989                       |

#### CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 1-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

| TABLE 1:    | Quantitative   | Solubility | Studies | of the     |
|-------------|----------------|------------|---------|------------|
| Acetic acid | 1-methylpropyl | ester (1)  | - Water | (2) System |
|             |                |            |         | _          |

| Reference                     | T/K     | Solubility | Method      |
|-------------------------------|---------|------------|-------------|
| Park and Hopkins (ref 1)      | 298     | (1) in (2) | unspecified |
| Doolittle (ref 2)             | 293     | mutual     | unspecified |
| Stephenson and Stuart (ref 3) | 273-364 | mutual     | GLC         |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

## 1. SOLUBILITY OF ACETIC ACID 1-METHYLPROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 1-methylpropyl ester (1) in water (2) are summarized in Table 2 with the exception of the approximate value of Park and Hopkins (ref 1) which is reported in v/v units and is therefore excluded from consideration. At 293 K, the only temperature where comparison is possible, the datum of Doolittle (ref 2) is only in fair agreement with the interpolated value of Stephenson and Stuart (ref 3). Consequently, in the absence of confirmatory studies, all the available data must be regarded as Tentative. For uniformity, the rounded data of Stephenson and Stuart (ref 3) have been chosen as the "Best" values.

| COMPONENTS:                                                                                                                                                                                       | EVALUATOR:                                                                                                                      |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| <ul> <li>(1) Acetic acid 1-methylpropyl<br/>ester (<i>sec-butyl acetate</i>);<br/>C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [105-46-4]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul> | G.T. Hefter, School of Mathematical<br>and Physical Sciences,<br>Murdoch University, Perth, W.A.,<br>Australia<br>January, 1989 |

## TABLE 2: Tentative Solubilities of Acetic acid 1-methylpropyl ester (1) in Water (2)

| T/K | Solubilit                               | ies                        |               |
|-----|-----------------------------------------|----------------------------|---------------|
|     | Reported values                         | "Best" values <sup>a</sup> |               |
|     | g(1)/100g sln                           | g(1)/100g sln              | $10^{3}x_{1}$ |
| 273 | 1.33 (ref 3)                            | 1.3                        | 2.1           |
| 283 | 0.88 <sup>*</sup> (ref 3)               | 0.9                        | 1.4           |
| 293 | 0.62 (ref 2), 0.86 <sup>*</sup> (ref 3) | 0.9                        | 1.4           |
| 298 | 0.82 <sup>*</sup> (ref 3)               | 0.8                        | 1.1           |
| 303 | 0.77 <sup>*</sup> (ref 3)               | 0.8                        | 1.1           |
| 313 | 0.66 <sup>*</sup> (ref 3)               | 0.7                        | 1.0           |
| 323 | 0.63 (ref 3)                            | 0.6                        | 1.0           |
| 333 | 0.61 <sup>*</sup> (ref 3)               | 0.6                        | 0.9           |
| 343 | 0.61 <sup>*</sup> (ref 3)               | 0.6                        | 0.9           |
| 353 | 0.61 <sup>*</sup> (ref 3)               | 0.6                        | 0.9           |
| 363 | 0.60 <sup>*</sup> (ref 3)               | 0.6                        | 0.9           |

<sup>a</sup> Rounded values of ref 3, see text.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 1-METHYLPROPYL ESTER (1)

As for the solubility of (1) in (2), the only data available for comparison of the solubilities of water (2) in acetic acid 1-methylpropyl ester (1) are those of Doolittle (ref 2) and Stephenson and Stuart (ref 3) at 293 K. However, unlike the  $H_2O$ -rich phase the datum of 1.65 g(2)/100 g sln reported by Doolittle is considerably higher than the value of 1.10 g(2)/100 g sln interpolated from the data of Stephenson and Stuart. In the absence of confirmatory studies it is not possible to choose between these data although it may be noted that the solubilities of Doolittle (ref 2) are often higher than reliable values for other systems. The interested user is referred to the Data Sheet for Stephenson and Stuart (ref 3) for what appear to be the most reliable experimental values available for the solubility of water in acetic acid 1-methylpropyl ester.

REFERENCES

1. Park, J. G.; Hopkins, M. B. Ind. Eng. Chem. <u>1930</u>, 22, 826-30.

- 2. Doolittle, A. K. Ind. Eng. Chem. <u>1935</u>, 27, 1169-79.
- 3. Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u>, 31, 56-70.

| <pre>COMPONENTS:<br/>(1) Acetic acid 1-methylpropyl<br/>ester (sec-butyl acetate);<br/>C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [105-46-4]<br/>(2) Water; H<sub>2</sub>O; [7732-18-5]<br/>VARIABLES:<br/>T/K = 298<br/>EXPERIMENTAL VALUES:<br/>The solubility of acetic acid 1-methy<br/>reported to be 1.0 mL(1)/100mL(2).</pre> | ORIGINAL MEASUREMENTS:<br>Park, J.G.; Hopkins, M.B.<br>Ind. Eng. Chem. <u>1930</u> , 22, 826-30.<br>PREPARED BY:<br>A. Skrzecz<br>/lpropyl ester in water at 25°C was |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|                                                                                                                                                                                                                                                                                                                                     |                                                                                                                                                                       |
| AUXILIARY                                                                                                                                                                                                                                                                                                                           | INFORMATION                                                                                                                                                           |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                                                                                                                         | SOURCE AND PURITY OF MATERIALS:                                                                                                                                       |
| The method was not specified.                                                                                                                                                                                                                                                                                                       | <ul> <li>(1) Source not specified, commer-<br/>cial samples; used as received;<br/>85-88% of ester,<br/>b.p. range 107-114°C.</li> <li>(2) Not specified.</li> </ul>  |
|                                                                                                                                                                                                                                                                                                                                     | ESTIMATED ERROR:                                                                                                                                                      |
|                                                                                                                                                                                                                                                                                                                                     | Not specified.                                                                                                                                                        |
|                                                                                                                                                                                                                                                                                                                                     | REFERENCES:                                                                                                                                                           |

| COMPONENTS:                                                                                                                                                                                                                                             | ORIGINAL MEASUREMENTS:                                                                                                                                                                                            |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <pre>(1) Acetic acid 1-methylpropyl     ester (sec-butyl acetate);     C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [105-46-4]</pre>                                                                                                                       | Doolittle, A.K.<br>Ind. End. Chem. <u>1935</u> , 27, 1169-79.                                                                                                                                                     |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                |                                                                                                                                                                                                                   |
| VARIABLES:                                                                                                                                                                                                                                              | PREPARED BY:                                                                                                                                                                                                      |
| T/K = 293                                                                                                                                                                                                                                               | A. Skrzecz                                                                                                                                                                                                        |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic                                                                             | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was                                                          |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic<br>reported to be 1.65 g(2)/100g sln.<br>value calculated by the compiler i | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was<br>The corresponding mole fraction, $x_2$ ,<br>s 0.0976. |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic<br>reported to be 1.65 g(2)/100g sln.<br>value calculated by the compiler i | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was<br>The corresponding mole fraction, $x_2$ ,<br>s 0.0976. |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic<br>reported to be 1.65 g(2)/100g sln.<br>value calculated by the compiler i | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was<br>The corresponding mole fraction, $x_2$ ,<br>s 0.0976. |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic<br>reported to be 1.65 g(2)/100g sln.<br>value calculated by the compiler i | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was<br>The corresponding mole fraction, $x_2$ ,<br>s 0.0976. |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 1-me<br>reported to be 0.62 g(1)/100g sln.<br>value calculated by the compiler i<br>The solubility of water in acetic<br>reported to be 1.65 g(2)/100g sln.<br>value calculated by the compiler i | thylpropyl ester in water at 20°C was<br>The corresponding mole fraction, $x_1$ ,<br>s 9.7 x 10 <sup>-4</sup> .<br>acid 1-methylpropyl ester at 20°C was<br>The corresponding mole fraction, $x_2$ ,<br>s 0.0976. |

# AUXILIARY INFORMATION

| METHOD/APPARATUS/PROCEDURE:   | SOURCE AND PURITY OF MATERIALS:                                                                                                      |
|-------------------------------|--------------------------------------------------------------------------------------------------------------------------------------|
| The method was not specified. | <pre>(1) Source not specified,<br/>commercial product; purity 82%,<br/>b.p. range 105-127°C, d<sub>4</sub><sup>20</sup> 0.858.</pre> |
|                               | (2) Not specified.                                                                                                                   |
|                               |                                                                                                                                      |
|                               | ESTIMATED ERROR:                                                                                                                     |
|                               | Not specified.                                                                                                                       |
|                               |                                                                                                                                      |
|                               |                                                                                                                                      |
|                               | REFERENCES:                                                                                                                          |
|                               |                                                                                                                                      |
|                               |                                                                                                                                      |
|                               |                                                                                                                                      |
|                               |                                                                                                                                      |

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                |                  |                                                                    |                                 |                  | 28.  |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------|------------------|--------------------------------------------------------------------|---------------------------------|------------------|------|
| COMPONEN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | TS:                            |                  | ORI                                                                | GINAL MEASUREM                  | ENTS:            |      |
| (1) Acetic acid 1-methylpropyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                | st               | ephenson, R.;                                                      | Stuart, J.                      |                  |      |
| ester (sec-butyl acetate);                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                |                  | Chem. Eng. Da                                                      | ta 1986.3                       | 1.               |      |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [105-46-4]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                |                  | 56-70.                                                             | <u></u> , ,                     | - /              |      |
| (2) Wa                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | ter; H <sub>2</sub> O; [7732-1 | 8-5]             |                                                                    |                                 |                  |      |
| VARIABLE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | S:                             |                  | PRE                                                                | PARED BY:                       |                  |      |
| T/K = 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 73 - 364                       |                  | z.                                                                 | Maczynska                       |                  |      |
| EXPERIME                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | NTAL VALUES:                   |                  | L                                                                  |                                 |                  |      |
| Mut                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | ual solubility of              | f acetic acid    | 1-me                                                               | thylpropyl est                  | er and wate      | er   |
| t/°C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | g(1)/10                        | 0g sln           |                                                                    | $x_1$ (comp                     | piler)           |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | (2)-rich phase                 | (1)-rich phas    | se                                                                 | (2)-rich phase                  | (1)-rich p       | hase |
| 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1.330                          | 99.17            |                                                                    | 0.002086                        | 0.9488           | 1    |
| 9.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 0.879                          | 99.05            |                                                                    | 0.001373                        | 0.9417           | ,    |
| 19.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.869                          | 98.94            |                                                                    | 0.001357                        | 0.9353           |      |
| 29.7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.753                          | 98.70            |                                                                    | 0.001175                        | 0.9217           | ,    |
| 39.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.663                          | 98.64            |                                                                    | 0.001034                        | 0.9183           |      |
| 50.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.629                          | 98.54            |                                                                    | 0.000981                        | 0.9128           |      |
| 60.1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.613                          | 98.40            |                                                                    | 0.000955                        | 0.9051           |      |
| 70.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.605                          | 98.38            |                                                                    | 0.000943                        | 0.9040           | 1    |
| 80.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.622                          | 98.16            |                                                                    | 0.000969                        | 0.8921           |      |
| 90.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | 0.604                          | 98.31            |                                                                    | 0.000941                        | 0.9002           |      |
| std. d                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | dev. 0.005                     | 0.01             |                                                                    |                                 |                  |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                | ΔΠΥΤΓΤΑΡΥ        |                                                                    |                                 |                  |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                | KUNILIARI J      |                                                                    |                                 |                  |      |
| METHOD/AI                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | PPARATUS/PROCEDUF              | æ:               | SOU                                                                | RCE AND PURITY                  | OF MATERIA       | LS:  |
| The analytical method was used.<br>Component (1) was equilibrated<br>with component (2) at a given<br>temperature in a thermostat. Each<br>layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile<br>(or sometimes propanol) to the<br>organic layer sample and measuring<br>by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher<br>boiling material (e.g. 1-hexanol) |                                | (1               | ) Source not sp<br>cial sample;<br>as received.<br>) Not specified | pecified, c<br>purity 99%<br>1. | ommer-<br>; used |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                | ESTIMATED ERROR: |                                                                    |                                 |                  |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                | Ac<br>fo         | curacy of metho<br>r solubility, s                                 | od 0.1 wt%<br>see above.        | or less,         |      |
| was usec<br>water la                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | a to determine (2<br>ayer.     | , in the         | REF                                                                | ERENCES:                        |                  |      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                |                  |                                                                    |                                 |                  |      |

| COMPC | DNENTS:                                                    | EVALUATOR:                          |
|-------|------------------------------------------------------------|-------------------------------------|
| (1)   | Acetic acid 2-methylpropyl                                 | G.T. Hefter, School of Mathematical |
|       | ester (isobutyl acetate);                                  | and Physical Sciences,              |
|       | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0] | Murdoch University, Perth, W.A.,    |
| (2)   | Water: H <sub>2</sub> O: [7732-18-5]                       | Australia                           |
| (2)   |                                                            | January, 1989                       |

### CRITICAL EVALUATION:

Quantitative solubility data for the acetic acid 2-methylpropyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Acetic acid 2-methylpropyl ester (1) - Water (2) System

| Reference                         | T/K     | Solubility | Method                     |
|-----------------------------------|---------|------------|----------------------------|
| Traube (ref 1)                    | 295     | (1) in (2) | unspecified                |
| Hemptinne (ref 2)                 | 298     | (1) in (2) | analytical                 |
| Fuehner (ref 3)                   | 293     | (1) in (2) | titration                  |
| Doolittle (ref 4)                 | 293     | mutual     | unspecified                |
| Frolov et al. (ref 5)             | 293     | mutual     | titration                  |
| Linek (ref 6)                     | 288-420 | mutual     | synthetic                  |
| Heyberger et al. (ref 7)          | 298,323 | mutual     | titration                  |
| Bomshtein et al. (ref 8)          | 293-353 | mutual     | analytical                 |
| Skrzecz (ref 9)                   | 291-360 | mutual     | synthetic,<br>Karl Fischer |
| Richon and Viallard (ref 10)      | 298     | (1) in (2) | refractometric             |
| Stephenson and Stuart<br>(ref 11) | 273-363 | mutual     | GLC                        |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF ACETIC ACID 2-METHYLPROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of acetic acid 2-methylpropyl ester (1) in water (2) are summarized in Table 2, with the following exceptions.

The datum of Heyberger et al. (ref 7) at 298K is lower than other studies and is rejected. The data of Bomshtein et al. (ref 8) over a wide temperature range are higher than other studies (ref 6,9,11) especially at lower temperatures (T < 343K) and show a quite different temperature dependence so are rejected. The data of Stephenson and Stuart (ref 11) at higher temperatures are rather scattered and appear lower than the other (continued next page)

| COMPONENTS: |                                                                  | EVALUATOR:                                                 |
|-------------|------------------------------------------------------------------|------------------------------------------------------------|
| (1)         | Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl acetate</i> ); | G.T. Hefter, School of Mathematical and Physical Sciences, |
|             | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0]       | Murdoch University, Perth, W.A.,                           |
| (2)         | Water; H <sub>2</sub> O; [7732-18-5]                             | Australia<br>January, 1989                                 |

studies (ref 6,9) but have been retained pending further independent investigations. The approximate value of Traube (ref 1) has, however, been excluded from consideration in view of the ready availability of more recent and precise data. Selected data are plotted in Figure 1.

TABLE 2:Tentative Solubilitiesof Acetic acid 2-methylpropyl ester (1) in Water (2)

| T/K | Solubilities                                                                                                           |                                  |                                |
|-----|------------------------------------------------------------------------------------------------------------------------|----------------------------------|--------------------------------|
|     | Reported values                                                                                                        | "Best" values (± $\sigma_{ m n}$ | ) <sup>a</sup>                 |
|     | g(1)/100g sln                                                                                                          | g(1)/100g sln                    | 10 <sup>3</sup> x <sub>1</sub> |
| 273 | 1.026 (ref 11)                                                                                                         | 1.03                             | 1.61                           |
| 283 | 0.827 (ref 11)                                                                                                         | 0.83                             | 1.29                           |
| 293 | 0.67 (ref 3), 0.67 (ref 4),<br>0.80 (ref 5),<br>0.765* (ref 6), 0.706 <sup>*</sup> (ref 9),<br>0.67* (ref 11)          | 0.71 ± 0.05                      | 1.11                           |
| 298 | 0.63 (ref 2). 0.740 <sup>*</sup> (ref 6),<br>0.668 <sup>*</sup> (ref 9), 0.693 (ref 10),<br>0.63 <sup>*</sup> (ref 11) | 0.67 ± 0.04                      | 1.04                           |
| 303 | 0.710 <sup>*</sup> (ref 6), 0.635 <sup>*</sup> (ref 9)<br>0.60 <sup>*</sup> (ref 11)                                   | 0.65 ± 0.05                      | 1.01                           |
| 313 | 0.695 <sup>*</sup> (ref 6), 0.587 <sup>*</sup> (ref 9),<br>0.53 <sup>*</sup> (ref 11)                                  | 0.60 ± 0.07                      | 0.94                           |
| 323 | 0.670 (ref 7), 0.695 <sup>*</sup> (ref 6),<br>0.567 <sup>*</sup> (ref 9), 0.51 <sup>*</sup> (ref 11)                   | 0.61 ± 0.08                      | 0.95                           |
| 333 | 0.702 <sup>*</sup> (ref 6), 0.58 <sup>*</sup> (ref 9),<br>0.51 <sup>*</sup> (ref 11)                                   | 0.60 ± 0.08                      | 0.94                           |
| 343 | 0.730 <sup>*</sup> (ref 6), 0.628 <sup>*</sup> (ref 9),<br>0.53 <sup>*</sup> (ref 11)                                  | 0.63 ± 0.08                      | 0,98                           |
| 353 | 0.780 <sup>*</sup> (ref 6), 0.718 <sup>*</sup> (ref 9),<br>0.55 <sup>*</sup> (ref 11)                                  | 0.68 ± 0.10                      | 1.06                           |
| 363 | 0.830 <sup>*</sup> (ref 6), 0.851 <sup>*</sup> (ref 9)                                                                 | $0.84 \pm 0.01^{b}$              | 1.31                           |
| 373 | 0.890 <sup>*</sup> (ref 6)                                                                                             | 0.89                             | 1.39                           |
| 393 | 1.030 <sup>*</sup> (ref 6)                                                                                             | 1.03                             | 1.61                           |
| 413 | 1.160* (ref 6)                                                                                                         | 1.16                             | 1.82                           |

<sup>a</sup> Obtained by averaging where appropriate.

<sup>b</sup> Tentative, see text.

| COMPONENTS: |                                                            | EVALUATOR:                          |
|-------------|------------------------------------------------------------|-------------------------------------|
| (1)         | Acetic acid 2-methylpropyl                                 | G.T. Hefter, School of Mathematical |
|             | <pre>ester (isobutyl acetate);</pre>                       | and Physical Sciences,              |
|             | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0] | Murdoch University, Perth, W.A.,    |
| (2)         | Water: H_O: [7732-18-5]                                    | Australia                           |
| (-)         |                                                            | January, 1989                       |

In Table 2,  $\sigma_n$  has no statistical significance. Mole fraction solubilities ( $x_2$ ) have the same status and (relative) percentage uncertainties as the mass % solubilities.



FIGURE 1. Selected data for the solubility of acetic acid 2-methylpropyl ester (1) in water (2): ref 6 ( $\bullet$ ); ref 8, rejected data, (O); ref 9 (X); ref 11 ( $\Box$ ). Solid line is a least square polynomial fitted to the "Best" values from Table 2.

2. SOLUBILITY OF WATER (2) IN ACETIC ACID 2-METHYLPROPYL ESTER (1)

All the available data for the solubility of water (2) in acetic acid 2-methylpropyl ester (1) are summarized in Table 3 with the following exceptions. The data of Doolittle (ref 4), Frolov *et al.* (ref 5) and Heyberger *et al.* (ref 6) at various temperatures are substantially higher than other studies and are rejected. The data of Bomshtein *et al.* (ref 8), as for the water-rich phase, are higher than other studies (ref 6,9,11) and are also rejected. The data of Stephenson and Stuart (ref 11) are somewhat lower than other studies (ref 6,9) at higher temperatures (T >323K) but, pending further independent investigations, have been retained. Selected data are plotted in Figure 2.

| СОМРС | DNENTS:                                                          | EVALUATOR:                                                 |
|-------|------------------------------------------------------------------|------------------------------------------------------------|
| (1)   | Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl acetate</i> ); | G.T. Hefter, School of Mathematical and Physical Sciences, |
|       | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0]       | Murdoch University, Perth, W.A.,                           |
| (2)   | Water: H_O: [7732-18-5]                                          | Australia                                                  |
|       |                                                                  | January, 1989 •                                            |

## TABLE 3: Recommended (R) and Tentative Solubilities of Water (2) in Acetic acid 2-methylpropyl ester (1)

| T/K | Solubilities                                                                        |                                  |  |
|-----|-------------------------------------------------------------------------------------|----------------------------------|--|
|     | Reported values                                                                     | "Best" values $(\pm \sigma_n)^a$ |  |
|     | g(2)/100g sln                                                                       | $g(2)/100g \ sln$ $10^2 x_2$     |  |
| 273 | 0.72 (ref 11)                                                                       | 0.72 4.5                         |  |
| 283 | 0.82 (ref 11)                                                                       | 0.82 5.1                         |  |
| 293 | 1.03 <sup>*</sup> (ref 9), 0.95 <sup>*</sup> (ref 11)                               | 0.99 ± 0.04 (R) 6.1              |  |
| 298 | 1.14 <sup>*</sup> (ref 9), 1.05 <sup>*</sup> (ref 11)                               | 1.10 ± 0.05 (R) 6.7              |  |
| 303 | 1.25 <sup>*</sup> (ref 9), 1.12 <sup>*</sup> (ref 11)                               | 1.18 ± 0.07 7.2                  |  |
| 313 | 1.33 <sup>*</sup> (ref 6), 1.44 <sup>*</sup> (ref 9),<br>1.21 <sup>*</sup> (ref 11) | 1.33 ± 0.09 8.0                  |  |
| 323 | 1.47 <sup>*</sup> (ref 6), 1.64 <sup>*</sup> (ref 9),<br>1.26 <sup>*</sup> (ref 11) | 1.5 ± 0.2 9.0                    |  |
| 333 | 1.70 <sup>*</sup> (ref 6), 1.87 <sup>*</sup> (ref 9),<br>1.32 <sup>*</sup> (ref 11) | 1.6 ± 0.2 9.5                    |  |
| 343 | 2.05 <sup>*</sup> (ref 6), 2.16 <sup>*</sup> (ref 9),<br>1.37 <sup>*</sup> (ref 11) | 1.9 ± 0.3 11                     |  |
| 353 | 2.42 <sup>*</sup> (ref 6), 2.55 <sup>*</sup> (ref 9),<br>1.42 <sup>*</sup> (ref 11) | 2.1 ± 0.5 12                     |  |
| 363 | 2.90 <sup>*</sup> (ref 6), 1.47 <sup>*</sup> (ref 11)                               | 2.2 ± 0.7 13                     |  |
| 373 | 3.42 <sup>*</sup> (ref 6)                                                           | 3.4 19                           |  |
| 393 | 4.47 <sup>*</sup> (ref 6)                                                           | 4.5 23                           |  |
| 413 | 5.62 <sup>*</sup> (ref 2)                                                           | 5.6 28                           |  |

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass solubilities.



| COMPO                            | ONENTS:                                                                                                                                                                | EVALUATOR:                                                                                                                      |  |
|----------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|--|
| (1)                              | Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl acetate</i> );<br>C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0]<br>Water; H <sub>2</sub> O; [7732-18-5] | G.T. Hefter, School of Mathematical<br>and Physical Sciences,<br>Murdoch University, Perth, W.A.,<br>Australia<br>January, 1989 |  |
| CRITICAL EVALUATION: (continued) |                                                                                                                                                                        |                                                                                                                                 |  |
| 8.                               | <ol> <li>Bomshtein, A. L.; Trofimov, A. N.; Gotlib, V. A.; Serafimov,</li> <li>L. A. Zh. Prikl. Khim. <u>1978</u>, 51, 440-2.</li> </ol>                               |                                                                                                                                 |  |
| 9.                               | Skrzecz, A. Pol. J. Chem. <u>1981</u> , 55, 1177-80; see also Skrzecz, A.<br>Thesis, I. Ch. F. PAN, Warszawa, <u>1979</u> .                                            |                                                                                                                                 |  |
| 10.                              | . Richon, D.; Viallard, A. Fluid Phase Equil. <u>1985</u> , 21, 279-93.                                                                                                |                                                                                                                                 |  |
| 11.                              | Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70.                                                                                                 |                                                                                                                                 |  |
|                                  |                                                                                                                                                                        |                                                                                                                                 |  |
| ACKNOWLEDGEMENT                  |                                                                                                                                                                        |                                                                                                                                 |  |

The Evaluator thanks Dr. Brian Clare for the graphics.

| COMPONENTS:                                                                                                             | ORIGINAL MEASUREMENTS:                                                                                 |
|-------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|
| (1) Acetic acid 2-methylpropyl                                                                                          | Traube, J.                                                                                             |
| ester (isobutyl acetate);                                                                                               | Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,                                                               |
| $C_6H_{12}O_2$ ; [110-19-0]                                                                                             | 2294-316.                                                                                              |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                |                                                                                                        |
| VARIABLES:                                                                                                              | PREPARED BY:                                                                                           |
| T/K = 295                                                                                                               | A. Skrzecz                                                                                             |
| EXPERIMENTAL VALUES:                                                                                                    |                                                                                                        |
| The solubility of acetic acid 2-methy                                                                                   | lpropyl ester in water at 22°C was                                                                     |
| reported to be 1 part of isobutyl acc<br>corresponding mass percent and mole f<br>compiler are 0.50 g(1)/100g sln and 7 | etate in 190-210 parts of water. The fraction, $x_1$ , values calculated by the $7.8 \times 10^{-4}$ . |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
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|                                                                                                                         |                                                                                                        |
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|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
| AUXILIARY                                                                                                               | INFORMATION                                                                                            |
| METHOD/APPARATUS/PROCEDURE:                                                                                             | SOURCE AND PURITY OF MATERIALS:                                                                        |
| The method was not specified.                                                                                           | (1) Not specified.                                                                                     |
|                                                                                                                         | (2) Not specified.                                                                                     |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         | ESTIMATED ERROR:                                                                                       |
|                                                                                                                         | Solv to $0.2 \sigma(1)/100\sigma$ old                                                                  |
|                                                                                                                         | Sory. 10.03 g(1)/100g SIN.                                                                             |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         | REFERENCES:                                                                                            |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |
|                                                                                                                         |                                                                                                        |

| COMPONENTS:<br>(1) Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl</i> acetate);<br>$C_6H_{12}O_2$ ; [110-19-0]<br>(2) Water; $H_2O$ ; [7732-18-5] | ORIGINAL MEASUREMENTS:<br>Hemptinne, A.<br>Z. Phys. Chem. <u>1894</u> , 13, 561-9. |
|------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
| VARIABLES:                                                                                                                                           | PREPARED BY:                                                                       |
| T/K = 298                                                                                                                                            | A. Skrzecz                                                                         |

The solubility of acetic acid 2-methylpropyl ester in water at  $25^{\circ}C$  was reported to be 6.332 g(1)/L sln.

| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                    | INFORMATION                                                                                                                      |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used. The<br>mixture of water with excess ester<br>was heated for some time in a water<br>bath and the ester phase was fil-<br>tered. A sample of known volume was<br>then transferred to a smaller<br>flask, heated with the known amount<br>of baryta until complete saponifi-<br>cation was obtained and then ti-<br>trated. No further details were re-<br>ported in the paper. | SOURCE AND PURITY OF MATERIALS:<br>(1) Not specified.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |

| ·····                                                                                                                                                           |                                                                                                                              |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|
| COMPONENTS:                                                                                                                                                     | ORIGINAL MEASUREMENTS:                                                                                                       |
| (1) Acetic acid 2-methylpropyl                                                                                                                                  | Fuehner, H.                                                                                                                  |
| ester ( <i>isobutyl acetate</i> );                                                                                                                              | Ber. Dtsch. Chem. Ges. <u>1924</u> ,                                                                                         |
| $C_6 R_{12} O_2; [110 - 19 - 0]$                                                                                                                                | 57, 510-5.                                                                                                                   |
| (2) Water; $H_2O$ ; $[7732-18-5]$                                                                                                                               |                                                                                                                              |
| VARIABLES:                                                                                                                                                      | PREPARED BY:                                                                                                                 |
| T/K = 293                                                                                                                                                       | A. Skrzecz                                                                                                                   |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 2-methy<br>reported to be 0.75 vol%, 0.67 g(1)/:<br>corresponding mole fraction, $x_1$ , valu<br>0.00104. | ylpropyl ester in water at 20 <sup>o</sup> C was<br>100g sln and 0.058 mol(1)/L sln. The<br>ne calculated by the compiler is |
|                                                                                                                                                                 |                                                                                                                              |
|                                                                                                                                                                 |                                                                                                                              |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                     | SOURCE AND PURITY OF MATERIALS:                                                                                              |
| The titration method was used. The ester was added from pipette to the                                                                                          | (1) Source not specified, commer-<br>cial product.                                                                           |
| flask with a constant amount of<br>water (50, 100 or 1000 mL) so long<br>as, on shaking, the mixture remain-<br>ed transparent.                                 | (2) Not specified.                                                                                                           |
|                                                                                                                                                                 | ESTIMATED ERROR:                                                                                                             |
|                                                                                                                                                                 | Soly. about $\pm 0.03 \ g(1) / 100 g$                                                                                        |
|                                                                                                                                                                 | (compiler).                                                                                                                  |
|                                                                                                                                                                 |                                                                                                                              |
|                                                                                                                                                                 | REFERENCES :                                                                                                                 |
|                                                                                                                                                                 |                                                                                                                              |
|                                                                                                                                                                 |                                                                                                                              |
|                                                                                                                                                                 |                                                                                                                              |
|                                                                                                                                                                 |                                                                                                                              |

| COMPONENTS:                                                                                                              | ORIGINAL MEASUREMENTS:                                        |  |  |
|--------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------|--|--|
| <pre>(1) Acetic acid 2-methylpropyl ester (isobutyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [110-19-0]</pre> | Doolittle, A.K.<br>Ind. End. Chem. <u>1935</u> , 27, 1169-79. |  |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                 |                                                               |  |  |
| VARIABLES:<br>T/K = 293                                                                                                  | PREPARED BY:<br>A. Skrzecz                                    |  |  |

The solubility of acetic acid 2-methylpropyl ester in water at  $20^{\circ}$ C was reported to be 0.67 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.00105.

The solubility of water in acetic acid 2-methylpropyl ester at 20°C was reported to be 1.64 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.0971.

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The method was not specified. The method was not specified. (1) Source not specified, commercial product; purity 96%, b.p. range 114-118°C,  $d_4^{20}$  0.870. (2) Not specified. ESTIMATED ERROR: Soly. about ±0.03 g(1)/100g sln and ±0.6 g(2)/100g sln (compiler). REFERENCES:

| NENTS: |  |  |
|--------|--|--|

|                                                                                                                                                                                                                                                                                                                                                                                                                                        | ·····                                                                                                                          |  |  |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|--|--|
| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                            | ORIGINAL MEASUREMENTS:                                                                                                         |  |  |
| <ul> <li>Acetic acid 2-methylpropyl</li> <li>ester (<i>isobutyl acetate</i>);</li> </ul>                                                                                                                                                                                                                                                                                                                                               | Frolov, A.F.; Loginova, M.A.<br>Fadeeva, G.S.; Ustavshchikov, B.F.                                                             |  |  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-19-0]                                                                                                                                                                                                                                                                                                                                                                             | Zh. Fiz. Khim. <u>1966</u> , 40, 145-7.                                                                                        |  |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                                                                                                                                                                                                               | Ustavshchikov, B.F.; Fadeeva, G.S.                                                                                             |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                        | Khim. Prom. <u>1967</u> , 43, 11-5.                                                                                            |  |  |
| VARIABLES:                                                                                                                                                                                                                                                                                                                                                                                                                             | PREPARED BY:                                                                                                                   |  |  |
| T/K = 293                                                                                                                                                                                                                                                                                                                                                                                                                              | 2. Maczynska                                                                                                                   |  |  |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 2-methylpropyl ester in water at 20°C was<br>reported to be 0.80 g(1)/100g sln. The corresponding mole fraction, $x_1$ ,<br>value calculated by the compiler is 0.00125.<br>The solubility of water in acetic acid 2-methylpropyl ester at 20°C was<br>reported to be 1.74 g(2)/100g sln. The corresponding mole fraction, $x_2$ ,<br>value calculated by the compiler is 0.102. |                                                                                                                                |  |  |
| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                              | INFORMATION                                                                                                                    |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                        | SOURCE AND DURTTY OF MATTERTALS.                                                                                               |  |  |
| The titration method was used. A<br>sample of one component was titrat-<br>ed by a second component at con-<br>stant temperature until a turbidity<br>was observed for 20-30 min. The<br>data were reported together with<br>the ternary system acetic acid<br>2-methylpropyl ester-water-                                                                                                                                             | (1) Source not specified;<br>distilled; b.p. $117^{\circ}C$ ,<br>$d_4^{20}$ 0.8695, $n_D^{18.8}$ 1.3910.<br>(2) Not specified. |  |  |
| 2-methylpropenamide (isobutyl acetate-water-methacrylamide).                                                                                                                                                                                                                                                                                                                                                                           | ESTIMATED ERROR:                                                                                                               |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                        | Soly. about ±0.1 g(1)/100g sln and<br>±0.7 g(2)/100g sln<br>(compiler).                                                        |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                        | REFERENCES:                                                                                                                    |  |  |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                             |               | ORIGINAL MEASUREMENTS:                                                                                                                                                                                                         |                                                               |  |  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------|--|--|
| (1) Acetic acid 2-methylpropyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                             |               | Linek, J.                                                                                                                                                                                                                      |                                                               |  |  |
| ester (isobutyl acetate);                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                             |               | Collect. Czech. C                                                                                                                                                                                                              | hem. Commun.                                                  |  |  |
| С <sub>6</sub> н                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | I <sub>12</sub> 0 <sub>2</sub> ; [110-19-0] |               | <u>1976</u> , 41, 1714-                                                                                                                                                                                                        | 6.                                                            |  |  |
| (2) Wat                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | cer; H <sub>2</sub> O; [7732-1              | .8-5]         |                                                                                                                                                                                                                                |                                                               |  |  |
| VARIABLES                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 3:                                          | <u></u>       | PREPARED BY:                                                                                                                                                                                                                   |                                                               |  |  |
| T/K = 28                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 38 - 420                                    |               | A. Skrzecz                                                                                                                                                                                                                     |                                                               |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               |                                                                                                                                                                                                                                |                                                               |  |  |
| EXPERIMEN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | TAL VALUES:                                 |               |                                                                                                                                                                                                                                |                                                               |  |  |
| Mutu                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | al solubility of                            | acetic acid   | 2-methylpropyl este                                                                                                                                                                                                            | er and water                                                  |  |  |
| t/°c                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | q(1)/10                                     | og sln        | qmoc) x                                                                                                                                                                                                                        | iler)                                                         |  |  |
| -, -                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | (2)-rich phase                              | (1)-rich phas | e (2)-rich phase                                                                                                                                                                                                               | (1)-rich phase                                                |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               |                                                                                                                                                                                                                                |                                                               |  |  |
| 14.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.761                                       | -             | 0.001188                                                                                                                                                                                                                       | -                                                             |  |  |
| 24.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.720                                       | -             | 0.001123                                                                                                                                                                                                                       | -                                                             |  |  |
| 35.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -                                           | 98.71         | -                                                                                                                                                                                                                              | 0.9223                                                        |  |  |
| 47.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.698                                       | -             | 0.001089                                                                                                                                                                                                                       | -                                                             |  |  |
| 61.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -                                           | 98.27         | -                                                                                                                                                                                                                              | 0.8981                                                        |  |  |
| 67.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.720                                       | -             | 0.001123                                                                                                                                                                                                                       | -                                                             |  |  |
| 74.9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.760                                       | -             | 0.001186                                                                                                                                                                                                                       | -                                                             |  |  |
| 75.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.761                                       | -             | 0.001188                                                                                                                                                                                                                       | -                                                             |  |  |
| 84.8                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.805                                       | -             | 0.001257                                                                                                                                                                                                                       | -                                                             |  |  |
| 85.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | -                                           | 97.36         | -                                                                                                                                                                                                                              | 0.8512                                                        |  |  |
| 93.2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 0.844                                       | -             | 0.001318                                                                                                                                                                                                                       | -                                                             |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | (con                                                                                                                                                                                                                           | tinued next page)                                             |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             | AUXILIARY 1   | INFORMATION                                                                                                                                                                                                                    |                                                               |  |  |
| METHOD/AF                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | PARATUS/PROCEDUR                            | ٤E:           | SOURCE AND PURITY                                                                                                                                                                                                              | OF MATERIALS:                                                 |  |  |
| ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, ,, , |                                             |               | (1) Commenter                                                                                                                                                                                                                  |                                                               |  |  |
| with the                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | e modification de                           | scribed by    | (1) Source not specified, technical<br>product: refluxed with acetic                                                                                                                                                           |                                                               |  |  |
| Matous,                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Novak, Sobr and                             | Pick          | anhydride, washed with saturat-<br>ed solution of $K_2CO_3$ and water,<br>dried and distilled; free of<br>acetic acid and alcohols, about<br>1.5% butyl acetate by glc; b.p.<br>117.5°C, $d_4^{20}$ 0.8715, $n_2^{20}$ 1.3902. |                                                               |  |  |
| of a giv                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ven composition t                           | ogether       |                                                                                                                                                                                                                                |                                                               |  |  |
| with a f                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ferrite magnet wa                           | s heated in   |                                                                                                                                                                                                                                |                                                               |  |  |
| connecte                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | ed into the circu                           | it of a       |                                                                                                                                                                                                                                |                                                               |  |  |
| thermost                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | at filled with t<br>The temperature         | riethylene    | (2) Distilled: sn                                                                                                                                                                                                              | ecific conductiv-                                             |  |  |
| was chan                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | nged continuously                           | and the       | (2) bischild, sp<br>ity $4\times10^{-6}$ ohr                                                                                                                                                                                   | $n^{-1}cm^{-1}$ .                                             |  |  |
| second p                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | hase in the ampo                            | ule was ob-   | ESTIMATED ERROR:                                                                                                                                                                                                               |                                                               |  |  |
| was not                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | observed.                                   | lydrorysis    | Momm +0 190 (aut)                                                                                                                                                                                                              | h \                                                           |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | Soly. about ±0.1                                                                                                                                                                                                               | nor).<br>g(1)/100g sln                                        |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             | [(2)-rich p]  | hase] and                                                                                                                                                                                                                      |                                                               |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | [(1)-rich p                                                                                                                                                                                                                    | hase] (compiler).                                             |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | DEFEDENCES.                                                                                                                                                                                                                    |                                                               |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | NEFERENCES:                                                                                                                                                                                                                    |                                                               |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                             |               | 1. Matous, J.; No<br>J.; Pick,J. C<br>Chem. Commun.                                                                                                                                                                            | vak, J.P.; Sobr,<br>ollect. Czech.<br><u>1972</u> , 37, 2653. |  |  |
| 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                             |               |                                                                                                                                                                                                                                |                                                               |  |  |

