COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 2,3-dimethylbutane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,3-Dimethylbutane (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	273-323	(2) in (1)	analytical
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer
Price (ref 3)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	298	(1) in (2)	GLC

The original data in all of 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. THE SOLUBILITY OF 2,3-DIMETHYLBUTANE (1) IN WATER (2)

The solubility data for 2,3-dimethylbutane in water (ref 2, 3) are listed in Table 2 and plotted in Figure 1. The datum of Krzyzanowska and Szeliga (ref 4) has been excluded from this Evaluation as it does not appear to be independent of that of Price (ref 3).

At 298K, where comparison is possible, agreement between the reported values is only fair. At other temperatures only the values of Price (ref 3) are available. Thus all values are classified as Tentative. It should be noted firstly that the increase in solubility at lower temperatures reported by Polak and Lu (ref 2) is larger than is usually observed in hydrocarbon-water systems (e.g. benzene in water), and secondly the values of Price (ref 3) are usually reliable over the entire temperature range studied.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values for the Solubility 2,3-Dimethylbutane (1) in Water (2)

T/K	Solubility values		
	Reported values[a] 10^3g(1)/100g sln	"Best" values (± σ_n)[b] 10^3g(1)/100g sln	$10^6 x_1$
273	3.29 (ref 2)	3.3	6.9
298	2.25 (ref 2), 1.91 (ref 3)	2.1 ± 0.2	4.4
303	1.9* (ref 3)	1.9	4.0
313	1.9* (ref 3)	1.9	4.0
323	2.1* (ref 3)	2.1	4.4
343	2.8* (ref 3)	2.8	5.9
363	3.5* (ref 3)	3.5	7.3
383	4.6* (ref 3)	4.6	9.6
403	7.5* (ref 3)	7.5	16
423	18* (ref 3)	18	38

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original measurements.

[b] Obtained by averaging where appropriate, σ_n has no statistical significance.

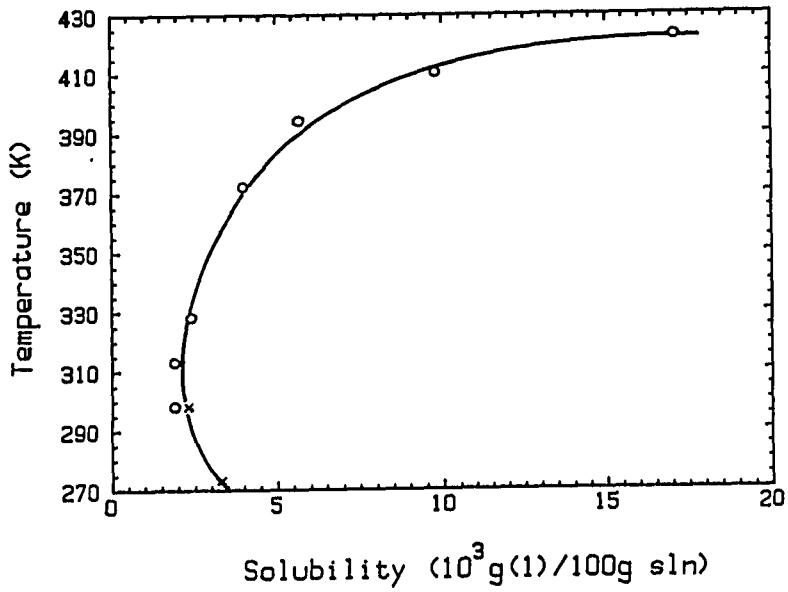

FIGURE 1. Solubility of 2,3-dimethylbutane in water: ref 2 (x); ref 3 (O).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,3-DIMETHYLBUTANE (1)

The reported solubility data for water in 2,3-dimethylbutane (ref 1, 2) are listed in Table 3. There are insufficient data to warrant plotting.

Agreement between the values at 273K is excellent but at 298K the datum of Englin *et al.* (ref 1) is about 50% (relative) higher than that of Polak and Lu (ref 2). In well characterized systems (e.g. water in benzene) the data of Englin *et al.* are generally satisfactory at T < 300K but are markedly higher than "Recommended" values at higher temperatures. The value of Polak and Lu (ref 2) is therefore preferred at 298K and at higher temperatures the data of Englin *et al.* should be regarded only as order of magnitude values.

TABLE 3: Recommended (R) and Tentative Values of the Solubility of Water (2) in 2,3-Dimethylbutane (1)

T/K	Solubility values		
	Reported values 10^3g(2)/100g sln	"Best" values 10^3g(2)/100g sln	"Best" values 10^4x_2
273	2.9 (ref 1), 3.0 (ref 2)	3.0 (R)	1.43 (R)
283	5.8 (ref 1)	5.8	2.8
293	11.0 (ref 1)	11	5
298	15[a] (ref 1), 9.0 (ref 2)	9	4
303	19.2 (ref 1)	20[b]	10[b]
313	32.3 (ref 1)	30[b]	14[b]
323	51.6 (ref 1)	50[b]	24[b]

[a] Graphically interpolated by the Evaluator; datum of Polak and Lu (ref 2) preferred, see text.

[b] Order-of-magnitude values only, see text.

REFERENCES

1. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

2. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

ACKNOWLEDGEMENT

The Evaluators thank Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 0-50°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,3-dimethylbutane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0029	1.4
10	0.0058	2.8
20	0.0110	5.26
30	0.0192	9.18
40	0.0323	15.4
50	0.0516	24.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
VARIABLES:	**PREPARED BY:**
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,3-dimethylbutane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	32.9[c]	6.87×10^{-6}
25[b]	22.5[c]	4.70×10^{-6}

Solubility of water in 2,3-dimethylbutane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	30[d]	1.43×10^{-4}
25[b]	90[e]	4.30×10^{-4}

[a-e]see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of 2,3-dimethylbutane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	19.1 ± 0.2	0.00191	3.99
40.1	19.2 ± 0.5	0.00192	4.01
55.1	23.7 ± 1.1	0.00237	4.95
99.1	40.1 ± 1.2	0.00401	8.38
121.3	56.8 ± 3.5	0.00568	11.87
137.3	97.9 ± 2.3	0.00979	20.46
149.5	171.0 ± 5.0	0.01710	35.75

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *12*, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimetylbutane in water at 25°C was reported to be 19.10 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00191 g(1)/100 g sln and 3.99×10^{-6}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. 0.48 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES: