COMPONENTS:

(1) Pentane; C_5H_{12}; [109-66-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta Katowice 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 25°C was reported to be 39 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0039 g(1)/100 g sln and 9.7 x 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.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.8 mg(1)/kg(2) (standard deviation from 7-9 determinations)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* 1979, *53*, 1298-1300.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of pentane between the gas and aqueous phase. $\alpha = 49 \pm 1$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 512.5$ mm of Hg and $\log C_g = \log p - 4.269 = -1.56$ expressed in moles per liter. Therefore $C_s = 5.63 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0040 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.0×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ± 10% (estimated by the compiler)

REFERENCES:

1. Hine, J.; Mooker, P.K. *J. Org. Chem.* 1975, *4*, 292.

COMPONENTS:

(1) Pentane; C_5H_{12}; [109-66-0]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Jonsson, J.A.; Vejrosta, J.; Novak, J.

Fluid Phase Equil. 1982, *9*, 279-86.

VARIABLES:

Temperature: 15-35°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of pentane in water

t/°C	mg(1)/kg sln	10^3g(1)/100g sln (compiler)	$10^5 x_1$ (compiler)
15	42.9	4.29	1.07
20	41.4	4.14	1.03
25	40.6	4.06	1.01
30	40.3	4.03	1.01
35	40.6	4.06	1.01

[a] Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapour concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analysed by gas chromatography. The method and apparatus are described in detail in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, > 99.8%, used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* 1982, *8*, 25-35.

COMPONENTS:

(1) Pentane; C_5H_{12}; [109-66-0]

(2) Sodium chloride; NaCl; [7647-14-5]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

Salinity: 1-360 g(2)/kg sln

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Pentane in Aqueous NaCl

Salinity g(2)/kg sln	10^3 g(1)/100 g sln	$10^6 x_1$ (compilers)
1.002	3.68	9.19
10.000	3.45	8.67
34.472[a]	2.76	7.05
50.030	2.26	5.84
125.100	1.09	2.95
199.900	0.591	1.67
279.800	0.264	0.777
358.700	0.201	0.614

[a] Artificial seawater, composition not specified but probably similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) commercial, 99 + % pure

ESTIMATED ERROR:

Temperature ± 1 K

Solubility ± 10 relative %

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

EVALUATOR:

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

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the system benzene (1) and water (2) have been reported in the references listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Benzene (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Herz (ref 1)	295	(1) in (2)	densimetric
Groschuff (ref 2)	278-350	(2) in (1)	titration
Clifford (ref 4)	284-328	(2) in (1)	analytical
Hill (ref 5)	273	(2) in (1)	cryoscopic
Hill (ref 6)	278-343	(1) in (2)	analytical
Jaeger (ref 7)	373-573	(1) in (2)	cloud-point
Milligan (ref 8)	298	(1) in (2)	analytical
Barbaudy (ref 9)	342	mutual	cloud-point
Uspenskii (ref 10)	283,295	mutual	titration, analytical
Rosenbaum and Walton (ref 11)	283-333	(2) in (1)	gasometric
Gross and Saylor (ref 12)	303	(1) in (2)	interferometric
Tarassenkow and Poloshinzewa (ref 13)	278-346	(2) in (1)	synthetic
Robertson (ref 14)	279	(2) in (1)	cryoscopic
Niini (ref 15)	293	mutual	refractometric, pycnometric
Saylor *et al.* (ref 16)	303-308	(1) in (2)	interferometric
Berkengeim (ref 18)	283-323	(2) in (1)	Karl Fischer
Staveley *et al.* (ref 19)	297-344	(2) in (1)	synthetic
Durand (ref 20,25)	289	(1) in (2)	synthetic
Stearns *et al.* (ref 21)	298	(1) in (2)	turbidimetric
Booth and Everson (ref 22,27)	298,333	(1) in (2)	residue volume
Joris *et al.* (ref 23,24)	283-299	(2) in (1)	radiotracer
Andrews and Keefer (ref 26)	298	(1) in (2)	spectrophotometric
Griswold *et al.* (ref 28)	298,323	mutual	cloud-point
Klevens (ref 29)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 30)	273-316	(1) in (2)	spectrophotometric
McBain and Lissant (ref 31)	298	(1) in (2)	synthetic
Staveley *et al.* (ref 32)	295-346	(2) in (1)	synthetic
Donahue and Bartell (ref 33)	298	mutual	interferometric
McDevit and Long (ref 34)	298	(1) in (2)	volumetric
Morrison and Billett (ref 35)	298	(1) in (2)	analytical
McCants *et al.* (ref 36)	311	mutual	titration
Hayashi and Sasaki (ref 37)	293,298	(1) in (2)	titration