| COMPONENTS:                                                                                                              | ORIGINAL MEASUREMENTS:                                                  |
|--------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|
| <pre>(1) Acetic acid 2-methylpropyl ester (isobutyl acetate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [110-19-0]</pre> | Linek, J.<br>Collect. Czech. Chem. Commun.<br><u>1976</u> , 41, 1714-6. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                 |                                                                         |
| EXPERIMENTAL VALUES: (continued)<br>Mutual solubility of acetic acid                                                     | 2-methylpropyl ester and water                                          |

| t/°C  | g(1)/10        | )0g sln        | $x_1$ (comp    | iler)          |
|-------|----------------|----------------|----------------|----------------|
|       | (2)-rich phase | (1)-rich phase | (2)-rich phase | (1)-rich phase |
| 99.7  | _              | 96.59          | _              | 0.8146         |
| 105.7 | -              | 96.19          | -              | 0.7966         |
| 111.5 | 0.968          | -              | 0.001514       | -              |
| 115.7 | 1.002          | -              | 0.001567       | -              |
| 122.4 | -              | ,95.39         | -              | 0.7624         |
| 140.3 | -              | 94.36          |                | 0.7218         |
| 147.1 | 1.206          | -              | 0.001890       | -              |

|                                                                              | <b>.</b>                                                                                                                                                                           | · · · · · ·             |                                                                            |                                                                             |
|------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------|----------------------------------------------------------------------------|-----------------------------------------------------------------------------|
| COMPONEN                                                                     | TS:                                                                                                                                                                                |                         | ORIGINAL MEASUREME                                                         | NTS:                                                                        |
| <ol> <li>Acetic acid 2-methylpropyl<br/>ester (isobutyl acetate);</li> </ol> |                                                                                                                                                                                    |                         | Heyberger, A.; Ho<br>Bulicka, J.; Pr                                       | racek, J.;<br>ochazka, J.                                                   |
| C <sub>6</sub> I                                                             | H <sub>12</sub> O <sub>2</sub> ; [110-19-0]                                                                                                                                        |                         | Collect. Czech. C                                                          | hem. Commun.                                                                |
| (2) Wat                                                                      | ter; H <sub>2</sub> O; [7732-1                                                                                                                                                     | 8-5]                    | <u>1977</u> , 42, 3355-                                                    | 62.                                                                         |
| VARIABLE                                                                     | s:                                                                                                                                                                                 |                         | PREPARED BY:                                                               | <u></u>                                                                     |
| T/K = 29                                                                     | 98 and 323                                                                                                                                                                         |                         | A. Skrzecz                                                                 |                                                                             |
| EXPERIMEN<br>Mutu                                                            | NTAL VALUES:<br>ual solubility of                                                                                                                                                  | acetic acid             | 2-methylpropyl este                                                        | r and water                                                                 |
| t/°C                                                                         | g(1)/10<br>(2)-rich phase                                                                                                                                                          | 0g sln<br>(1)-rich phas | $x_1$ (comp:<br>se (2)-rich phase                                          | iler)<br>(1)-rich phase                                                     |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
| 50                                                                           | 0.400<br>0.670 <sup>b</sup>                                                                                                                                                        | 98.840°<br>96.400°      | 0.001045                                                                   | 0.8059                                                                      |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    | AUXILIARY               | INFORMATION                                                                |                                                                             |
| METHOD/AI                                                                    | PPARATUS/PROCEDUR                                                                                                                                                                  | Е:                      | SOURCE AND PURITY O                                                        | OF MATERIALS:                                                               |
| The tit<br>samples<br>bidity o<br>phase ap<br>were rep                       | METHOD/APPARATUS/PROCEDURE:<br>The titration method was used. The<br>samples were titrated until a tur-<br>bidity or droplets of the second<br>phase appeared. The data and method |                         | (1) Source not spe<br>grade; shaken<br>distilled from<br>addition of ch    | ecified, technical<br>with $Na_2CO_3(aq)$ ,<br>m $H_2O$ after<br>hloroform. |
| ternary<br>2-methyl<br>acid.                                                 | system acetic ac<br>lpropyl ester-wat                                                                                                                                              | id<br>er-acetic         | (2) Not specified.                                                         |                                                                             |
| ucru.                                                                        |                                                                                                                                                                                    |                         | ESTIMATED ERROR:                                                           |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         | Soly. about ±0.2 <sup>a</sup> ,<br>±1.9 <sup>c</sup> g(1)/1<br>(compiler). | ±0.1 <sup>b</sup> and<br>00g sln                                            |
|                                                                              |                                                                                                                                                                                    |                         | REFERENCES:                                                                |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |
|                                                                              |                                                                                                                                                                                    |                         |                                                                            |                                                                             |

| СОМРО | NENTS:                                                  | ORIGINAL MEASUREMENTS:                                            |
|-------|---------------------------------------------------------|-------------------------------------------------------------------|
| (1)   | Acetic acid 2-methylpropyl<br>ester (isobutyl acetate); | Bomshtein, A.L.; Trofimov, A.N.;<br>Gotlib, V.A.; Serafimov, L.A. |

Zh. Prikl. Khim. <u>1978</u>, 51, 440-2.

C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [110-19-0] (2) Water; H<sub>2</sub>O; [7732-18-5]

VARIABLES:

T/K = 293 - 353

PREPARED BY: A. Skrzecz

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EXPERIMENTAL VALUES:
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Mutual solubility of acetic acid 2-methylpropyl ester and water

| t/°C | х              | 51             | g(1)/100g sl   | n (compiler)   |
|------|----------------|----------------|----------------|----------------|
|      | (2)-rich phase | (1)-rich phase | (2)-rich phase | (1)-rich phase |
| 20   | 0.00161        | 0.92458        | 1.03           | 98.751         |
| 25   | 0.00158        | 0.91784        | 1.01           | 98.631         |
| 30   | 0.00155        | 0.91118        | 0.99           | 98.511         |
| 40   | 0.00149        | 0.89919        | 0.95           | 98.291         |
| 50   | 0.00142        | 0.88692        | 0.91           | 98.061         |
| 60   | 0.00136        | 0.87493        | 0.87           | 97.831         |
| 70   | 0.00131        | 0.86321        | 0.84           | 97.601         |
| 80   | 0.00125        | 0.85174        | 0.80           | 97.371         |

Authors' smoothing equations:

| g(1)/100g | sln = | 1.109 |   | 0.0039 | t/°C | (2)-rich | phase |
|-----------|-------|-------|---|--------|------|----------|-------|
| g(2)/100g | sln = | 0.812 | + | 0.0229 | t/°C | (1)-rich | phase |

## AUXILIARY INFORMATION

| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                    | SOURCE AND PURITY OF MATERIALS:                                                                                                                                           |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| The analytical methods were used.<br>The component (1) was analyzed by<br>saponification and the component<br>(2) was analyzed by the Karl<br>Fischer method. The experiments<br>were made at normal pressure. | <ul> <li>(1) Source not specified; distil-<br/>led; without impurities by glc,<br/>b.p. 117.7°C, n<sub>D</sub><sup>20</sup> 1.390.</li> <li>(2) Not specified.</li> </ul> |
|                                                                                                                                                                                                                | ESTIMATED ERROR:                                                                                                                                                          |
|                                                                                                                                                                                                                | Soly. ±(0.1 - 0.4) g(1)/100g sln<br>in both phases (compiler).                                                                                                            |
|                                                                                                                                                                                                                | REFERENCES:                                                                                                                                                               |
|                                                                                                                                                                                                                |                                                                                                                                                                           |
|                                                                                                                                                                                                                |                                                                                                                                                                           |

| COMPONENTS:<br>(1) Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl</i> acetate);<br>$C_6H_{12}O_2$ ; [110-19-0]<br>(2) Water; $H_2O$ ; [7732-18-5] | ORIGINAL MEASUREMENTS:<br>Skrzecz, A.<br>Pol. J. Chem. <u>1981</u> , 55, 1177-80.<br>Skrzecz, A.<br>Thesis, Inst. Phys. Chem., Pol.<br>Acad. Sci., Warszawa, <u>1979</u> . |
|------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| VARIABLES:                                                                                                                                           | PREPARED BY:                                                                                                                                                               |
| T/K = 291 - 360                                                                                                                                      | A. Skrzecz                                                                                                                                                                 |

Mutual solubility of acetic acid 2-methylpropyl ester and water

| T/K                | $x_1$          |                | g(1)/100g sln  |                |
|--------------------|----------------|----------------|----------------|----------------|
|                    | (2)-rich phase | (1)-rich phase | (2)-rich phase | (1)-rich phase |
| 290.8 <sup>a</sup> | _              | 0.9404         |                | 99.027         |
| 293.3              | 0.00110        | -              | 0.705          | -              |
| 297.6              | -              | 0.9317         | -              | 98.876         |
| 304.1              | 0.00098        | -              | 0.629          | -              |
| 316.9              | 0.00090        | -              | 0.577          | -              |
| 324.8              | -              | 0.9008         | -              | 98.321         |
| 333.6              | 0.00090        | -              | 0.577          | -              |
| 342.4              | -              | 0.8765         | -              | 97.861         |
| 342.6              | 0.00098        | -              | 0.629          | -              |
| 352.1              | 0.00110        | -              | 0.705          | -              |

<sup>a</sup> By the Karl Fischer method.

| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | INFORMATION                                                                                                                                                                                                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The synthetic method of Alexejew<br>and the analytical method were<br>used. An ampoule with the solution<br>of fixed concentration was placed<br>in a glass tube connected with a<br>thermostat filled completely with<br>distilled water. During the meas-<br>urements the temperature of the<br>bath was changed continuously and<br>the appearance and disappearance of<br>turbidity within the ampoule was<br>observed visually. For the analyti- | <pre>SOURCE AND PURITY OF MATERIALS: (1) POCH, pure grade;    distilled; purity 99.98% by    glc, 0.11 wt% water by the    Karl Fischer method. (2) Distilled.  ESTIMATED ERROR: Temp. ±(0.2-0.6)°C. Soly. see above.</pre> |
| determined using a Karl Fischer<br>titration procedure. The amount of<br>water in the pure ester was taken<br>into account.                                                                                                                                                                                                                                                                                                                                                          | REFERENCES:                                                                                                                                                                                                                 |

| COMPONENTS:                                                                       |                                                                                                               | ORIGINAL MEASURE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | MENTS:                                                                                                     |                                                                                        |
|-----------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|
| (1) Acetic acid 2-methylpropyl                                                    |                                                                                                               | Skrzecz, A.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                            |                                                                                        |
| ester                                                                             | (isobuty) .                                                                                                   | acetate);                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Pol. J. Chem.                                                                                              | <u>1981</u> , 55, 1177-80.                                                             |
| $C_{6}n_{12}$                                                                     | $0_2, [110^{-19^{-19^{-19^{-19^{-19^{-19^{-19^{-19$                                                           | 0]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Skrzecz, A.                                                                                                |                                                                                        |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                          |                                                                                                               | 2-10-5]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Thesis, Inst. Phys. Chem., Pol.<br>Acad. Sci., Warszawa, <u>1979</u> .                                     |                                                                                        |
| XPERIMENT                                                                         | CAL VALUES:                                                                                                   | (continued)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                                            |                                                                                        |
| Mutual                                                                            | solubility                                                                                                    | of acetic acid                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 2-methylpropyl es                                                                                          | ter and water                                                                          |
|                                                                                   |                                                                                                               | Υ.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | g(1)/1                                                                                                     | 00g sln                                                                                |
| T/K                                                                               |                                                                                                               | A1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                                                                                            |                                                                                        |
| т/к                                                                               | 2)-rich pha                                                                                                   | se (1)-rich pha                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | se (2)-rich phase                                                                                          | e (1)-rich phase                                                                       |
| т/к<br>                                                                           | 2)-rich pha                                                                                                   | se (1)-rich pha:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | se (2)-rich phase                                                                                          | e (1)-rich phase                                                                       |
| 7/K<br>(<br>                                                                      | 2)-rich pha                                                                                                   | se (1)-rich pha:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | se (2)-rich phase                                                                                          | e (1)-rich phase                                                                       |
| 7/K<br>(<br>353.2<br>359.7                                                        | 2)-rich pha:<br>-<br>-                                                                                        | 0.8559<br>0.8397                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | se (2)-rich phase<br>                                                                                      | 97.455<br>97.124                                                                       |
| 7/K<br>353.2<br>359.7<br>                                                         | 2)-rich pha:<br>-<br>-                                                                                        | 0.8559<br>0.8397                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | se (2)-rich phase<br>                                                                                      | 97.455<br>97.124                                                                       |
| T/K<br>353.2<br>359.7<br>Author's<br>$x_1 = 1.5$                                  | 2)-rich pha:<br>-<br>-<br>: smoothing 0<br>088x10 <sup>-3</sup> - 2                                           | 0.8559<br>0.8397<br>equations:<br>.50x10 <sup>-5</sup> (T/K -                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 273.15) + 2.51x10                                                                                          | e (1)-rich phase<br>97.455<br>97.124<br>-7 $(T/K - 273.15)^2$                          |
| T/K<br>353.2<br>359.7<br>Author's<br>$x_1 = 1.5$<br>st.                           | 2)-rich pha:<br>-<br>-<br>s smoothing<br>088x10 <sup>-3</sup> - 2<br>dev. = 9.5                               | $\begin{array}{c}  & \begin{array}{c}  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & & \\  & & \\$        | 273.15) + 2.51x10<br>- rich phase                                                                          | 97.455<br>97.124<br>-7 $(T/K - 273.15)^2$                                              |
| $\frac{T/K}{353.2}$ $\frac{359.7}{4000}$ Author's $x_1 = 1.5$<br>$x_2 = 0.00$     | 2)-rich phas<br>-<br>-<br>s smoothing<br>088x10 <sup>-3</sup> - 2<br>dev. = 9.55<br>50721 + 4.19              | $\begin{array}{c}  & 1 \\  & 5e & (1) - rich \ phase \\  & 0.8559 \\  & 0.8397 \\  & \\  & equations: \\  & .50x10^{-5} \ (T/K - 5x \ 10^{-6} \ (2) \\  & 02x10^{-4} \ (T/K - 2) \\  & \\  & \hline \end{array}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 273.15) + 2.51x10<br>                                                                                      | e (1)-rich phase<br>97.455<br>97.124<br>$(T/K - 273.15)^2$<br>$(T/K - 273.15)^2$       |
| T/K<br>353.2<br>359.7<br>Author's<br>$x_1 = 1.5$<br>st.<br>$x_2 = 0.0$<br>st.     | 2)-rich phas<br>-<br>-<br>s smoothing<br>088x10 <sup>-3</sup> - 2<br>dev. = 9.5<br>50721 + 4.19<br>dev. = 2.3 | $\begin{array}{c} \text{ase (1)-rich phase} \\ 0.8559 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\$                 | 273.15) + 2.51x10<br>                                                                                      | e (1)-rich phase<br>97.455<br>97.124<br>$^{-7} (T/K - 273.15)^2$<br>$(T/K - 273.15)^2$ |
| $\frac{T/K}{353.2}$ 359.7<br>Author's<br>$x_1 = 1.5$<br>st.<br>$x_2 = 0.0$<br>st. | 2)-rich phas<br>-<br>-<br>s smoothing<br>088x10 <sup>-3</sup> - 2<br>dev. = 9.5<br>50721 + 4.19<br>dev. = 2.3 | $\begin{array}{c} \text{ase (1)-rich phase} \\ 0.8559 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.8397 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\ 0.837 \\$ | 273.15) + 2.51x10<br>                                                                                      | e (1)-rich phase<br>97.455<br>97.124<br>-7 $(T/K - 273.15)^2$<br>$(T/K - 273.15)^2$    |
| T/K<br>353.2<br>359.7<br>Author's<br>$x_1 = 1.5$<br>st.<br>$x_2 = 0.0$<br>st.     | -<br>-<br>-<br>smoothing<br>088x10 <sup>-3</sup> - 2<br>dev. = 9.5<br>50721 + 4.19<br>dev. = 2.3              | $\begin{array}{c} \text{a. 8559} \\ \text{0.8559} \\ \text{0.8397} \\ \text{equations:} \\ \text{.50x10^{-5}} (T/K - 5 \times 10^{-6} (2)) \\ \text{0.2x10^{-4}} (T/K - 2) \\ \text{0.2x10^{-3}} (1) \\ \end{array}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | -<br>-<br>-<br>-<br>-<br>273.15) + 2.51x10<br>-rich phase<br>73.15) + 9.52x10 <sup>-6</sup><br>-rich phase | e (1)-rich phase<br>97.455<br>97.124<br>-7 $(T/K - 273.15)^2$<br>$(T/K - 273.15)^2$    |

|                                                                                                                                                                                          | 500                                                                                                     |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
| COMPONENTS:                                                                                                                                                                              | ORIGINAL MEASUREMENTS:                                                                                  |
| (1) Acetic acid 2-methylpropyl<br>ester ( <i>isobutyl acetate</i> );<br>$C_6H_{12}O_2$ ; [110-19-0]<br>(2) Water: H.O: [7732-18-5]                                                       | Richon, D.; Viallard, A.<br><i>Fluid Phase Equilib.</i> <u>1985</u> , 21,<br>279-93.                    |
|                                                                                                                                                                                          |                                                                                                         |
| T/K = 298                                                                                                                                                                                | A. Skrzecz                                                                                              |
| EXPERIMENTAL VALUES:<br>The solubility of acetic acid 2-methy<br>reported to be 0.00601 mol(1)/100g(2)<br>and mole fraction, $x_1$ , values calcula<br>0.693 g(1)/100g sln and 0.001082. | vlpropyl ester in water at 298.1 K was<br>. The corresponding mass per cent<br>.ted by the compiler are |

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                      |  |  |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| METHOD/APPARATUS/PROCEDURE:<br>The refractometric method was used.<br>The Phoenix model 1-2000T differen-<br>tial refractometer from Texas In-<br>struments was used and the solubil-<br>ity was determined from a charac-<br>teristic calibration curve as de-<br>scribed in the thesis of Richon<br>(ref 1). | <pre>SOURCE AND PURITY OF MATERIALS: (1) Fluka (puriss); purified by    preparation gas chromatographic    method; purity &gt;99.5%, water    content was negligible. (2) Distilled. (2) Distilled. ESTIMATED ERROR: Soly. about ±0.04 g(1)/100g sln    (compiler). REFERENCES: 1. Richon, D. Thesis, University    de Clermont-Ferrand, 1974.</pre> |  |  |

| COMPONENT                                                         |                                                                                                                                             |                            |                                               | NITTO -                           |  |
|-------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|-----------------------------------------------|-----------------------------------|--|
| (1) Apphin paid a mathematical                                    |                                                                                                                                             | ORIGINAL MEASUREMENTS:     |                                               |                                   |  |
| (1) Acetic acid 2-methylpropyl                                    |                                                                                                                                             | Stephenson, R.; Stuart, J. |                                               |                                   |  |
| ester (isobutyl acetate);                                         |                                                                                                                                             | J. Chem. Eng. Dat          | a <u>1986</u> , 31,                           |                                   |  |
| C6.                                                               | m <sub>12</sub> 0 <sub>2</sub> , [110 19 0]                                                                                                 |                            | 50 /0.                                        |                                   |  |
| (2) Wa                                                            | ter; H <sub>2</sub> 0; [7732-1                                                                                                              | 8-5]                       |                                               |                                   |  |
| VARIABLE                                                          | S:                                                                                                                                          |                            | PREPARED BY:                                  |                                   |  |
| T/K = 2                                                           | 73 - 363                                                                                                                                    |                            | Z. Maczynska                                  |                                   |  |
| EXPERIME<br>Mut                                                   | NTAL VALUES:<br>ual solubility of                                                                                                           | acetic acid                | 2-methylpropyl este                           | er and water                      |  |
| t/°C                                                              | g(1)/10                                                                                                                                     | 0g sln                     |                                               | viler)                            |  |
| 0, 0                                                              | (2)-rich phase                                                                                                                              | (1)-rich phas              | e (2)~rich phase                              | (1)-rich phase                    |  |
| <u></u>                                                           |                                                                                                                                             |                            |                                               | · · · · · · · · · · · · · · · · · |  |
| 0                                                                 | 1.03                                                                                                                                        | 99.28                      | 0.00161                                       | 0.9553                            |  |
| 10.0                                                              | 0.83                                                                                                                                        | • 99.18                    | 0.00130                                       | 0.9494                            |  |
| 19.7                                                              | 0.66                                                                                                                                        | 99.05                      | 0.00103                                       | 0.9417                            |  |
| 29.9                                                              | 0.61                                                                                                                                        | 98.88                      | 0.00095                                       | 0.9319                            |  |
| 39.7                                                              | 0.54                                                                                                                                        | 98.79                      | 0.00084                                       | 0.9268                            |  |
| 50.0                                                              | 0.49                                                                                                                                        | 98.74                      | 0.00076                                       | 0.9240                            |  |
| 60.5                                                              | 0.57                                                                                                                                        | 98.71                      | 0.00089                                       | 0.9223                            |  |
| 70.1                                                              | 0.53                                                                                                                                        | 98.64                      | 0.00082                                       | 0.9183                            |  |
| 80.2                                                              | 0.55                                                                                                                                        | 98.35                      | 0.00086                                       | 0.9024                            |  |
| 90.2                                                              | -                                                                                                                                           | 98.51                      | -                                             | 0.9111                            |  |
| std. d                                                            | dev. 0.02                                                                                                                                   | 0.01                       |                                               |                                   |  |
|                                                                   |                                                                                                                                             |                            |                                               |                                   |  |
|                                                                   |                                                                                                                                             | AUXILIARY I                | NFORMATION                                    |                                   |  |
| METHOD/AI                                                         | PPARATUS/PROCEDUR                                                                                                                           | E:                         | SOURCE AND PURITY                             | OF MATERIALS:                     |  |
| The ana                                                           | lytical method wa                                                                                                                           | s used.                    | (1) Source not specified, commer-             |                                   |  |
| Componer<br>with con                                              | nt (1) was equili<br>mponent (2) at a                                                                                                       | brated<br>given            | cial sample; purity 99%; used as received.    |                                   |  |
| temperat                                                          | ture in a thermos                                                                                                                           | tat. Each                  |                                               |                                   |  |
| (1) was                                                           | layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile                                       |                            | (2) Not specified.                            |                                   |  |
| weighed                                                           |                                                                                                                                             |                            |                                               |                                   |  |
| (or sometimes propanol) to the organic layer sample and measuring |                                                                                                                                             |                            | <u>,                                     </u> |                                   |  |
| by a Gou                                                          | by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator). |                            | ESTIMATED ERROR:                              |                                   |  |
| (Chromos<br>3390 A 1                                              |                                                                                                                                             |                            | Accuracy of metho<br>for solubility, s        | d 0.1 wt% or less,<br>ee above.   |  |
| A simila<br>boiling                                               | ar procedure but<br>material (e.g. 1                                                                                                        | a higher<br>-hexanol)      |                                               |                                   |  |
| was used<br>water la                                              | d to determine (2<br>ayer.                                                                                                                  | ) in the                   | REFERENCES                                    |                                   |  |
|                                                                   |                                                                                                                                             |                            | WEL DIVERCED .                                |                                   |  |
|                                                                   |                                                                                                                                             |                            |                                               |                                   |  |
|                                                                   |                                                                                                                                             | [                          |                                               |                                   |  |
|                                                                   |                                                                                                                                             |                            |                                               |                                   |  |

| COMPONENTS:                                                                                                      | EVALUATOR:                                                                                        |
|------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| (1) Butanoic acid ethyl ester<br>(ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[105-54-4] | G.T. Hefter, School of Mathematical<br>and Physical Sciences,<br>Murdoch University, Perth, W.A., |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                         | Australia<br>January, 1989                                                                        |

#### CRITICAL EVALUATION:

Quantitative solubility data for the butanoic acid ethyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

#### TABLE 1: Quantitative Solubility Studies of the Butanoic acid ethyl ester (1) - Water (2) System

| entre second sec |         |            |                |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|------------|----------------|
| Reference                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | T/K     | Solubility | Method         |
| Traube (ref 1)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 295     | (1) in (2) | unspecified    |
| Hemptinne (ref 2)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 298     | (1) in (2) | analytical     |
| Bancroft (ref 3)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 293     | mutual     | titration      |
| Fuehner (ref 4)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 295     | (1) in (2) | titration      |
| Doolittle (ref 5)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 293     | mutual     | unspecified    |
| Rao and Rao (ref 6)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 303     | mutual     | titration      |
| Venkataratnam <i>et al</i> . (ref 7)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 303     | mutual     | titration      |
| Rao and Rao (ref 8)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 303     | mutual     | titration      |
| Richon and Viallard (ref 9)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 298     | (1) in (2) | refractometric |
| Stephenson and Stuart<br>(ref 10)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 273-364 | mutual     | GLC            |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

### 1. SOLUBILITY OF BUTANOIC ACID ETHYL ESTER (1) IN WATER (2)

All the available data for the solubility of butanoic acid ethyl ester (1) in water (2) are summarized in Table 2 with the following exclusions.

The data of Hemptinne (ref 2) and Bancroft (ref 3), expressed in w/v and v/v units have been excluded from consideration. The data of Traube (ref 1) and Doolittle (ref 5) at *ca*. 293 K have been rejected as they are considerably lower than other reported values (ref 4,9,10). The data of Rao *et al.* (ref 6-8), whilst not rejected, have for the purpose of uniformity not been included in calculating the "Best" values.

| COMPONENTS:                          |                                                                   | EVALUATOR:                          |  |
|--------------------------------------|-------------------------------------------------------------------|-------------------------------------|--|
| (1)                                  | Butanoic acid ethyl ester                                         | G.T. Hefter, School of Mathematical |  |
|                                      | (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; | and Physical Sciences,              |  |
|                                      | [105-54-4]                                                        | Murdoch University, Perth, W.A.,    |  |
| (2) Water: $H_{-0}$ : $[7732-18-5]$  | Australia                                                         |                                     |  |
| $(2)$ water, $m_2^2$ , $[,,52,10,5]$ |                                                                   | January, 1989                       |  |

TABLE 2:

The remaining data (Table 2) are in general in good agreement although the lack of independent studies over a wide temperature range precludes Recommendation at most temperatures.

of Butanoic acid ethyl ester (1) in Water (2)

Recommended (R) and Tentative Solubilities

T/K Solubilities Reported values "Best" values  $(\pm \sigma_n)^a$ g(1)/100g sln g(1)/100g sln  $10^{3}x_{1}$ 1.06 (ref 10) 273 1.1 1.7 0.81\* (ref 10) 283 0.8 1.3  $0.616^b$  (ref 4), 0.68 (ref 10)  $0.65 \pm 0.03$  (R) 293 1.01 0.666 (ref 9), 0.63<sup>\*</sup> (ref 10) 298  $0.65 \pm 0.02 (R)$ 1.01  $0.8^{c}$  (ref 6-8),  $0.58^{*}$  (ref 10) 303 0.58 0.9  $0.51^*$  (ref 10) 0.5 0.8 313 0.47<sup>\*</sup> (ref 10) 0.5 323 0.8 0.46<sup>\*</sup> (ref 10) 333 0.5 0.7 0.46<sup>\*</sup> (ref 10) 0.5 343 0.7 0.46<sup>\*</sup> (ref 10) 0.5 353 0.7 363 0.44<sup>\*</sup> (ref 10) 0.4 0.7

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

<sup>b</sup> 295 К.

<sup>c</sup> Not included in calculation of "Best" value, see text.

2. SOLUBILITY OF WATER (2) IN BUTANOIC ACID ETHYL ESTER (1)

All the available data for the solubility of water (2) in butanoic acid ethyl ester (1) are summarized in Table 3. In general, agreement is satisfactory although the lack of independent studies over a wide temperature range precludes Recommendation of any of the "Best" values.

|                                                                                                                                          | ·····                                                                  |                                                    | <u> </u>       |  |
|------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------|----------------------------------------------------|----------------|--|
| COMP                                                                                                                                     | ONENTS:                                                                | EVALUATOR:                                         |                |  |
| (1)                                                                                                                                      | Butanoic acid ethyl ester                                              | G.T. Hefter, School of Mathematical                |                |  |
|                                                                                                                                          | (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;      | and Physical Sciences,                             | _              |  |
|                                                                                                                                          | [105-54-4]                                                             | Murdoch University, Perth, W.A                     | A.,            |  |
| (2)                                                                                                                                      | Water; H <sub>2</sub> O; [7732-18-5]                                   | January, 1989                                      |                |  |
|                                                                                                                                          |                                                                        |                                                    |                |  |
| CRIT                                                                                                                                     | ICAL EVALUATION: (continued)                                           |                                                    |                |  |
|                                                                                                                                          | <u>TABLE 3: Tentat</u><br>of Water (2) in Butanoi                      | <u>ive Solubilities</u><br>Ic acid ethyl ester (1) |                |  |
| T/K                                                                                                                                      | Sol                                                                    | ubilities                                          |                |  |
|                                                                                                                                          | Reported values                                                        | "Best" values $(\pm \sigma_n)^a$                   |                |  |
|                                                                                                                                          | g(2)/100g sln                                                          | g(2)/100g sln 10 <sup>2</sup>                      | <sup>K</sup> 2 |  |
| 273                                                                                                                                      | 0.56 (ref 10)                                                          | 0.6 4                                              |                |  |
| 283                                                                                                                                      | 0.70 <sup>*</sup> (ref 10)                                             | 0.7 4                                              |                |  |
| 293                                                                                                                                      | 0.75 (ref 5), 0.86 (ref 10)                                            | 0.80 ± 0.06 4.9                                    |                |  |
| 298                                                                                                                                      | 0.92 <sup>*</sup> (ref 10)                                             | 0.9 6                                              |                |  |
| 303                                                                                                                                      | 1.1 (ref 6), 0.6 (ref 7,8),<br>0.98 <sup>*</sup> (ref 10)              | 0.9 ± 0.2 6                                        |                |  |
| 313                                                                                                                                      | 1.09 <sup>*</sup> (ref 10)                                             | 1.1 7                                              |                |  |
| 323                                                                                                                                      | 1.16 <sup>*</sup> (ref 10)                                             | 1.2 7                                              |                |  |
| 333                                                                                                                                      | 1.21 <sup>*</sup> (ref 10)                                             | 1.2 7                                              |                |  |
| 343                                                                                                                                      | 1.23 <sup>*</sup> (ref 10)                                             | 1.2 7                                              |                |  |
| 353                                                                                                                                      | 1.29 <sup>*</sup> (ref 10)                                             | 1.3 8                                              |                |  |
| 363                                                                                                                                      | 1.30 <sup>*</sup> (ref 10)                                             | 1.3 8                                              |                |  |
|                                                                                                                                          |                                                                        |                                                    |                |  |
| a (                                                                                                                                      | Obtained by averaging where approp                                     | riate; $\sigma_{ m n}$ has no statistical          |                |  |
| significance. Mole fraction solubilities $(x_2)$ have the same status and (relative) percentage uncertainties as the mass  solubilities. |                                                                        |                                                    |                |  |
| REFE                                                                                                                                     | RENCES                                                                 |                                                    |                |  |
| 1.                                                                                                                                       | Traube, J. Ber. Dtsch. Chem. Ges                                       | . <u>1884</u> , 17, 2294-2316.                     |                |  |
| 2.                                                                                                                                       | Hemptinne, A. Z. Phys. Chem. <u>1894</u> , 13, 561-9.                  |                                                    |                |  |
| з.                                                                                                                                       | Bancroft, W. D. Phys. Rev. <u>1895</u> , 3, 114-36.                    |                                                    |                |  |
| 4.                                                                                                                                       | Fuehner, H. Ber. Dtsch. Chem. Ges. <u>1924</u> , 57, 510-5.            |                                                    |                |  |
| 5.                                                                                                                                       | Doolittle, A. K. Ind. Eng. Chem. <u>1935</u> , 27, 1169-79.            |                                                    |                |  |
| 6.                                                                                                                                       | Rao, J. R.; Rao, C. V. J. Appl. Chem. <u>1957</u> , 7, 435-9.          |                                                    |                |  |
| 7.                                                                                                                                       | Venkataratnam, A.; Rao, J. R.; 1<br><u>1957</u> , 7, 102-10.           | Rao, C. V. Chem. Eng. Sci.                         |                |  |
| 8.                                                                                                                                       | Rao, J. R.; Rao, C. V.; J. Appl                                        | . Chem. <u>1959</u> , 9, 69-73.                    |                |  |
| 9.                                                                                                                                       | Richon, D.; Viallard, A. Fluid A                                       | Phase Equil. <u>1985</u> , 21, 279 <b>-</b> 93.    |                |  |
| 10.                                                                                                                                      | Stephenson, R.; Stuart, J. J. Chem. Eng. Data <u>1986</u> , 31, 56-70. |                                                    |                |  |
|                                                                                                                                          |                                                                        |                                                    |                |  |

| COMPONENTS:                                                                                                                                                                                          | ORIGINAL MEASUREMENTS:                                                                                                              |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| (1) Butanoic acid ethyl ester                                                                                                                                                                        | Traube, J.                                                                                                                          |
| (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[105-54-4]                                                                                                                      | Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,<br>2294-316.                                                                               |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                             |                                                                                                                                     |
| VARIABLES:                                                                                                                                                                                           | PREPARED BY:                                                                                                                        |
| T/K = 295                                                                                                                                                                                            | A. Skrzecz                                                                                                                          |
| EXPERIMENTAL VALUES:<br>The solubility of butanoic acid ethyl<br>to be 1 part of ethyl butyrate in 190<br>ing mass percent and mole fraction, x<br>are 0.50 g(1)/100g sln and 7.8 x 10 <sup>-4</sup> | ester in water at $22^{\circ}$ C was reported<br>0-210 parts of water. The correspond-<br>$x_1$ , values calculated by the compiler |
| AUXILIARY                                                                                                                                                                                            | INFORMATION                                                                                                                         |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                          | SOURCE AND PURITY OF MATERIALS:                                                                                                     |
| The method was not specified.                                                                                                                                                                        | (1) Not specified.                                                                                                                  |
|                                                                                                                                                                                                      | (2) Not specified.                                                                                                                  |
|                                                                                                                                                                                                      | (2)                                                                                                                                 |
|                                                                                                                                                                                                      | ESTIMATED ERROR:                                                                                                                    |
|                                                                                                                                                                                                      | Soly. ±0.03 g(1)/100g sln.                                                                                                          |
|                                                                                                                                                                                                      |                                                                                                                                     |
|                                                                                                                                                                                                      | REFERENCES:                                                                                                                         |

| COMPONENTS:                                                                                                       | ORIGINAL MEASUREMENTS:                                          |
|-------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------|
| <pre>(1) Butanoic acid ethyl ester  (ethyl butyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;  [105-54-4]</pre> | Hemptinne, A.<br><i>Z. Phys. Chem.</i> <u>1894</u> , 13, 561-9. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                          |                                                                 |
| VARIABLES:                                                                                                        | PREPARED BY:                                                    |
| T/K = 298                                                                                                         | A. Skrzecz                                                      |

The solubility of butanoic acid ethyl ester in water at  $25^{\circ}$ C was reported to be 6.862 g(1)/L sln.