(Table 1 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 1 (continued)

Reference	T/K	Solubility	Method
Umano and Hayano (ref 38)	459-554	(2) in (1)	volumetric
Wing and Johnston (ref 39)	298	(2) in (1)	radiotracer
Arnold *et al.* (ref 40)	273-342	(1) in (2)	spectrophotometric
Brady and Huff (ref 41)	298	(1) in (2)	vapor pressure
Pavia (ref 42)	282-388	(2) in (1)	Karl Fischer
Alexander (ref 43)	273-338	(1) in (2)	spectrophotometric
Rebert and Kay (ref 44)	556-580^a	mutual	synthetic
Caddock and Davies (ref 45)	293	(2) in (1)	radiotracer
Kudchadker and McKetta (ref 46)	311-411^a	(1) in (2)	not specified
Franks *et al.* (ref 48)	290-336	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 49)	426-537^a	(1) in (2)	cloud-point
Jones and Monk (ref 50)	298-308	(2) in (1)	radiotracer
McAuliffe (ref 51,60)	298	(1) in (2)	GLC
Schatzberg (ref 52)	293	(2) in (1)	Karl Fischer
Udovenko and Aleksandrova (ref 53)	293-353	(1) in (2)	not specified
Hoegfeldt and Bolander (ref 54)	298	(2) in (1)	Karl Fischer
Thompson and Snyder (ref 55)	311-477^a	mutual	analytical
Englin *et al.* (ref 56)	273-323	(2) in (1)	analytical
Connolly (ref 57)	533-573^a	(1) in (2)	cloud-point
Johnson *et al.* (ref 58)	298	(2) in (1)	Karl Fischer
Masterton and Gendrano (ref 59)	298	(2) in (1)	Karl Fischer
Moule and Thurston (ref 61)	282-323	(2) in (1)	radiotracer
Taha *et al.* (ref 62)	298	(1) in (2)	vapor pressure
Alwani and Schneider (ref 63)	523-636^a	mutual	synthetic
Gregory *et al.* (ref 64)	308	(2) in (1)	Karl Fischer
O'Grady (ref 65)	561-566^a	mutual	volumetric
Worley (ref 66)	298	(1) in (2)	spectrophotometric
Burd and Braun (ref 67)	359-473^a	(2) in (1)	GLC
Roddy and Coleman (ref 68)	298	(2) in (1)	gravimetric
Corby and Elworthy (ref 71)	293	(1) in (2)	spectrophotometric
Pierotti and Liabastre (ref 72)	278-319	(1) in (2)	GLC
Ben-Naim *et al.* (ref 73)	283-323	(1) in (2)	spectrophotometric
Bradley *et al.* (ref 74)	298-328^a	(1) in (2)	spectrophotometric
Filyas (ref 75)	568	(2) in (1)	not specified
Karlsson (ref 76)	287-308	(2) in (1)	Karl Fischer
Leinonen and Mackay (ref 77)	298	(1) in (2)	GLC

(Table 1 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 1 (continued)

Reference	T/K	Solubility	Method
Polak and Lu (ref 78)	273,298	mutual	GLC
Sultanov and Skripka (ref 79,89)	498-533[a]	(2) in (1)	not specified
Brown and Wasik (ref 80)	278-293	(2) in (1)	GLC
Goldman (ref 81)	283-313	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 82)	298	(1) in (2)	GLC
Mackay and Shiu (ref 83)	298	(1) in (2)	GLC
Sada *et al.* (ref 84)	298	(1) in (2)	titration
Budantseva *et al.* (ref 85)	293	mutual	GLC
Kirchnerova and Cave (ref 87)	298	(2) in (1)	Karl Fischer
Price (ref 88)	298	(1) in (2)	GLC
Korenman and Aref'eva (ref 90,91)	293,298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 92)	298	(1) in (2)	GLC
May *et al.* (ref 93)	298	(1) in (2)	GLC
Singh and Sah (ref 94)	303	(2) in (1)	titration
Bittrich *et al.* (ref 95)	293-333	mutual	GLC
Banerjee *et al.* (ref 97)	298	(1) in (2)	radiotracer
Schwarz (ref 98)	297	(1) in (2)	chromatographic
Sanemasa *et al.* (ref 100)	288-318	(1) in (2)	spectrophotometric
Sanemasa *et al.* (ref 101)	278-318	(1) in (2)	spectrophotometric
Tsonopoulos and Wilson (ref 102)	313-473[a]	mutual	GLC, Karl Fischer
Sanemasa *et al.* (ref 103)	298	(1) in (2)	spectrophotometric

[a] Pressure also varied, see Table 4

Quantitative solubility data for the benzene-heavy water (D_2O) system are given in the papers by Ben-Naim *et al.* (ref 73), in terms of the Ostwald absorption coefficient, and Backx and Goldman (ref 99). However, these data have not been determined under comparable conditions and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for experimental values. Solubility data may also be calculated from the calorimetric data of Gill *et al.* (ref 86). Bröllos *et al.* (ref 69) have also reported data on a critical locus in the D_2O-benzene system (*cf.* Section 3 below).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

Critical phenomena in the benzene-water system have been reported by Alwani and Schneider (ref 63), Roof (ref 70) and Scheffer (ref 108). These data are discussed along with the solubility data at elevated pressures in Section 3 below.

The extensive information available for the solubility of benzene in brine solutions is considered in a separate Critical Evaluation immediately following the benzene-water Data Sheets.

Apart from the papers by Roof (ref 70) and Scheffer (ref 108) which did not contain sufficient information to justify their inclusion; and the work of Horiba (ref 3), Vermillion (ref 17), Thompson (ref 47) and Herz (ref 107) which were not available for inspection, the original data in all of the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The data of Gorbachev *et al.* (ref 109, 110) are noted but arrived too late to be included in this Evaluation.

In the benzene-water system the mutual solubilities are sufficiently low at atmospheric pressures to enable data reported on w/v fractions (or equivalent) to be converted to mass percent solubilities with reasonable precision by assuming solution densities to be the same as the pure solvents. These conversions are given on the Data Sheets and data are included in this Evaluation. The data of Herz (ref 1), Jaeger (ref 7), Milligan (ref 8), Durand (ref 20,25), Booth and Everson (ref 22,27), Jones and Monk (ref 50) and Sada *et al.* (ref 84) given in v/v fractions have not been converted and so have been excluded.

For convenience, further discussion of this system will be divided into three parts: the solubility of benzene in water and of water in benzene at atmospheric pressure, and their mutual solubilities at higher temperatures and pressures.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation of the original measurements compiled in the data sheets are indicated by an asterisk (*). The uncertainty limits (given as standard deviations, σ_n) attached to the mean "Best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits. Where relevant, 95% confidence intervals have been calculated for the mass percentage solubilities, as error estimates using the *t*-distribution and are given along with the mean values. Error estimates have not been included for mole fraction

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

solubilities because of space limitations but may be assumed to be the same (proportionately) as those given for the mass percentage solubilities. The letter (*R*) indicates "Recommended" data. Data are "Recommended" if σ_n is less than 5% (relative) of the average solubility. All other data are regarded as Tentative.

1. THE SOLUBILITY OF BENZENE (1) IN WATER (2) AT ATMOSPHERIC PRESSURE

Table 1 shows a plethora of studies of the solubility of benzene in water: 29 independent values have been reported at 298K! Most of the data are in good agreement enabling solubilities to be "Recommended" over almost the entire liquid range at atmospheric pressure.

The data of Niini (ref 15), Stearns *et al.* (ref 21), McBain and Lissant (ref 31), Hayashi and Sasaki (ref 37), Kudchadker and McKetta (ref 46, atmospheric pressure data only), Udovenko and Aleksandrova (ref 53), Worley (ref 68), Pierotti and Liabastre (ref 72), Krasnoshchekova and Gubergrits (ref 82), Korenman and Aref'eva (ref 90,91), Schwarz (ref 98) and Sanemasa *et al.* (ref 100,101,103), reported mainly at 293 or 298K, disagree markedly with other studies and have therefore been rejected.