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                  | |
|---|---|---|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used. The<br>mixture of water with excess ester<br>was heated for some time in a water<br>bath and the ester phase was fil-<br>tered. A sample of known volume<br>was then transferred to a smaller<br>flask, heated with the known amount<br>of baryta until complete saponifi-<br>cation was obtained and then ti-<br>trated. No further details were<br>reported in the paper. | SOURCE AND PURITY OF MATERIALS:<br>(1) Not specified.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |
| COMPONENTS:                                                                                                                    | ORIGINAL MEASUREMENTS:              |  |
|--------------------------------------------------------------------------------------------------------------------------------|-------------------------------------|--|
| (1) Butanoic acid ethyl ester                                                                                                  | Bancroft, W.D.                      |  |
| (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[105-54-4]                                                | Phys. Rev. <u>1895</u> , 3, 114-36. |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                       |                                     |  |
| VARIABLES:                                                                                                                     | PREPARED BY:                        |  |
| T/K = 293                                                                                                                      | A. Skrzecz                          |  |
| EXPERIMENTAL VALUES:<br>The solubility of butanoic acid ethyl ester in water at 20°C was reported<br>to be 0.08 mL(1)/10mL(2). |                                     |  |
| to be 0.04-0.05 mL(2)/10mL(1).                                                                                                 |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
| AUXILIARY INFORMATION                                                                                                          |                                     |  |
| METHOD/APPARATUS/PROCEDURE:                                                                                                    | SOURCE AND PURITY OF MATERIALS:     |  |
| 10 mL of solvent in a test tube was<br>titrated with the second component                                                      | CaCl <sub>2</sub> , distilled.      |  |
| until the solution became cloudy.                                                                                              | (2) Not specified.                  |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                | ESTIMATED ERROR:                    |  |
|                                                                                                                                | Soly. ±0.01 mL.                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                | REFERENCES:                         |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |
|                                                                                                                                |                                     |  |

| COMPONENTS:                                                                                                       | ORIGINAL MEASUREMENTS:                                            |
|-------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|
| <pre>(1) Butanoic acid ethyl ester  (ethyl butyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;  [105-54-4]</pre> | Fuehner, H.<br>Ber. Dtsch. Chem. Ges. <u>1924</u> ,<br>57, 510-5. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                          |                                                                   |
| VARIABLES:                                                                                                        | PREPARED BY:                                                      |
| T/K = 295                                                                                                         | A. Skrzecz                                                        |

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# EXPERIMENTAL VALUES:

The solubility of butanoic acid ethyl ester in water at 22°C was reported to be 0.725 vol%, 0.616 g(1)/100g sln and 0.0531 mol(1)/L sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 9.60 x 10<sup>-4</sup>.

| AUXILIARY INFORMATION                                                                                                                                                                                                                         |                                                                                                                                                                  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used. The<br>ester was added from a pipette to<br>the flask with a constant amount of<br>water (50, 100 or 1000 mL) so long<br>as, on shaking, the mixture remain-<br>ed transparent. | SOURCE AND PURITY OF MATERIALS:<br>(1) Source not specified, commer-<br>cial product.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |
|                                                                                                                                                                                                                                               |                                                                                                                                                                  |

| COMPONENTS:                                                                                                       | ORIGINAL MEASUREMENTS:                                        |
|-------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------|
| <pre>(1) Butanoic acid ethyl ester  (ethyl butyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;  [105-54-4]</pre> | Doolittle, A.K.<br>Ind. End. Chem. <u>1935</u> , 27, 1169-79. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                          |                                                               |
| VARIABLES:                                                                                                        | PREPARED BY:                                                  |
| T/K = 293                                                                                                         | A. Skrzecz                                                    |

The solubility of butanoic acid ethyl ester in water at 20°C was reported to be 0.49 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 7.6 x  $10^{-4}$ .

The solubility of water in butanoic acid ethyl ester at  $20^{\circ}C$  was reported to be 0.75 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.046.

| AUXILIARY INFORMATION                                        |                                                                                      |
|--------------------------------------------------------------|--------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The method was not specified. | SOURCE AND PURITY OF MATERIALS:<br>(1) Source not specified,                         |
|                                                              | commercial product; purity 99%,<br>b.p. range $107-131^{\circ}C$ , $d_4^{20}$ 0.880. |
|                                                              | (2) Not specified.                                                                   |
|                                                              | ESTIMATED ERROR:                                                                     |
|                                                              | Not specified.                                                                       |
|                                                              | REFERENCES:                                                                          |
|                                                              |                                                                                      |

| СОМРО | NENTS:                                                                                                                | ORIGINAL MEASUREMENTS:                                         |
|-------|-----------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------|
| (1)   | Butanoic acid ethyl ester<br>( <i>ethyl butyrate</i> ); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[105-54-4] | Rao, J.R.; Rao, C.V.<br>J. Appl. Chem. <u>1957</u> , 7, 435-9. |
| (2)   | Water; H <sub>2</sub> O; [7732-18-5]                                                                                  |                                                                |
| VARIA | BLES:                                                                                                                 | PREPARED BY:                                                   |
| Т/К   | = 303                                                                                                                 | A. Skrzecz                                                     |

The solubility of butanoic acid ethyl ester in water at  $30^{\circ}$ C was reported to be 0.8 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.0012.

The solubility of water in butanoic acid ethyl ester at  $30^{\circ}$ C was reported to be 1.1 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.067.

| AUXILIARY 1                                                                                                                                                                             | INFORMATION                                                                                                                                                                                                                                     |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used.<br>The data and method were reported<br>together with the ternary system<br>butanoic acid ethyl ester-water-<br>methanol. | SOURCE AND PURITY OF MATERIALS:<br>(1) Naarden, reagent grade; b.p.<br>121.5°C, d <sup>30</sup> 0.8685, n <sub>D</sub> <sup>30</sup> 1.3880.<br>(2) Distilled; free from CO <sub>2</sub> .<br>ESTIMATED ERROR:<br>Temp. ±0.02°C.<br>REFERENCES: |
|                                                                                                                                                                                         |                                                                                                                                                                                                                                                 |

| 316                                                                                                                                                                                              |                                                                                                                                   |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|
| COMPONENTS:                                                                                                                                                                                      | ORIGINAL MEASUREMENTS:                                                                                                            |
| <pre>(1) Butanoic acid ethyl ester   (ethyl butyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;   [105-54-4]</pre>                                                                              | Venkataratnam, A.; Rao, J.R.;<br>Rao, C.V.<br><i>Chem. Eng. Sci.</i> <u>1957</u> , 7, 102-10.                                     |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                         |                                                                                                                                   |
| VARIABLES:                                                                                                                                                                                       | PREPARED BY:                                                                                                                      |
| T/K = 303                                                                                                                                                                                        | A. Skrzecz                                                                                                                        |
| to be 0.8 g(1)/100g sln. The correspon<br>lated by the compiler is 0.0012.<br>The solubility of water in butanoic at<br>to be 0.6 g(2)/100g sln. The correspon<br>lated by the compiler is 0.04. | anding mole fraction, $x_1$ , value calcu-<br>acid ethyl ester at 30°C was reported<br>anding mole fraction, $x_2$ , value calcu- |

# AUXILIARY INFORMATION

The titration method described by Othmer, White and Trueger (ref 1) was used. The data were reported together with the ternary system butanoic acid ethyl ester-water-2-propanone (ethyl butyrate-wateracetone).

# SOURCE AND PURITY OF MATERIALS:

- (1) Naarden, analytical grade; used as received; b.p.  $121.5^{\circ}$ C,  $d^{30}$  0.8685,  $n^{30}$  1.3880.
- (2) Distilled; free of CO<sub>2</sub>.

ESTIMATED ERROR:

Not specified.

# **REFERENCES:**

 Othmer, D.F.; White, R.E.; Trueger, E. Ind. Eng. Chem. <u>1941</u>, 33, 1240.

| COMPONENTS:                                                                                                             | ORIGINAL MEASUREMENTS:                                         |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------|
| <pre>(1) Butanoic acid ethyl ester<br/>(ethyl butyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;<br/>[105-54-4]</pre> | Rao, R.J.; Rao, C.V.<br>J. Appl. Chem. <u>1959</u> , 9, 69-73. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                |                                                                |
| VARIABLES:                                                                                                              | PREPARED BY:                                                   |
| T/K = 303                                                                                                               | A. Skrzecz                                                     |

The solubility of butanoic acid ethyl ester in water at  $30^{\circ}$ C was reported to be 0.8 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 0.0012.

The solubility of water in butanoic acid ethyl ester at  $30^{\circ}$ C was reported to be 0.6 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.04.

| AUXILIARY INFORMATION                                                                                                                                                                                                         |                                                                                                                                                                                                         |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>Presumably the titration method<br>described by Rao and Rao (ref 1)<br>was used. The data were reported<br>together with the ternary system<br>butanoic acid ethyl ester-water-<br>1-propanol. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Naarden, analytical grade;    b.p. 121.5°C, d<sup>30</sup> 0.8685,    n<sub>D</sub><sup>30</sup> 1.3880. (2) Distilled.  ESTIMATED ERROR: Not specified.</pre> |
|                                                                                                                                                                                                                               | REFERENCES:<br>1. Rao, R.J.; Rao, C.V. J. Appl.<br>Chem. <u>1957</u> , 7, 435.                                                                                                                          |

| COMPONENTS:                                                                     | ORIGINAL MEASUREMENTS:                            |
|---------------------------------------------------------------------------------|---------------------------------------------------|
| (1) Butanoic acid ethyl ester                                                   | Richon, D.; Viallard, A.                          |
| (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[105-54-4] | Fluid Phase Equilib. <u>1985</u> , 21,<br>279-93. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                        |                                                   |
| VARIABLES:                                                                      | PREPARED BY:                                      |
| T/K = 298                                                                       | A. Skrzecz                                        |

The solubility of butanoic acid ethyl ester in water at 298.1 K was reported to be 0.00577 mol(1)/100g(2). The corresponding mass per cent and mole fraction,  $x_1$ , values calculated by the compiler are 0.666 g(1)/100g sln and 0.001038.

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric method was used. The Phoenix model 1-2000T differential refractometer from Texas Instruments was used and the solubility was determined from a characteristic calibration curve as described in the thesis of Richon (ref 1).

#### SOURCE AND PURITY OF MATERIALS:

- BDH: purified by preparation gas chromatographic method; purity >99.5%, water content was negligible.
- (2) Distilled.

ESTIMATED ERROR:

Not specified.

**REFERENCES:** 

1. Richon, D. *Thesis*, University de Clermont-Ferrand, <u>1974</u>.

| COMPONENTS:                                                       | ORIGINAL MEASUREMENTS:                      |
|-------------------------------------------------------------------|---------------------------------------------|
| <pre>(1) Butanoic acid ethyl ester</pre>                          | Stephenson, R.; Stuart, J.                  |
| (ethyl butyrate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; | <i>J. Chem. Eng. Data</i> <u>1986</u> , 31, |
| [105-54-4]                                                        | 56-70.                                      |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                          |                                             |
| VARIABLES:                                                        | PREPARED BY:                                |
| T/K = 273 - 364                                                   | Z. Maczynska                                |

Mutual solubility of butanoic acid ethyl ester and water

EXPERIMENTAL VALUES:

| t/°C | g(1)/10        | )0g sln        | $x_1$ (compiler) |                |  |
|------|----------------|----------------|------------------|----------------|--|
|      | (2)-rich phase | (1)-rich phase | (2)-rich phase   | (1)-rich phase |  |
| 0    | 1.06           | 99.44          | 0.00166          | 0.9650         |  |
| 9.5  | 0.81           | 99.32          | 0.00126          | 0.9577         |  |
| 20.0 | 0.69           | 99.21          | 0.00108          | 0.9512         |  |
| 31.0 | 0.58           | 98.98          | 0.00090          | 0.9377         |  |
| 39.9 | 0.52           | 98.93          | 0.00081          | 0.9348         |  |
| 50.0 | 0.46           | 98.78          | 0.00072          | 0.9262         |  |
| 60.4 | 0.46           | 98.83          | 0.00072          | 0.9291         |  |
| 70.2 | 0.46           | 98.72          | 0.00072          | 0.9228         |  |
| 80.3 | 0.46           | 98.82          | 0.00072          | 0.9285         |  |
| 90.5 | 0.44           | 98.74          | 0.00068          | 0.9240         |  |

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                      |  |  |  |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|--|--|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used.<br>Component (1) was equilibrated<br>with component (2) at a given<br>temperature in a thermostat. Each<br>layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile<br>(or sometimes propanol) to the<br>organic layer sample and measuring<br>by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher<br>boiling material (e.g. 1-hexanol)<br>was used to determine (2) in the<br>water layer. | <pre>INFORMATION SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer- cial sample; purity 99%; used as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less, for colubility goo above</pre> |  |  |  |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | REFERENCES:                                                                                                                                                                                                                          |  |  |  |  |

| COMPONENTS: |                                                            | EVALUATOR:                          |  |
|-------------|------------------------------------------------------------|-------------------------------------|--|
| (1)         | Formic acid 3-methyl-1-butyl                               | G.T. Hefter, School of Mathematical |  |
|             | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-45-2] | Murdoch University, Perth, W.A.,    |  |
| (2)         | Water; H <sub>2</sub> O; [7732-18-5]                       | Australia<br>January, 1989          |  |

#### CRITICAL EVALUATION:

Quantitative solubility data for the formic acid 3-methyl-1-butyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

| TABLE 1     | : Quantitative  | <u>Solubility</u> | Studies | <u>of the</u> |
|-------------|-----------------|-------------------|---------|---------------|
| Formic acid | 3-methyl-1-buty | l_ester (1)       | - Water | (2) System    |

| Reference                     | T/K     | Solubility | Method      |
|-------------------------------|---------|------------|-------------|
| Traube (ref 1)                | 295     | (1) in (2) | unspecified |
| Trofimov (ref 2)              | 293-363 | mutual     | GLC         |
| Stephenson and Stuart (ref 3) | 273-364 | mutual     | GLC         |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF FORMIC ACID 3-METHYL-1-BUTYL ESTER (1) IN WATER (2)

All the available data for the solubility of formic acid 3-methyl-1butyl ester (1) in water (2) are summarized in Table 2 and plotted in Figure 1. The data are in poor agreement with the two major studies (ref 2,3) showing a quite different temperature dependence. In the absence of confirmatory studies it is not possible at this stage to prefer either data set although it may be noted that ester solubilities in water do *not* usually show a monotonic increase with temperature as observed by Trofimov (ref 2). This system clearly warrants further study.

TABLE 2: Solubilities ofFormic acid 3-methyl-1-butyl ester (1) in Water (2)

| T/K | Solubilities                                        |                           |                 |  |  |  |
|-----|-----------------------------------------------------|---------------------------|-----------------|--|--|--|
|     | Reported values                                     | "Best" values (± $\sigma$ | n) <sup>a</sup> |  |  |  |
|     | g(1)/100g sln                                       | g(1)/100g sln             | $10^4 x_1$      |  |  |  |
| 273 | 0.198 (ref 3)                                       | 0.2                       | 3               |  |  |  |
| 283 | 0.15 <sup>*</sup> (ref 3)                           | 0.2                       | 3               |  |  |  |
| 293 | $0.31^{b}$ (ref 1), 0.244 (ref 2),<br>0.13* (ref 3) | 0.19 ± 0.06               | 2.9             |  |  |  |

| COMPONENTS: |                                                                                                                                   | EVALUATOR:                                                                                                     |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|
| (1)         | Formic acid 3-methyl-1-butyl<br>ester ( <i>isopentyl formate</i> );<br>C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-45-2] | G.T. Hefter, School of Mathematical<br>and Physical Sciences,<br>Murdoch University, Perth, W.A.,<br>Australia |
| (2)         | Water; H <sub>2</sub> O; [7732-18-5]                                                                                              | January, 1989                                                                                                  |

CRITICAL EVALUATION: (continued)

| T/K | Solubilit                                            | zies                             |
|-----|------------------------------------------------------|----------------------------------|
|     | Reported values                                      | "Best" values $(\pm \sigma_n)^a$ |
|     | g(1)/100g sln                                        | $g(1)/100g \ sln \ 10^4 x_1$     |
| 298 | 0.25 <sup>*</sup> (ref 2), 0.12 <sup>*</sup> (ref 3) | 0.2 ± 0.1 3                      |
| 303 | 0.26 <sup>*</sup> (ref 2), 0.12 <sup>*</sup> (ref 3) | 0.2 ± 0.1 3                      |
| 313 | 0.28 <sup>*</sup> (ref 2), 0.11 <sup>*</sup> (ref 3) | 0.2 ± 0.1 3                      |
| 323 | 0.29 <sup>*</sup> (ref 2), 0.11 <sup>*</sup> (ref 3) | 0.2 ± 0.1 3                      |
| 333 | 0.34 <sup>*</sup> (ref 2), 0.11 <sup>*</sup> (ref 3) | _ c _                            |
| 343 | 0.46 <sup>*</sup> (ref 2), 0.11 <sup>*</sup> (ref 3) | _ c _                            |
| 353 | 0.66* (ref 2), 0.12* (ref 3)                         | _ c _                            |
| 363 | 0.95 <sup>*</sup> (ref 2), 0.13 <sup>*</sup> (ref 3) | _ <sup>c</sup> _                 |

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass solubilities.

<sup>b</sup> 295 K, not included in calculation of average.

С

Disagreement too marked for meaningful calculation of "Best" values.