The approximate solubilities of Griswold *et al.* (ref 28), Taha *et al.* (ref 62) and Budantseva *et al.* (ref 85) have been excluded from consideration because of the abundance of more precise values.

All other data on the solubility of benzene in water are included in Table 2. Also included in Table 2 are the mean "Best" values and the 95% confidence intervals.

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Benzene (1) in Water (2)

	Solubility values		
T/K	Reported values[a] g(1)/100g sln	"Best" values ± σ_n (C.I.)[b] g(1)/100g sln	$10^4 x_1$
273[c]	0.153 (ref 5), 0.185 (ref 43), 0.168 (ref 78)	0.169 ± 0.013(0.032)[c]	3.90
278	0.181* (ref 30), 0.172 (ref 40), 0.182* (ref 43), 0.185 (ref 80)	0.180 ± 0.005(0.005)(*R*)	4.15(*R*)
283	0.175 (ref 10), 0.180 (ref 30), 0.173* (ref 40), 0.179* (ref 43), 0.181* (ref 80)	0.178 ± 0.003(0.004)(*R*)	4.11(*R*)

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

T/K	Solubility values Reported values[a] g(1)/100g sln	"Best" values ± σ_n(C.I.)[b] g(1)/100g sln	 10^4x_1
288	0.178* (ref 30), 0.173 (ref 40), 0.178* (ref 43), 0.170* (ref 48), 0.179* (ref 80)	0.176 ± 0.003(0.004)(*R*)	4.06(*R*)
293	0.178* (ref 30), 0.171 (ref 40), 0.178* (ref 43), 0.172* (ref 48), 0.177* (ref 80), 0.179 (ref 95).	0.176 ± 0.003(0.003)(*R*)	4.06(*R*)
298	0.174 (ref 26), 0.186 (ref 29), 0.179 (ref 30), 0.182 (ref 33), 0.172 (ref 35), 0.180 (ref 37), 0.175* (ref 40), 0.176 (ref 41), 0.180* (ref 43), 0.173* (ref 48), 0.178 (ref 51,60), 0.170 (ref 71), 0.177 (ref 77), 0.176 (ref 78), 0.178 (ref 83), 0.174 (ref 88), 0.174 (ref 92), 0.179 (ref 93), 0.175 (ref 97)	0.177 ± 0.004(0.002)(*R*)	4.09(*R*)
303	0.185 (ref 12), 0.184 (ref 16), 0.184* (ref 30), 0.177 (ref 40), 0.182* (ref 43), 0.176* (ref 48)	0.181 ± 0.004(0.005)(*R*)	4.18(*R*)
308	0.190 (ref 16), 0.189* (ref 30), 0.182 (ref 40), 0.187* (ref 43), 0.181* (ref 48)	0.186 ± 0.004(0.006)(*R*)	4.30(*R*)
313	0.195* (ref 30), 0.188 (ref 40), 0.194* (ref 43), 0.188* (ref 48), 0.203 (ref 95), 0.192[d] (ref 102)	0.193 ± 0.005(0.006)(*R*)	4.46(*R*)
318	0.197 (ref 40), 0.203* (ref 43), 0.196* (ref 48), 0.201[d] (ref 102)	0.199 ± 0.003(0.006)(*R*)	4.60(*R*)
323	0.205* (ref 40), 0.212* (ref 43), 0.205* (ref 48), 0.209[d] (ref 102)	0.208 ± 0.003(0.006)(*R*)	4.81(*R*)
328	0.216* (ref 40), 0.223* (ref 43), 0.216* (ref 48), 0.220[d] (ref 102)	0.219 ± 0.003(0.006)(*R*)	5.06(*R*)
333	0.227* (ref 40), 0.238* (ref 43), 0.228* (ref 48), 0.231[d] (ref 102)	0.231 ± 0.004(0.007)(*R*)	5.34(*R*)
338	0.242* (ref 40), 0.236* (ref 43), 0.241* (ref 48), 0.245[d] (ref 102)	0.241 ± 0.003(0.006)(*R*)	5.57(*R*)
343	0.281 (ref 9), 0.261* (ref 40), 0.259[d] (ref 102)	0.267 ± 0.010(0.03) (*R*)	6.17

a Values marked with an asterisk (*) have been graphically interpolated by the Evaluator from the authors' original data.
b Obtained by averaging; figures in parentheses are the 95% confidence intervals (*t* - test). *c* Refers to supercooled liquid (1).
d Calculated from original authors' fitting equation over the range of their experimental investigation.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

Figure 1 plots the mean solubility values as a function of temperature. Using non-linear regression, these values can be fitted to an equation of the form:

$$s(\text{g(1)/100g sln}) = 5.5773 - 4.6067 \times 10^{-2}T + 1.2504 \times 10^{-4}T^2 - 1.0489 \times 10^{-7}T^3 \qquad [1]$$

(Range T: 273-343K, std. error of estimate = 0.0008 g(1)/100g sln., correlation coefficient = 0.9995).

A similar equation was obtained by Arnold *et al.* (ref 40) from a least squares treatment of their own data:

$$s(\text{g(1)/100g sln}) = 0.1784 - 7.436 \times 10^{-4}t + 1.906 \times 10^{-5}t^2 + 1.217 \times 10^{-7}t^3 \qquad [2]$$

(Range t: 5-70°C, std. dev. 0.0028 g(1)/100g sln).

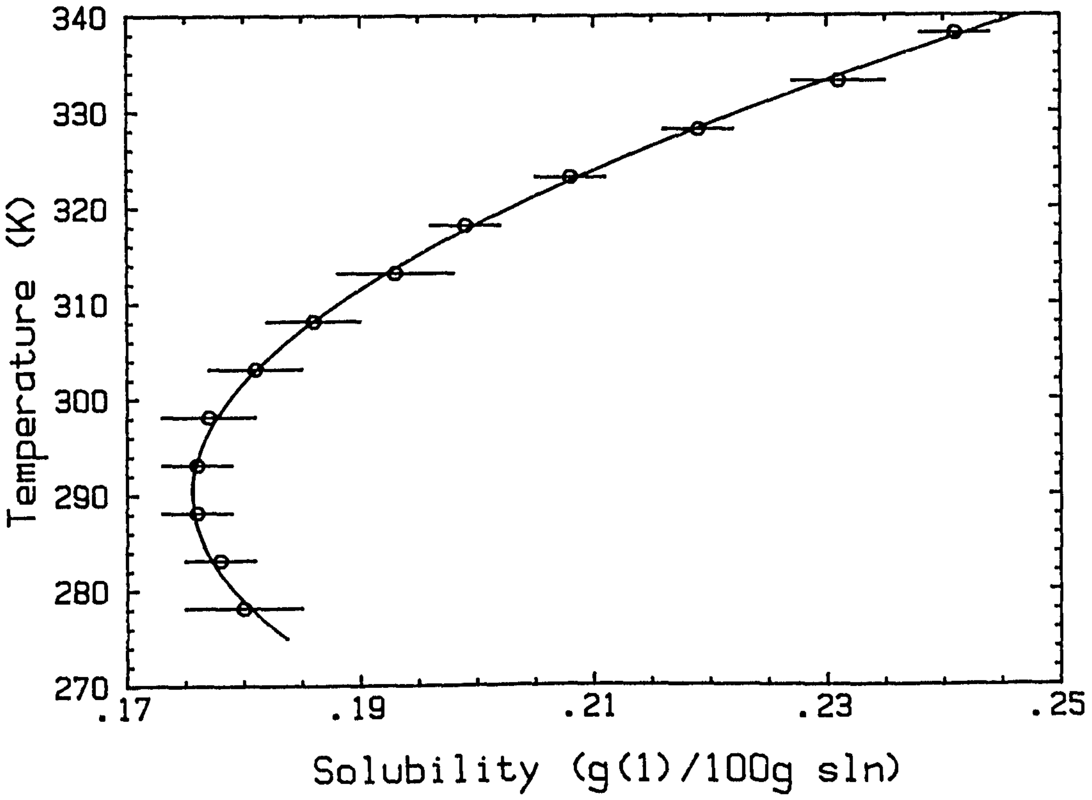

FIGURE 1. Solubility of benzene in water: "Best" values. Error bars represent $\pm\sigma_n$.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

Solubilities calculated from equation [2] are generally 2% (relative) lower than those obtained from equation [1], *i.e.* within the limits of precision of the Recommended values in Table 2.