FIGURE 1. Selected data for the solubility of formic acid 3-methyl-1-butyl ester (1) in water (2): ref 2 ( $\bullet$ ); ref 3 (0). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

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| COMPONENTS: |                                                            | EVALUATOR:                          |  |
|-------------|------------------------------------------------------------|-------------------------------------|--|
| (1)         | Formic acid 3-methyl-1-butyl                               | G.T. Hefter, School of Mathematical |  |
|             | <pre>ester (isopentyl formate);</pre>                      | and Physical Sciences,              |  |
|             | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-45-2] | Murdoch University, Perth, W.A.,    |  |
| (2)         | Water: H <sub>2</sub> O: [7732-18-5]                       | Australia                           |  |
| (-)         |                                                            | January, 1989                       |  |

#### CRITICAL EVALUATION: (continued)

# 2. SOLUBILITY OF WATER (2) IN FORMIC ACID 3-METHYL-1-BUTYL ESTER (1)

Only Trofimov (ref 2) and Stephenson and Stuart (ref 3) have reported solubilities of water (2) in formic acid 3-methyl-1-butyl ester (1). Their data are summarized in Table 3 and plotted in Figure 2. As for the  $H_2O$ -rich phase, the data of refs 2 and 3 are not in very good agreement although they both show an increase in solubility with increasing temperature. The average "Best" values should be regarded as very Tentative pending further studies.

|                 | $\mathbf{T}$ | ABLE | 3: T   | entat: | <u>ive Solubilities</u> |       |     |
|-----------------|--------------|------|--------|--------|-------------------------|-------|-----|
| <u>of Water</u> | (2)          | in   | Formic | acid   | 3-methyl-1-butyl        | ester | (1) |

| T/K                   | Solubilit                          | ies           |                    |
|-----------------------|------------------------------------|---------------|--------------------|
|                       | Reported values                    | "Best" values | $(\pm \sigma_n)^a$ |
|                       | g(2)/100g sln                      | g(2)/100g sln | $10^2 x_2$         |
| 273 0.80*             | (ref 3)                            | 0.8           | 5                  |
| 283 0.92*             | (ref 3)                            | 0.9           | 6                  |
| 293 0.535             | (ref 2), 1.05 <sup>*</sup> (ref 3) | 0.8 ± 0.3     | 5                  |
| 298 0.58*             | (ref 2), 1.13 <sup>*</sup> (ref 3) | 0.9 ± 0.3     | 6                  |
| 303 0.63*             | (ref 2), 1.19 <sup>*</sup> (ref 3) | 0.9 ± 0.3     | 6                  |
| 313 0.725             | (ref 2), 1.35 <sup>*</sup> (ref 3) | 1.0 ± 0.3     | 6                  |
| 323 0.83*             | (ref 2), 1.53 <sup>*</sup> (ref 3) | 1.2 ± 0.4     | 7                  |
| 333 0.934             | (ref 2), 1.70 <sup>*</sup> (ref 3) | 1.3 ± 0.4     | 8                  |
| 343 1.05*             | (ref 2), 1.91 <sup>*</sup> (ref 3) | 1.5 ± 0.4     | 9                  |
| 353 1.18 <sup>*</sup> | (ref 2), 2.11 <sup>*</sup> (ref 3) | 1.6 ± 0.5     | 9                  |
| 363 1.32*             | (ref 2), 2.35 <sup>*</sup> (ref 3) | 1.8 ± 0.5     | 11                 |

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.



| ົ | 2 | Λ |
|---|---|---|
| J | 2 | 4 |

| COMPONENTS:                                                                                                                                                                                 | ORIGINAL MEASUREMENTS:                                                                                                                               |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| (1) Formic acid 3-methyl-1-butyl                                                                                                                                                            | Traube, J.                                                                                                                                           |
| ester (isopentyl formate);                                                                                                                                                                  | Ber. Dtsch. Chem. Ges. <u>1884</u> , 17,<br>2294-216                                                                                                 |
| $C_6 R_{12} O_2$ ; [110-45-2]                                                                                                                                                               | 2294-310.                                                                                                                                            |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                    |                                                                                                                                                      |
| VARIABLES:                                                                                                                                                                                  | PREPARED BY:                                                                                                                                         |
| T/K = 295                                                                                                                                                                                   | A. Skrzecz                                                                                                                                           |
| EXPERIMENTAL VALUES:<br>The solubility of formic acid 3-methy<br>reported to be 1 part of isopentyl for<br>corresponding mass percent and mole for<br>compiler are 0.31 g(1)/100g sln and 4 | yl-1-butyl ester in water at 22°C was<br>prmate in 325 parts of water. The<br>fraction, $x_1$ , values calculated by the<br>4.8 x 10 <sup>-4</sup> . |
| AUXILIARY                                                                                                                                                                                   | INFORMATION                                                                                                                                          |
|                                                                                                                                                                                             |                                                                                                                                                      |
| merrod/APPARATUS/PROCEDURE:                                                                                                                                                                 | SOURCE AND PURITY OF MATERIALS:                                                                                                                      |
| The method was not specified.                                                                                                                                                               | (1) Not specified.                                                                                                                                   |
|                                                                                                                                                                                             | (2) Not specified.                                                                                                                                   |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             | ESTIMATED ERROR:                                                                                                                                     |
|                                                                                                                                                                                             | Not specified.                                                                                                                                       |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             | REFERENCES:                                                                                                                                          |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             |                                                                                                                                                      |
|                                                                                                                                                                                             |                                                                                                                                                      |

| COMPONENT                                                                                                | rs:                                                                                                                                                                                                                                         | ORIGINAL MEASUREMENTS:                                                                                                                                                  |  |
|----------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| (1) Formic acid 3-methyl-1-butyl                                                                         |                                                                                                                                                                                                                                             | Trofimov, A.N.                                                                                                                                                          |  |
| ester (isopentyl formate);<br>C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-45-2]                 |                                                                                                                                                                                                                                             | Gidroliz. Lesokhim. Prom. <u>1969</u> ,<br>22(8), 9.                                                                                                                    |  |
| (2) Wat                                                                                                  | er; H <sub>2</sub> O; [7732-18-5]                                                                                                                                                                                                           |                                                                                                                                                                         |  |
| VARIABLES                                                                                                |                                                                                                                                                                                                                                             | PREPARED BY:                                                                                                                                                            |  |
| T/K = 29                                                                                                 | 93 - 363                                                                                                                                                                                                                                    | A. Skrzecz                                                                                                                                                              |  |
|                                                                                                          |                                                                                                                                                                                                                                             |                                                                                                                                                                         |  |
| EXPERIMEN<br>Mutua                                                                                       | TAL VALUES:<br>al solubility of formic acid                                                                                                                                                                                                 | 3-methyl-1-butyl ester and water                                                                                                                                        |  |
| t/°C                                                                                                     | <i>X</i> 1                                                                                                                                                                                                                                  | g(1)/100g sln (compiler)                                                                                                                                                |  |
|                                                                                                          | (2)-rich phase (1)-rich pha                                                                                                                                                                                                                 | se (2)-rich phase (1)-rich phase                                                                                                                                        |  |
| 20                                                                                                       | 0.00038 0.9665                                                                                                                                                                                                                              | 0.244 99.465                                                                                                                                                            |  |
| 40                                                                                                       | 0.00047 0.9550                                                                                                                                                                                                                              | 0.302 99.275                                                                                                                                                            |  |
| 60                                                                                                       | 0.00049 0.9427                                                                                                                                                                                                                              | 0.315 99.066                                                                                                                                                            |  |
| 90.2 <sup>a</sup>                                                                                        | 0.0015 0.9200                                                                                                                                                                                                                               | 0.96 98.669                                                                                                                                                             |  |
|                                                                                                          |                                                                                                                                                                                                                                             |                                                                                                                                                                         |  |
|                                                                                                          | AUXILIARY                                                                                                                                                                                                                                   | INFORMATION                                                                                                                                                             |  |
| METHOD/AP                                                                                                | PARATUS/PROCEDURE:                                                                                                                                                                                                                          | SOURCE AND PURITY OF MATERIALS:                                                                                                                                         |  |
| The anal<br>two-phas<br>thermost<br>netic st<br>and mixe<br>temperat<br>arated f<br>glc. The<br>than 2%. | ytical method was used. The<br>e mixture was placed in a<br>ated apparatus with a mag-<br>irrer and reflux condenser<br>d for 1 h. (at the boiling<br>ure for 1/2 h. only), sep-<br>or 20 min, and analyzed by<br>ester hydrolysis was less | <ul> <li>(1) Source not specified; properties were described in the publication of Trofimov, Chashchin and Botsharnikov (ref 1).</li> <li>(2) Not specified.</li> </ul> |  |
|                                                                                                          |                                                                                                                                                                                                                                             | ESTIMATED ERROR:                                                                                                                                                        |  |
|                                                                                                          |                                                                                                                                                                                                                                             | Soly. ±1.5% (max. relative<br>error of analysis).                                                                                                                       |  |
|                                                                                                          |                                                                                                                                                                                                                                             | REFERENCES:<br>1. Trofimov, A.N.; Chashchin, A.;<br>Botsharnikov, E.V. Gidroliz.<br>Lesokhim. Prom. <u>1968</u> , (5).                                                  |  |

| COMPONENTS:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                   | ORIGINAL MEASUREME | INTS:                             |                  |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|--------------------|-----------------------------------|------------------|
| (1) Formic acid 3-methyl-1-butyl                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                   | Stephenson, R.; S  | tuart, J.                         |                  |
| <pre>ester (isopentyl formate);</pre>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                   | J. Chem. Eng. Dat  | a <u>1986</u> , 31,               |                  |
| C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [110-45-2]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                   | 56-70.             |                                   |                  |
| (2) Wa                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | ter; H <sub>2</sub> 0; [7732-1                                    | .8-5]              |                                   |                  |
| VARIABLE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | S:                                                                |                    | PREPARED BY:                      |                  |
| T/K = 2                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 73 - 364                                                          |                    | Z. Maczynska                      |                  |
| EXPERIME                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | NTAL VALUES:                                                      |                    | 4 <u></u>                         |                  |
| Mutu                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | al solubility of                                                  | formic acid 3      | -methyl-1-butyl est               | er and water     |
| t/°C                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | g(1)/10                                                           | 0g sln             | x <sub>1</sub> (comp              | iler)            |
| •                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | (2)-rich phase                                                    | (1)-rich phas      | e (2)-rich phase                  | (1)-rich phase   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
| 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 0.198                                                             | 99.24              | 0.000307                          | 0.9529           |
| 9.3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 0.151                                                             | <b>`98.91</b>      | 0.000234                          | 0.9336           |
| 19.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.108                                                             | 98.92              | 0.000168                          | 0.9342           |
| 31.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.116                                                             | 98.80              | 0.000180                          | 0.9274           |
| 39.6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.111                                                             | 98.66              | 0.000172                          | 0.9195           |
| 50.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.135                                                             | 98.51              | 0.000209                          | 0.9111           |
| 60.4                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | -                                                                 | 98.25              | -                                 | 0.8970           |
| 70.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.115                                                             | 98.08              | 0.000178                          | 0.8879           |
| 80.3                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.082                                                             | 97.93              | 0.000127                          | 0.8800           |
| 90.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 0.131                                                             | 97.64              | 0.000203                          | 0.8651           |
| std. d                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | lev. 0.005                                                        | 0.02               |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
| l de la constante de |                                                                   |                    |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | ΔΙΙΥΤΓΤΑΡΥ ΤΝΕΟΡΜΑΤΤΟΝ                                            |                    |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
| METHOD/AI                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | METHOD/APPARATUS/PROCEDURE:                                       |                    | SOURCE AND PURITY                 | OF MATERIALS:    |
| The anal                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | lytical method wa                                                 | s used.            | (1) Source not specified, commer- |                  |
| with con                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | nt (1) was equili<br>mponent (2) at a                             | brated<br>given    | cial sample;<br>as received.      | purity 96%; used |
| temperat                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | ture in a thermos                                                 | tat. Each          | (2) Not an official               |                  |
| (1) was                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | determined by ad                                                  | ding a             | (2) Not specified                 | •                |
| weighed                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | amount of aceton                                                  | itrile             |                                   |                  |
| organic                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | (or sometimes propanol) to the organic layer sample and measuring |                    |                                   |                  |
| by a Gow-Mac thermal conductivity                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                   | ESTIMATED ERROR:   |                                   |                  |
| (Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                   | Accuracy of method | d 0.1 wt% or less,                |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   | tor solubility, s  |                                   |                  |
| boiling material (e.g. 1-hexanol)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                                                                   |                    |                                   |                  |
| was used to determine (2) in the water layer.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                   | PEEPENCES.         |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   | KELEKERGEG +       |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   | [                  |                                   |                  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                   |                    |                                   |                  |

| COMPONENTS:                                                                                                        | ORIGINAL MEASUREMENTS:                                                              |
|--------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| <pre>(1) Formic acid pentyl ester   (pentyl formate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;   [638-49-3]</pre> | Stephenson, R.; Stuart, J.<br><i>J. Chem. Eng. Data</i> <u>1986</u> , 31,<br>56-70. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                           |                                                                                     |
| VARIABLES:                                                                                                         | PREPARED BY:                                                                        |
| T/K = 273 - 364                                                                                                    | Z. Maczynska                                                                        |
|                                                                                                                    |                                                                                     |

Mutual solubility of formic acid pentyl ester and water

| t/°C     | g(1)/100g sln  |                | $x_1$ (compiler) |                |  |
|----------|----------------|----------------|------------------|----------------|--|
|          | (2)-rich phase | (1)-rich phase | (2)-rich phase   | (1)-rich phase |  |
| 0        | 0.36           | 99.01          | 0.00056          | 0.9394         |  |
| 9.1      | 0.31           | 99.03          | 0.00048          | 0.9406         |  |
| 19.9     | 0.27           | 98.93          | 0.00042          | 0.9348         |  |
| 30.9     | 0.26           | 98.89          | 0.00040          | 0.9325         |  |
| 39.6     | 0.26           | 98.75          | 0.00040          | 0.9245         |  |
| 50.0     | 0.27           | 98.66          | 0.00042          | 0.9195         |  |
| 60.1     | 0.24           | 98.63          | 0.00037          | 0.9178         |  |
| 70.2     | 0.27           | 98.51          | 0.00042          | 0.9111         |  |
| 80.0     | 0.29           | 98.51          | 0.00045          | 0.9111         |  |
| 90.5     | 0.26           | 97.59          | 0.00040          | 0.8626         |  |
| std. dev | v. 0.01        | 0.02           |                  |                |  |

| AUXILIARY                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | INFORMATION                                                                                                                                                                                                                                          |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used.<br>Component (1) was equilibrated<br>with component (2) at a given<br>temperature in a thermostat. Each<br>layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile<br>(or sometimes propanol) to the<br>organic layer sample and measuring<br>by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher<br>boiling material (e.g. 1-hexanol)<br>was used to determine (2) in the<br>water layer. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer-<br/>cial sample; purity 95%; used<br/>as received. (2) Not specified.  ESTIMATED ERROR: Accuracy of method 0.1 wt% or less,<br/>for solubility, see above.  REFERENCES:</pre> |

| СОМРС                             | DNENTS:                                                                                           | EVALUATOR:                                                    |
|-----------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------|
| (1)                               | Pentanoic acid methyl ester<br>(methyl valerate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; | G.T. Hefter, School of Mathematical<br>and Physical Sciences, |
|                                   | [624-24-8]                                                                                        | Murdoch University, Perth, W.A.,                              |
| (2) Water; $H_{2}O$ ; [7732-18-5] | Australia                                                                                         |                                                               |
|                                   |                                                                                                   | January, 1989                                                 |

## CRITICAL EVALUATION:

Quantitative solubility data for the pentanoic acid methyl ester (1) water (2) system have been reported in the publications listed in Table 1.

#### TABLE 1: Quantitative Solubility Studies of the Pentanoic acid methyl ester (1) - Water (2) System

| Reference                     | T/K     | Solubility | Method    |
|-------------------------------|---------|------------|-----------|
| Bomshtein et al. (ref 1)      | 293-353 | mutual     | titration |
| Stephenson and Stuart (ref 2) | 273-363 | mutual     | GLC       |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

#### 1. SOLUBILITY OF PENTANOIC ACID METHYL ESTER (1) IN WATER (2)

All the available data are summarized in Table 2 and plotted in Figure As can be seen the values are in poor agreement, showing an opposite 1. dependence on temperature. Although ester solubilities in water commonly exhibit a minimum when plotted against temperature (as found for the present system by Stephenson and Stuart (ref 2)), in the absence of any independent studies it is not possible to prefer any one data set. Consequently, no "Best" values have been derived and this system clearly requires further study. The interested user is referred to the relevant Data Sheets for further information.

|     | <u>TABLE 2: Reported Solubilities</u><br>of Pentanoic acid methyl ester (1) in Water (2) |
|-----|------------------------------------------------------------------------------------------|
| Т/К | Reported Solubilities                                                                    |
|     | g(1)/100g sln                                                                            |
| 273 | 0.80 (ref 2)                                                                             |
| 283 | 0.63 <sup>*</sup> (ref 2)                                                                |
| 293 | 0.06 (ref 1), 0.52 <sup>*</sup> (ref 2)                                                  |
| 298 | 0.13 <sup>*</sup> (ref 1), 0.49 <sup>*</sup> (ref 2)                                     |
| 303 | 0.19 (ref 1), 0.47 <sup>*</sup> (ref 2)                                                  |
| 313 | 0.32 (ref 1), 0.45 <sup>*</sup> (ref 2)                                                  |
|     |                                                                                          |



| COMPONENTS:                                                                                                      | EVALUATOR:                                                 |
|------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------|
| <ol> <li>Pentanoic acid methyl ester<br/>(methyl valerate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> </ol> | G.T. Hefter, School of Mathematical and Physical Sciences, |
| [624-24-8]                                                                                                       | Murdoch University, Perth, W.A.,                           |
| (2) Water: H <sub>2</sub> O: [7732-18-5]                                                                         | Australia                                                  |
| (2,                                                                                                              | January, 1989                                              |

CRITICAL EVALUATION: (continued)

#### SOLUBILITY OF WATER (2) IN PENTANOIC ACID METHYL ESTER (1) 2.

All the available data (ref 1,2) for the solubility of water (2) in pentanoic acid methyl ester (1) are summarized in Table 3 and plotted in As for the  $H_2O$ -rich phase, the data of Bomshtein et al. (ref 1) Figure 2. differ markedly from those of Stephenson and Stuart (ref 2), albeit both studies at least give a similar dependence on temperature in this phase although the data are rather scattered. In the absence of confirmatory studies it is not possible at this stage to prefer one of these sets and no "Best" values have been calculated. Nevertheless, it may be noted that the solubilities of water in the organic-rich phase reported by Bomshtein et al. in other systems are often higher than reliable values. This system clearly requires re-investigation. The interested user is referred to the relevant Data Sheets for further information.

|            | of Water (2) in Pentanoic acid methyl ester (1)      |
|------------|------------------------------------------------------|
| <b>т/к</b> | Reported Solubilities<br>g(2)/100 g sln              |
| 273        | 0.56 (ref 2)                                         |
| 283        | 0.64* (ref 2)                                        |
| 293        | 2.30 (ref 1), 0.76 <sup>*</sup> (ref 2)              |
| 298        | 2.45 <sup>*</sup> (ref 1), 0.90 <sup>*</sup> (ref 2) |
| 303        | 2.60 (ref 1), 1.02* (ref 2)                          |
| 313        | 2.80 (ref 1), 1.05 (ref 2)                           |
| 323        | 3.10 (ref 1), 1.06 (ref 2)                           |
| 333        | 3.40 (ref 1), 1.09 (ref 2)                           |
| 343        | 4.10 (ref 1), 1.14 (ref 2)                           |
| 353        | 5.50 (ref 1), 1.30 (ref 2)                           |
| 363        | 1.55 (ref 2)                                         |



| COMPONENTS:                                                                                                        | ORIGINAL MEASUREMENTS:                                                                            |
|--------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| <pre>(1) Pentanoic acid methyl ester (methyl valerate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [624-24-8]</pre> | Bomshtein, A.L.; Trofimov, A.N.;<br>Serafimov, L.A.<br>Zh. Prikl. Khim. <u>1978</u> , 51, 1280-2. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                           |                                                                                                   |
| VARIABLES:                                                                                                         | PREPARED BY:                                                                                      |
| T/K = 293 - 353                                                                                                    | A. Skrzecz                                                                                        |