Gill *et al.* (ref 86) present an alternative equation derived from calorimetric studies of the enthalpy and heat capacity of solution of benzene in water between 288 and 303 K.

$$\ell n\{x_1(T)/x_1(T^{\dagger})\} = (\Delta C^{\infty}_{p,\mathrm{sln}}/R)\{\ell n(T/T^{\dagger}) + (T^{\dagger}/T) - 1\} \qquad [3]$$

$$(\Delta C^{\infty}_{p,\mathrm{sln}} = 225\ \mathrm{J\ K^{-1}\ mol^{-1}},\ T^{\dagger} = 289.0\ \mathrm{K},\ \ell n\ x_1(T^{\dagger}) = -7.843)$$

where $\Delta C^{\infty}_{p,\mathrm{sln}}$ is the infinite dilution heat capacity for benzene in water and $T^{\dagger}$ the temperature of the solubility minimum. Solubilities calculated from this equation are in good agreement (typically lower by 2% relative) with equation [1] over the range 288-303 K. However, they show a systematically increasing deviation at higher temperatures rising to -5.3% at 333 K, *i.e.* slightly outside the precision limits of the recommended values although well within the 95% confidence interval.

Consistent with these findings, application of the van't Hoff equation to the recommended solubilities (Table 2) gives $\Delta H^{\infty}_{\mathrm{sln}} = 2.07$ kJ mol^{-1} and $\Delta C^{\infty}_{p,\mathrm{sln}} = 232$ J K^{-1} mol^{-1} for the dissolution of benzene in water in good agreement with the experimental values of Gill *et al.* No evidence was found for any dependence of $\Delta C^{\infty}_{p,\mathrm{sln}}$ on temperature.

Finally, it is worthwhile noting that Green and Frank (ref 96) have concluded from Henry's law measurements and other thermodynamic data that benzene dissolves in water in monomeric form. These authors also show that solubility determinations based on the measurement of benzene in the vapor-phase by UV spectrophotometry (*e.g.* ref 73) may be seriously in error.

2. THE SOLUBILITY OF WATER (2) IN BENZENE (1) AT ATMOSPHERIC PRESSURE

Despite the many studies of the solubility of water in benzene the reported values are in only fair agreement. This is probably a reflection of the difficulties of quantitating the relatively low water solubility. Thus, the *absolute* uncertainty in the averaged solubility of (2) in (1) is virtually independent of the magnitude of the solubility thereby increasing the *relative* uncertainty at lower solubilities.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

The wealth of publications reporting solubility as a function of temperature (ref 2, 5, 6, 13, 19, 32, 56, 61, 81) enables a particularly critical appraisal of all reported solubilities. Hence data which might be acceptable in less well investigated systems have been rejected if they deviate significantly from averaged values. This procedure has a small effect on the mean value but often results in a substantial decrease in the uncertainty (σ_n).

On this basis the data of Clifford (ref 4), Rosenbaum and Walton (ref 11; data below 303 K retained), Tarassenkow and Poloshinzewa (ref 13; data above 283 K retained), Berkengeim (ref 18), Joris *et al.* (ref 23, 24), Wing and Johnston (ref 39), Englin *et al.* (ref 56; data below 303 K retained), Budantseva *et al.* (ref 85) and Bittrich (ref 95) have been rejected. Most of these data are lower than the mean values. The approximate values of Griswold *et al.* (ref 28) and McCants *et al.* (ref 36) have also been excluded as more precise data are available. All other data are included in Table 3.

It is interesting to note that the average solubilities reported in the more recent studies (ref 58, 59, 61, 64, 68, 76, 78, 81, 87, 94, 102) tend to be somewhat higher than the overall average and with considerably smaller σ_n (see Table 3). The reasons for these differences are unclear but could be due to improved analytical or purification techniques. If only the more recent data are considered then the averaged values could be "Recommended" between 283 and 298 K. However, comparison of the earlier data (with ref 58 arbitrarily chosen as the cut off) with the more recent values by standard statistical procedures (*t*-test or *F*-test) indicates that these two data sets differ significantly ($P < 0.05$) only at 298 K and possibly 288 K. Further careful measurements are required to resolve this situation.