Mutual solubility of pentanoic acid methyl ester and water

| t/°C | (2)-rich phase | (1)-rich phase | g(1)/100g sl:<br>(2)-rich phase | n (compiler)<br>(1)-rich phase |
|------|----------------|----------------|---------------------------------|--------------------------------|
| 20   | 0.0001         | 0.8683         | 0.06                            | 97.70                          |
| 30   | 0.0003         | 0.8532         | 0.19                            | 97.40                          |
| 40   | 0.0005         | 0.8434         | 0.32                            | 97.20                          |
| 50   | 0.0007         | 0.8291         | 0.45                            | 96.90                          |
| 60   | 0.0009         | 0.8151         | 0.58                            | 96.60                          |
| 70   | 0.0012         | 0.7840         | 0.77                            | 95.90                          |
| 80   | 0.0015         | 0.7272         | 0.96                            | 94.50                          |

| AUXILIARY INFORMATION                                                                                                                      |                                                                                                                                                                                                                                        |  |  |
|--------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| METHOD/APPARATUS/PROCEDURE:<br>The titration method was used at<br>constant temperature. No further<br>details were reported in the paper. | SOURCE AND PURITY OF MATERIALS:<br>(1) Source not specified; distil-<br>led; without impurities by glc,<br>b.p. 127.2°C, n <sub>D</sub> <sup>0</sup> 1.398.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |  |  |
|                                                                                                                                            |                                                                                                                                                                                                                                        |  |  |

| COMPONENTS:                                                                                                             | ORIGINAL MEASUREMENTS:                                                       |
|-------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
| (1) Pentanoic acid methyl ester<br>(methyl valerate); $C_6H_{12}O_2$ ;<br>[624-24-8]<br>(2) Water; $H_2O$ ; [7732-18-5] | Stephenson, R.; Stuart, J.<br>J. Chem. Eng. Data <u>1986</u> , 31,<br>56-70. |
| VARIABLES:<br>T/K = 273 - 363                                                                                           | PREPARED BY:<br>Z. Maczynska                                                 |

Mutual solubility of pentanoic acid methyl ester and water

| t/°C     | g(1)/100g sln  |                | $x_1$ (compiler) |                |
|----------|----------------|----------------|------------------|----------------|
|          | (2)-rich phase | (1)-rich phase | (2)-rich phase   | (1)-rich phase |
| 0        | 0.80           | 99.44          | 0.00125          | 0.9650         |
| 9.2      | 0.64           | 99.37          | 0.00100          | 0.9607         |
| 19.5     | 0.53           | 99.25          | 0.00083          | 0.9535         |
| 29.5     | 0.45           | 98.98          | 0.00070          | 0.9377         |
| 39.8     | 0.47           | 98.95          | 0.00073          | 0.9360         |
| 50.0     | 0.46           | 98.95          | 0.00072          | 0.9360         |
| 60.1     | 0.44           | 98.90          | 0.00068          | 0.9331         |
| 70.2     | 0.46           | 98.88          | 0.00072          | 0.9319         |
| 80.3     | 0.46           | 98.67          | 0.00072          | 0.9200         |
| 90.5     | 0.45           | 98.43          | 0.00070          | 0.9067         |
| std. dev | 7. 0.01        | 0.02           |                  |                |

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                    |  |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used.<br>Component (1) was equilibrated<br>with component (2) at a given<br>temperature in a thermostat. Each<br>layer was sampled with a syringe;<br>(1) was determined by adding a<br>weighed amount of acetonitrile<br>(or sometimes propanol) to the<br>organic layer sample and measuring<br>by a Gow-Mac thermal conductivity<br>gc the (1)/acetonitrile peak ratio<br>(Chromosorb 101 packing and a HP<br>3390 A recorder-integrator).<br>A similar procedure but a higher<br>boiling material (e.g. 1-hexanol)<br>was used to determine (2) in the<br>water layer. | <pre>SOURCE AND PURITY OF MATERIALS: (1) Source not specified, commer-<br/>cial sample; purity 99%; used<br/>as received. (2) Not specified. ESTIMATED ERROR: Accuracy of method 0.1 wt% or less,<br/>for solubility, see above. REFERENCES:</pre> |  |  |

| OMPONENTS:                                                                         |                                                                                                                               | ORIGINAL MEASUREME                                                                                                          | NTS:                                                                                                                                                               |                                                                                                                            |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| (1) Prop                                                                           | <pre>) Propanoic acid, 2,2-dimethyl-,<br/>methyl ester<br/>(methyl trimethylacetate);</pre>                                   |                                                                                                                             | Stephenson, R.; Stuart, J.<br>J. Chem. Eng. Data <u>1986</u> , 31,<br>56-70.                                                                                       |                                                                                                                            |
| metr<br>(met                                                                       |                                                                                                                               |                                                                                                                             |                                                                                                                                                                    |                                                                                                                            |
| с <sub>6</sub> н <sub>1</sub>                                                      | 2 <sup>0</sup> 2; [598-98-1]                                                                                                  |                                                                                                                             |                                                                                                                                                                    |                                                                                                                            |
| 2) Wate                                                                            | er; H <sub>2</sub> O; [7732-18-5                                                                                              | 5]                                                                                                                          |                                                                                                                                                                    |                                                                                                                            |
| RIABLES:                                                                           | . <u> </u>                                                                                                                    |                                                                                                                             | PREPARED BY:                                                                                                                                                       |                                                                                                                            |
| T/K = 273                                                                          | - 364                                                                                                                         |                                                                                                                             | 2. Maczynska                                                                                                                                                       |                                                                                                                            |
| Mutual                                                                             | solubility of 2,2-                                                                                                            | -dimethylpr                                                                                                                 | opanoic acid methyl                                                                                                                                                | ester and wate                                                                                                             |
| Mutual<br><br>t/°C                                                                 | g(1)/100g<br>(2)-rich phase (1)                                                                                               | -dimethylpr<br>sln<br>-rich phase                                                                                           | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase                                                                                                    | ester and wate<br>iler)<br>(1)-rich phase                                                                                  |
| Mutual<br><br>t/°C<br>                                                             | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)                                                                         | -dimethylpr<br>sln<br>-rich phase                                                                                           | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126                                                                                         | ester and wate<br>iler)<br>(1)-rich phase                                                                                  |
| Mutual<br>                                                                         | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66                                                         | -dimethylpr<br>sln<br>-rich phas<br>99.51<br>99.43                                                                          | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103                                                                              | ester and wate<br>iler)<br>(1)-rich phase<br>0.9692<br>0.9643                                                              |
| Mutual<br><br>t/°C<br><br>0<br>9.7<br>19.7                                         | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56                                                 | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34                                                                | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087                                                                   | ester and wate<br>iler)<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589                                                    |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7                                         | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51                                         | -dimethylpr<br>sln<br>-rich phas<br>99.51<br>99.43<br>99.34<br>99.20                                                        | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079                                                        | ester and wate<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506                                                   |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7<br>40.0                                 | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51<br>0.45                                 | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34<br>99.20<br>99.07                                              | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079<br>0.00070                                             | . ester and wate<br>iler)<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506<br>0.9429                              |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7<br>40.0<br>50.1                         | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51<br>0.45<br>0.43                         | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34<br>99.20<br>99.07<br>98.97                                     | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079<br>0.00070<br>0.00067                                  | . ester and wate<br>iler)<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506<br>0.9429<br>0.9371                    |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7<br>40.0<br>50.1<br>60.5                 | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51<br>0.45<br>0.43<br>0.42                 | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34<br>99.20<br>99.07<br>98.97<br>98.99                            | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079<br>0.00070<br>0.00067<br>0.00065                       | ester and wate<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506<br>0.9429<br>0.9371<br>0.9382                     |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7<br>40.0<br>50.1<br>60.5<br>70.4         | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51<br>0.45<br>0.43<br>0.42<br>0.39         | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34<br>99.20<br>99.07<br>98.97<br>98.99<br>98.99                   | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079<br>0.00079<br>0.00070<br>0.00065<br>0.00061            | ester and wate<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506<br>0.9429<br>0.9371<br>0.9382<br>0.9331           |
| Mutual<br>t/°C<br>0<br>9.7<br>19.7<br>29.7<br>40.0<br>50.1<br>60.5<br>70.4<br>80.5 | solubility of 2,2-<br>g(1)/100g<br>(2)-rich phase (1)<br>0.81<br>0.66<br>0.56<br>0.51<br>0.45<br>0.43<br>0.42<br>0.39<br>0.41 | -dimethylpr<br>sln<br>-rich phase<br>99.51<br>99.43<br>99.34<br>99.20<br>99.07<br>98.97<br>98.99<br>98.99<br>98.90<br>98.82 | opanoic acid methyl<br>x <sub>1</sub> (comp<br>e (2)-rich phase<br>0.00126<br>0.00103<br>0.00087<br>0.00079<br>0.00070<br>0.00067<br>0.00065<br>0.00061<br>0.00064 | ester and wate<br>(1)-rich phase<br>0.9692<br>0.9643<br>0.9589<br>0.9506<br>0.9429<br>0.9371<br>0.9382<br>0.9331<br>0.9285 |

std. dev. 0.02

0.02

AUXILIARY INFORMATION

SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: The analytical method was used. (1) Source not specified, commer-Component (1) was equilibrated cial sample; purity 99%; used with component (2) at a given as received. temperature in a thermostat. Each layer was sampled with a syringe; (2) Not specified. (1) was determined by adding a weighed amount of acetonitrile (or sometimes propanol) to the organic layer sample and measuring by a Gow-Mac thermal conductivity ESTIMATED ERROR: gc the (1)/acetonitrile peak ratio Accuracy of method 0.1 wt% or less, (Chromosorb 101 packing and a HP for solubility, see above. 3390 A recorder-integrator). A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the water layer. **REFERENCES:** 

|                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                             |                                                                                                                                                          | 33                                                         |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------|
| <pre>COMPONENTS: (1) Propanoic acid, 2-methyl-,     ethyl ester         (ethyl isobutyrate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;         [97-62-1] (2) Water; H<sub>2</sub>O; [7732-18-5]</pre>              |                                                                                                                                                                                                                                                             | ORIGINAL MEASUREME<br>Stephenson, R.; S<br>J. Chem. Eng. Dat<br>56-70.                                                                                   | NTS:<br>Stuart, J.<br>Sa <u>1986</u> , <i>31</i> ,         |
|                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                             |                                                                                                                                                          |                                                            |
| VARIABLES:                                                                                                                                                                                                         |                                                                                                                                                                                                                                                             | PREPARED BY:                                                                                                                                             |                                                            |
| T/K = 273 - 36                                                                                                                                                                                                     | 4                                                                                                                                                                                                                                                           | Z. Maczynska                                                                                                                                             |                                                            |
| EXPERIMENTAL VA<br>Mutual solu<br>t/°C<br>(2)-r                                                                                                                                                                    | LUES:<br>bility of 2-methylprop<br>g(1)/100g sln<br>ich phase (1)-rich pha                                                                                                                                                                                  | anoic acid ethyl est<br>x <sub>1</sub> (comp<br>se (2)-rich phase                                                                                        | er and water<br>iler)<br>(1)-rich phase                    |
| <u> </u>                                                                                                                                                                                                           | <u> </u>                                                                                                                                                                                                                                                    |                                                                                                                                                          |                                                            |
| 0 1                                                                                                                                                                                                                | .01 99.41                                                                                                                                                                                                                                                   | 0.00158                                                                                                                                                  | 0.9631                                                     |
| 10.0 0                                                                                                                                                                                                             | .// 99.33                                                                                                                                                                                                                                                   | 0.00120                                                                                                                                                  | 0.9583                                                     |
| 19.8 0                                                                                                                                                                                                             | .68 99.18                                                                                                                                                                                                                                                   | 0.00108                                                                                                                                                  | 0.9494                                                     |
| 29.7 0                                                                                                                                                                                                             | .58 98.90<br>51 08.97                                                                                                                                                                                                                                       | 0.00090                                                                                                                                                  | 0.9331                                                     |
| 40.1 0                                                                                                                                                                                                             | .51 98.87<br>45 98.84                                                                                                                                                                                                                                       | 0.00079                                                                                                                                                  | 0.9314                                                     |
| 60.2 0                                                                                                                                                                                                             | AA 98.87                                                                                                                                                                                                                                                    | 0.00070                                                                                                                                                  | 0.9296                                                     |
| 70.4 0                                                                                                                                                                                                             | .45 98.84                                                                                                                                                                                                                                                   | 0.00070                                                                                                                                                  | 0.9296                                                     |
| 80.5 0                                                                                                                                                                                                             | .44 98.54                                                                                                                                                                                                                                                   | 0.00068                                                                                                                                                  | 0.9128                                                     |
| 90.5 0                                                                                                                                                                                                             | .38 98.49                                                                                                                                                                                                                                                   | 0.00059                                                                                                                                                  | 0.9100                                                     |
| std. dev. 0                                                                                                                                                                                                        | .01 0.01                                                                                                                                                                                                                                                    |                                                                                                                                                          |                                                            |
| ······                                                                                                                                                                                                             | AUXILIARY                                                                                                                                                                                                                                                   | INFORMATION                                                                                                                                              |                                                            |
| METHOD/APPARATU                                                                                                                                                                                                    | S/PROCEDURE:                                                                                                                                                                                                                                                | SOURCE AND PURITY                                                                                                                                        | OF MATERIALS:                                              |
| The analytical<br>Component (1)<br>with component<br>temperature in<br>layer was samp<br>(1) was determ<br>weighed amount<br>(or sometimes<br>organic layer<br>by a Gow-Mac ti<br>gc the (1)/ace<br>(Chromosorb 10 | method was used.<br>was equilibrated<br>(2) at a given<br>a thermostat. Each<br>led with a syringe;<br>ined by adding a<br>of acetonitrile<br>propanol) to the<br>sample and measuring<br>mermal conductivity<br>tonitrile peak ratio<br>l packing and a HP | <ul> <li>(1) Source not sp<br/>cial sample;<br/>as received.</li> <li>(2) Not specified</li> <li>ESTIMATED ERROR:</li> <li>Accuracy of method</li> </ul> | ecified, commer-<br>purity 99%; used<br>d 0.1 wt% or less, |

# ESTIMATED ERROR:

**REFERENCES:** 

A similar procedure but a higher boiling material (e.g. 1-hexanol) was used to determine (2) in the

water layer.

| COMPONENTS:                              |                                                                      | EVALUATOR:                          |
|------------------------------------------|----------------------------------------------------------------------|-------------------------------------|
| (1)                                      | Propanoic acid propyl ester                                          | G.T. Hefter, School of Mathematical |
|                                          | (propyl propionate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; | and Physical Sciences,              |
|                                          | [106-36-5]                                                           | Murdoch University, Perth, W.A.,    |
| (2) Water: H <sub>2</sub> O: [7732-18-5] | Australia                                                            |                                     |
| <b>v</b> – <b>v</b>                      |                                                                      | January, 1989                       |

#### CRITICAL EVALUATION:

Quantitative solubility data for the propanoic acid propyl ester (1) - water (2) system have been reported in the publications listed in Table 1.

| <u>TABLE 1: Ouantitative Solubility Studies of the</u><br>Propanoic acid propyl ester (1) - Water (2) System |                  |            |            |
|--------------------------------------------------------------------------------------------------------------|------------------|------------|------------|
| Reference                                                                                                    | T/K              | Solubility | Method     |
| Hemptinne (ref 1)                                                                                            | . 298            | (1) in (2) | analytical |
| Rayman (ref 2)                                                                                               | 273-303          | (1) in (2) | volumetric |
| Mozzhukhin <i>et al</i> . (ref 3)                                                                            | 293              | mutual     | titration  |
| Bomshtein et al. (ref 4)                                                                                     | 293-353          | mutual     | titration  |
| Stephenson and Stuart<br>(ref 5)                                                                             | 273 <b>-</b> 364 | mutual     | GLC        |

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. SOLUBILITY OF PROPANOIC ACID PROPYL ESTER (1) IN WATER (2)

All the available data for the solubility of propanoic acid propyl ester (1) in water (2) are summarized in Table 2 except for the value of Mozzhukhin et al. (ref 3) which is significantly lower than all other reports and is therefore rejected. Selected data (ref 4,5) are also plotted in Figure 1. Although the independent studies which cover the widest temperature range (ref 4,5) are in good agreement with each other and the values of Rayman (ref 2) at T < 303, they diverge markedly at higher temperatures. In the absence of confirmatory studies it is not possible to prefer either data set at this stage and no "Best" values have been derived at higher temperatures. Further studies of this system are clearly desirable.

| СОМРО | DNENTS:                                                                                                           | EVALUATOR:                                                                                        |
|-------|-------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
| (1)   | Propanoic acid propyl ester<br>(propyl propionate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ;<br>[106-36-5] | G.T. Hefter, School of Mathematical<br>and Physical Sciences,<br>Murdoch University, Perth, W.A., |
| (2)   | Water; H <sub>2</sub> O; [7732-18-5]                                                                              | Australia<br>January, 1989                                                                        |

CRITICAL EVALUATION: (continued)

# TABLE 2: Recommended (R) and Tentative Solubilities of Propanoic acid propyl ester (1) in Water (2)

| T/K | Solubilities                                                                                     |                                              |  |
|-----|--------------------------------------------------------------------------------------------------|----------------------------------------------|--|
|     | Reported values                                                                                  | "Best" values $(\pm \sigma_n)^a$             |  |
|     | g(1)/100g sln                                                                                    | g(1)/100g sln 10 <sup>3</sup> x <sub>1</sub> |  |
| 273 | 1.05 (ref 2), 1.01 (ref 5)                                                                       | 1.03 ± 0.02 (R) 1.61                         |  |
| 283 | 0.84 (ref 2), 0.79 <sup>*</sup> (ref 5)                                                          | 0.82 ± 0.03 (R) 1.28                         |  |
| 293 | 0.68 (ref 2), 0.51 (ref 4),<br>0.64* (ref 5)                                                     | 0.61 ± 0.07 0.95                             |  |
| 298 | 0.56 (ref 1), 0.68 <sup>*</sup> (ref 2),<br>0.61 <sup>*</sup> (ref 4), 0.59 <sup>*</sup> (ref 5) | 0.61 ± 0.04 0.95                             |  |
| 303 | 0.60 (ref 2), 0.71 (ref 4),<br>0.54 <sup>*</sup> (ref 5)                                         | 0.62 ± 0.07 0.97                             |  |
| 313 | 1.02 (ref 4), 0.48 <sup>*</sup> (ref 5)                                                          | 0.8 ± 0.3 1.2                                |  |
| 323 | 1.21 (ref 4), 0.44 <sup>*</sup> (ref 5)                                                          | 0.8 ± 0.4 1.2                                |  |
| 333 | 1.78 (ref 4), 0.42 <sup>*</sup> (ref 5)                                                          | _ <i>b</i> _ <i>b</i>                        |  |
| 343 | 2.59 (ref 4), 0.41 <sup>*</sup> (ref 5)                                                          | _ b _ b                                      |  |
| 353 | 3.50 (ref 4), 0.40 <sup>*</sup> (ref 5)                                                          | _ b _ b                                      |  |
| 363 | 0.39 <sup>*</sup> (ref 5)                                                                        | _ b _ b                                      |  |

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_1)$  have the same status and (relative) percentage uncertainties as the mass % solubilities.

<sup>b</sup> See text.

| COMPONENTS:                                                                                                        | EVALUATOR:                                                 |  |
|--------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------|--|
| <ol> <li>Propanoic acid propyl ester<br/>(propyl propionate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> </ol> | G.T. Hefter, School of Mathematical and Physical Sciences, |  |
| [106-36-5]                                                                                                         | Murdoch University, Perth, W.A.,<br>Australia              |  |
| (2) water; $H_20$ ; [//32-18-5]                                                                                    | January, 1989                                              |  |





FIGURE 1. Selected data for the solubility of propanoic acid propyl ester (1) in water (2): ref 4 ( $\bullet$ ); ref 5 (O). Solid lines are least squares polynomial fits and are included only for illustrative purposes.

2. SOLUBILITY OF WATER (2) IN PROPANOIC ACID PROPYL ESTER (1)

All the available solubility data for water (2) in propanoic acid propyl ester (1) are summarized in Table 3 except for the value of Mozzhukhin et al. (ref 3) which is an order of magnitude higher than other studies (ref 4,5) and is therefore rejected. The data are also plotted in Figure 2.

As for the  $H_2O$  rich phase, the data of Bomshtein *et al.* (ref 4) and Stephenson and Stuart (ref 5) are in good agreement near 298 K but differ markedly at higher temperatures. Again, in the absence of other independent studies it is not possible to prefer either data set and so no "Best" values have been derived at T > 333 K. Further studies of this system are clearly desirable.

| COMPONENTS:                              |                                                                                                     | EVALUATOR:                                                 |
|------------------------------------------|-----------------------------------------------------------------------------------------------------|------------------------------------------------------------|
| (1)                                      | Propanoic acid propyl ester<br>(propyl propionate); C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; | G.T. Hefter, School of Mathematical and Physical Sciences, |
|                                          | [106-36-5]                                                                                          | Murdoch University, Perth, W.A.,                           |
| (2) Water: H <sub>2</sub> O: [7732-18-5] | Australia                                                                                           |                                                            |
| $(2)$ mater, $n_2 o$ , $[1102 10 o]$     |                                                                                                     | January, 1989                                              |

CRITICAL EVALUATION: (continued)

# TABLE 3: Recommended (R) and Tentative Solubilitiesof Water (2) in Propanoic acid propyl ester (1)

| T/K | Solubilit                                            | ies                              |                |
|-----|------------------------------------------------------|----------------------------------|----------------|
|     | Reported values                                      | "Best" values $(\pm \sigma_n)^a$ |                |
|     | g(2)/100g sln                                        | g(2)/100g sln                    | $10^2 x_2$     |
| 273 | 0.63 (ref 5)                                         | 0.6                              | 4              |
| 283 | 0.71 <sup>*</sup> (ref 5)                            | 0.7                              | 4              |
| 293 | 0.90 (ref 4), 0.81 <sup>*</sup> (ref 5)              | 0.86 ± 0.05 (R)                  | 5.3            |
| 298 | 1.00 <sup>*</sup> (ref 4), 0.88 <sup>*</sup> (ref 5) | 0.94 ± 0.06                      | 5.8            |
| 303 | 1.10 (ref 4), 0.93 <sup>*</sup> (ref 5)              | 1.02 ± 0.09                      | 6.2            |
| 313 | 1.40 (ref 4), 1.03 <sup>*</sup> (ref 5)              | 1.2 ± 0.2                        | 7              |
| 323 | 1.50 (ref 4), 1.12 <sup>*</sup> (ref 5)              | 1.3 ± 0.2                        | 8              |
| 333 | 1.90 (ref 4), 1.19 <sup>*</sup> (ref 5)              | 1.5 ± 0.4                        | 9              |
| 343 | 2.80 (ref 4), 1.25 <sup>*</sup> (ref 5)              | _ b                              | _ b            |
| 353 | 3.90 (ref 4), 1.28 <sup>*</sup> (ref 5)              | _ b                              | _ <i>b</i>     |
| 363 | 1.31 <sup>*</sup> (ref 5)                            | _ b                              | _ <sup>b</sup> |

<sup>a</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance. Mole fraction solubilities  $(x_2)$  have the same status and (relative) percentage uncertainties as the mass solubilities.

<sup>b</sup> No "Best" values derived, see text.



| COMPONENTS:                                                                                                           | ORIGINAL MEASUREMENTS:                                          |
|-----------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------|
| (1) Propanoic acid propyl ester<br>(propyl propionate); $C_6H_{12}O_2$ ;<br>[106-36-5]<br>(2) Water: H=0: [7732-18-5] | Hemptinne, A.<br><i>Z. Phys. Chem.</i> <u>1894</u> , 13, 561-9. |
| VARIABLES:<br>T/K = 298                                                                                               | PREPARED BY:<br>A. Skrzecz                                      |

The solubility of propanoic acid propyl ester in water at  $25^{\circ}C$  was reported to be 5.623 g(1)/L sln.

| AUXILIARY INFORMATION                                                                                                                                                                                                                                                                                                                                                                                                                      |                                                                                                                                  |  |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------|--|
| METHOD/APPARATUS/PROCEDURE:<br>The analytical method was used. The<br>mixture of water with excess ester<br>was heated for some time in a water<br>bath and the ester phase was fil-<br>tered. A sample of known volume was<br>then transferred to a smaller<br>flask, heated with the known amount<br>of baryta until complete saponifi-<br>cation was obtained and then ti-<br>trated. No further details were<br>reported in the paper. | SOURCE AND PURITY OF MATERIALS:<br>(1) Not specified.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Not specified.<br>REFERENCES: |  |

|  |  |  | _ |
|--|--|--|---|

| COMPONENTS:                                                                                                          | ORIGINAL MEASUREMENTS:                                |  |
|----------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------|--|
| <pre>(1) Propanoic acid propyl ester (propyl propionate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [106-36-5]</pre> | Rayman, J.<br><i>Thesis</i> , Budapest, <u>1906</u> . |  |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                             |                                                       |  |
| VARIABLES:                                                                                                           | PREPARED BY:                                          |  |
| T/K = 273 - 303 G.T. Hefter                                                                                          |                                                       |  |
| EXPERIMENTAL VALUES:                                                                                                 |                                                       |  |
| Solubility of propanoic acid propyl ester in water                                                                   |                                                       |  |
|                                                                                                                      |                                                       |  |

| t/°C | g(1)/100g(2) | g(1)/100g solution<br>(compiler) | x <sub>1</sub><br>(compiler) |
|------|--------------|----------------------------------|------------------------------|
|      |              | - <u></u>                        |                              |
| ο.   | 1.09         | 1.05                             | 0.00164                      |
| 10.  | 0.85         | 0.84                             | 0.00131                      |
| 20.  | 0.69         | 0.68                             | 0.00106                      |
| 30.  | 0.60         | 0.60                             | 0.00094                      |

These data have also been published in (ref 2).

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volumetric method was used. A known volume (1) was mixed with a known volume of (2) in an apparatus similar to that described in (ref 1). After a suitable period of time, the volume of undissolved (1) was measured. This undissolved volume was kept as small as possible to minimize the error arising from the solubility of (2) in (1).

# SOURCE AND PURITY OF MATERIALS:

 Kahlbaum or Merck; washed with salt water; dried over CaCl<sub>2</sub> or CuSO<sub>4</sub>; purity not stated.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

### **REFERENCES:**

1. Winkler, L. Z. Phys. Chem. <u>1906</u>, 55, 360.

 Hill, A.E. International Critical Tables (Washburn, E.W., Ed.) McGraw Hill, New York, <u>1928</u>, Vol. 3, 387-98.

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| COMPONENTS:                                                                                                                                                                                     | ORIGINAL MEASUREMENTS:                                                                                                    |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------|--|
| <ul> <li>(1) Propanoic acid propyl ester</li> <li>(propyl propionate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</li> <li>[106-36-5]</li> <li>(2) Water; H<sub>2</sub>O; [7732-18-5]</li> </ul> | Mozzhukhin, A.S.; Serafimov, L.A.;<br>Mitropol'skaya, V.A.; Sankina,<br>L.M.<br>Zh. Fiz. Khim. <u>1967</u> , 41, 1687-90. |  |
| VARIABLES:<br>T/K = 293                                                                                                                                                                         | PREPARED BY:<br>A. Skrzecz                                                                                                |  |

The solubility of propanoic acid propyl ester in water at 20°C was reported to be 0.1 g(1)/100g sln. The corresponding mole fraction,  $x_1$ , value calculated by the compiler is 1.6 x  $10^{-4}$ .

The solubility of water in propanoic acid propyl ester at  $20^{\circ}$ C was reported to be 6.5 g(2)/100g sln. The corresponding mole fraction,  $x_2$ , value calculated by the compiler is 0.31.

| AUXILIARY INFORMATION                                                                                                                                                                                                                   |                                                                                                                                                                                                                                                                                                                       |  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                                                             | SOURCE AND PURITY OF MATERIALS:                                                                                                                                                                                                                                                                                       |  |
| The titration method described by<br>Mozzhukhin, Serafimov, Mitropol'-<br>skaya and Rudakovskaya (ref 1) was<br>used. The data were reported to-<br>gether with the ternary system<br>propanoic acid propyl ester-water-<br>1-propanol. | <ol> <li>By Mozzhukhin, Mitropl'skaya,<br/>Serafimov, Torubarov and<br/>Rudakovskaya (ref 2): synthe-<br/>sized; distilled; impurities</li> <li>&lt;0.5wt% by glc, 0.01wt% H<sub>2</sub>O,<br/>b.p.121°C, d<sub>4</sub><sup>20</sup> 0.8826,<br/>n<sub>D</sub><sup>0</sup> 1.3933.</li> <li>Not specified.</li> </ol> |  |
|                                                                                                                                                                                                                                         | ESTIMATED ERBOR:                                                                                                                                                                                                                                                                                                      |  |
|                                                                                                                                                                                                                                         | Temp. $\pm 0.1^{\circ}$ C by (ref 1).                                                                                                                                                                                                                                                                                 |  |
|                                                                                                                                                                                                                                         | REFERENCES:                                                                                                                                                                                                                                                                                                           |  |
|                                                                                                                                                                                                                                         | <ol> <li>Mozzhukhin, A.S.; Serafimov,<br/>L.A.; Mitropol'skaya, V.A.;<br/>Rudakovskaya, T.S. Khim. Tekh-<br/>nol. Topl. Masel <u>1966</u>, 4, 11.</li> </ol>                                                                                                                                                          |  |
|                                                                                                                                                                                                                                         | <ol> <li>Mozzhukhin, A.S.; Mitropl'skaya,<br/>V.A.; Serafimov, L.A.;<br/>Torubarov, A.I.; Rudakovskaya,<br/>T.S. Zh. Fiz. Khim. <u>1967</u>, 41,<br/>227.</li> </ol>                                                                                                                                                  |  |

|                                                                                                             |                                                         |                                                     | r                                                               |                                                                    |
|-------------------------------------------------------------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------------------|--------------------------------------------------------------------|
| COMPONENTS:                                                                                                 |                                                         | ORIGINAL MEASUREMENTS:                              |                                                                 |                                                                    |
| <pre>(1) Propanoic acid propyl ester   (propyl propionate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;</pre> |                                                         | Bomshtein, A.L.; Trofimov, A.N.;<br>Serafimov, L.A. |                                                                 |                                                                    |
| [106-36-5]                                                                                                  |                                                         | Zh. Prikl. Khim.                                    | <u>1978</u> , 51, 1280-2.                                       |                                                                    |
| (2) Wat                                                                                                     | er; H <sub>2</sub> O; [7732-1                           | 8-5]                                                |                                                                 |                                                                    |
| VARIABLES                                                                                                   | 5:                                                      |                                                     | PREPARED BY:                                                    |                                                                    |
| T/K = 29                                                                                                    | 93 - 353                                                |                                                     | A. Skrzecz                                                      |                                                                    |
| EXPERIMEN                                                                                                   | TAL VALUES:                                             |                                                     |                                                                 | ·                                                                  |
| ł                                                                                                           | Mutual solubility                                       | of propanoic                                        | acid propyl ester                                               | and water                                                          |
| t/°C                                                                                                        | x                                                       | 1                                                   | q(1)/100q s                                                     | ln (compiler)                                                      |
|                                                                                                             | (2)-rich phase                                          | (1)-rich phas                                       | e (2)-rich phase                                                | (1)-rich phase                                                     |
| 20                                                                                                          | 0.0008                                                  | 0.9448                                              | 0.51                                                            | 99.10                                                              |
| 30                                                                                                          | 0.0011                                                  | 0.9331                                              | 0.71                                                            | 98.90                                                              |
| 40                                                                                                          | 0.0016                                                  | 0.9162                                              | 1.02                                                            | 98.60                                                              |
| 50                                                                                                          | 0.0019                                                  | 0.9106                                              | 1.21                                                            | 98.50                                                              |
| 60                                                                                                          | 0.0028                                                  | 0.8890                                              | 1.78                                                            | 98.10                                                              |
| 70                                                                                                          | 0.0041                                                  | 0.8434                                              | 2.59                                                            | 97.20                                                              |
| 80                                                                                                          | 0.0056                                                  | 0.7927                                              | 3.50                                                            | 96.10                                                              |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
| AUXILIARY INFORMATION                                                                                       |                                                         | NFORMATION                                          |                                                                 |                                                                    |
| METHOD/APPARATUS/PROCEDURE:                                                                                 |                                                         | SOURCE AND PURITY OF MATERIALS:                     |                                                                 |                                                                    |
| The titr<br>constant<br>details                                                                             | ation method was<br>temperature. No<br>were reported in | used at<br>further<br>the paper.                    | (1) Source not sp<br>led; without<br>b.p. 122.9 <sup>o</sup> C, | pecified; distil-<br>impurities by glc,<br>$n_{\rm D}^{20}$ 1.392. |
|                                                                                                             |                                                         |                                                     | (2) Not specified                                               | 1.                                                                 |
|                                                                                                             |                                                         |                                                     | ESTIMATED ERROR:                                                |                                                                    |
|                                                                                                             |                                                         |                                                     | Not specified.                                                  |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
|                                                                                                             |                                                         |                                                     | REFERENCES:                                                     |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |
|                                                                                                             |                                                         |                                                     |                                                                 |                                                                    |

| COMPONENTS:                                                                                                            | ORIGINAL MEASUREMENTS:                                                              |
|------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| <pre>(1) Propanoic acid propyl ester  (propyl propionate); C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>;  [106-36-5]</pre> | Stephenson, R.; Stuart, J.<br><i>J. Chem. Eng. Data</i> <u>1986</u> , 31,<br>56-70. |
| (2) Water; H <sub>2</sub> O; [7732-18-5]                                                                               |                                                                                     |
| VARIABLES:                                                                                                             | PREPARED BY:                                                                        |
| T/K = 273 - 364                                                                                                        | Z. Maczynska                                                                        |

| t/°C    | g(1)/100g sln  |                | $x_1$ (compiler) |                |
|---------|----------------|----------------|------------------|----------------|
|         | (2)-rich phase | (1)-rich phase | (2)-rich phase   | (1)-rich phase |
| 0       | 1.01           | 99.37          | 0.00158          | 0.9607         |
| 9.1     | 0.80           | 99.30          | 0.00125          | 0.9565         |
| 19.3    | 0.66           | 99.20          | 0.00103          | 0.9506         |
| 29.6    | 0.52           | 99.06          | 0.00081          | 0.9423         |
| 39.5    | 0.50           | 98.88          | 0.00078          | 0.9319         |
| 50.0    | 0.43           | 98.76          | 0.00067          | 0.9251         |
| 60.3    | 0.43           | 98.78          | 0.00067          | 0.9262         |
| 70.6    | 0.44           | 98.78          | 0.00068          | 0.9262         |
| 80.3    | 0.44           | 98.79          | 0.00068          | 0.9268         |
| 90.5    | 0.36           | 98.69          | 0.00056          | 0.9211         |
| std. de | v. 0.01        | 0.02           |                  |                |

| AUXILIARY INFORMATION                                                                                                                                                                                                                               |  |  |  |  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|--|--|
| SOURCE AND PURITY OF MATERIALS:<br>(1) Source not specified, commer-<br>cial sample; purity 98%; used<br>as received.<br>(2) Not specified.<br>ESTIMATED ERROR:<br>Accuracy of method 0.1 wt% or less,<br>for solubility, see above.<br>REFERENCES: |  |  |  |  |
|                                                                                                                                                                                                                                                     |  |  |  |  |
|                                                                                                                                                                                                                                                     |  |  |  |  |

| COMPONENTS:                                                                                                                                                                                           | ORIGINAL MEASUREMENTS:                                                                                                       |  |  |  |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------|--|--|--|
| (1) Acetic acid 2-ethoxyethyl                                                                                                                                                                         | Doolittle, A.K.                                                                                                              |  |  |  |
| ester (2-ethoxyethyl acetate);<br>CcHecOc: [111-15-9]                                                                                                                                                 | Ind. End. Chem. <u>1935</u> , 27, 1169-79.                                                                                   |  |  |  |
| (2) Water; $H_2O$ ; [7732-18-5]                                                                                                                                                                       |                                                                                                                              |  |  |  |
| VARIABLES:                                                                                                                                                                                            | PREPARED BY:                                                                                                                 |  |  |  |
| T/K = 293                                                                                                                                                                                             | A. Skrzecz                                                                                                                   |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
| The solubility of acetic acid 2-ethoxyethyl ester in water at 20°C was reported to be 24.7 g(1)/100g sln. The corresponding mole fraction, $x_1$ , value calculated by the compiler is 0.0428.        |                                                                                                                              |  |  |  |
| The solubility of water in acetic acid 2-ethoxyethyl ester at $20^{\circ}$ C was reported to be 9.4 g(2)/100g sln. The corresponding mole fraction, $x_2$ , value calculated by the compiler is 0.43. |                                                                                                                              |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
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|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
| AUXILIARY INFORMATION                                                                                                                                                                                 |                                                                                                                              |  |  |  |
| METHOD/APPARATUS/PROCEDURE:                                                                                                                                                                           | SOURCE AND PURITY OF MATERIALS:                                                                                              |  |  |  |
| The method was not specified.                                                                                                                                                                         | (1) Source not specified, commer-<br>cial product; purity 96%, b.p.<br>range 145-166°C, d <sup>2</sup> 4 <sup>0</sup> 0.974. |  |  |  |
|                                                                                                                                                                                                       | (2) Not specified.                                                                                                           |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
|                                                                                                                                                                                                       | ESTIMATED ERROR:                                                                                                             |  |  |  |
|                                                                                                                                                                                                       | Not specified.                                                                                                               |  |  |  |
|                                                                                                                                                                                                       |                                                                                                                              |  |  |  |
|                                                                                                                                                                                                       | REFERENCES:                                                                                                                  |  |  |  |
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