TABLE 3: Recommended (*R*) and Tentative Values of the Solubility of Water (2) in Benzene (1)

T/K	Solubility values		
	Reported values[a] g(2)/100g sln	"Best" values ± σ_n (C.I.)[b] g(2)/100g sln	10^3x_2
273	0.029* (ref 2), 0.0400 (ref 56), 0.0302 (ref 78)	0.033 ± 0.005(0.012)	1.4
278	0.032* (ref 2), 0.034* (ref 6), 0.035 (ref 14), 0.042* (ref 56)	0.036 ± 0.004(0.006)	1.6

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 3 (continued)

T/K	Solubility values Reported values[a] g(2)/100g sln	"Best" values ± σ_n (C.I.)[b] g(2)/100g sln	$10^3 x_2$
283	0.038* (ref 2), 0.042* (ref 6), 0.051 (ref 10), 0.0451 (ref 11), 0.040 (ref 18), 0.0425* (ref 42), 0.0446 (ref 56), 0.045 (ref 61), 0.0440 (ref 81)	0.044 ± 0.003(0.002) [0.0445 ± 0.0005][b]	1.9 [1.93]
288	0.045* (ref 2), 0.052* (ref 6), 0.057* (ref 10), 0.050* (ref 11), 0.043* (ref 13), 0.046* (ref 18), 0.0510* (ref 42), 0.051* (ref 56), 0.0530 (ref 61), 0.0533 (ref 76), 0.0522 (ref 81)	0.050 ± 0.004(0.003) [0.0528 ± 0.0005][b]	2.2 [2.29]
293	0.055* (ref 2), 0.064* (ref 6), 0.064* (ref 10), 0.0573 (ref 11), 0.054* (ref 13), 0.059 (ref 15), 0.053 (ref 18), 0.053* (ref 32), 0.0603* (ref 42), 0.052 (ref 45), 0.0532 (ref 52), 0.0582 (ref 56), 0.0635* (ref 61), 0.0631 (ref 76), 0.0618 (ref 81), 0.0586 (ref 95)	0.058 ± 0.006(0.003) [0.062 ± 0.002][b]	2.5 [2.69]
298	0.066* (ref 2), 0.077* (ref 6), 0.065* (ref 11), 0.065* (ref 13), 0.069* (ref 19), 0.067* (ref 32), 0.072 (ref 33), 0.0710* (ref 42), 0.066* (ref 54), 0.065 (ref 56), 0.0719 (ref 58), 0.0715 (ref 59), 0.0740* (ref 61), 0.0747 (ref 68), 0.0725* (ref 76), 0.0691 (ref 78), 0.0725 (ref 81), 0.0719 (ref 87)	0.070 ± 0.004(0.002) [0.0722 ± 0.0016][b]	3.0 [3.13]
303	0.080* (ref 2), 0.090* (ref 6), 0.077* (ref 13), 0.082* (ref 19), 0.083* (ref 32), 0.0828* (ref 42), 0.0860* (ref 61), 0.0854 (ref 76), 0.082 (ref 81), 0.082 (ref 94)	0.083 ± 0.003 (0.002) (*R*) [0.084 ± 0.002][b]	3.60(*R*) [3.64]
308	0.095* (ref 2), 0.105* (ref 6), 0.089* (ref 13), 0.097* (ref 19), 0.097* (ref 32), 0.0970* (ref 42), 0.102 (ref 61), 0.097 (ref 64), 0.102 (ref 76), 0.0979 (ref 81)	0.098 ± 0.004 (0.003) (*R*) [0.099 ±0.002][b]	4.23(*R*) [4.30]
313	0.114 (ref 2), 0.122* (ref 6), 0.102 (ref 13), 0.114* (ref 19), 0.114* (ref 32), 0.112* (ref 42), 0.118* (ref 61), 0.110 (ref 81), 0.112 (ref 102)	0.113 ± 0.005 (0.004) (*R*)	4.87(*R*)
318	0.134* (ref 2), 0.140* (ref 6), 0.126 (ref 13), 0.135* (ref 19), 0.135* (ref 32), 0.131* (ref 42), 0.138 (ref 61), 0.133[c] (ref 102)	0.134 ± 0.004 (0.004) (*R*)	5.78(*R*)

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 3 (continued)

/K	Solubility values		
	Reported values^a g(2)/100g sln	"Best" values ± σ_n(C.I.)^b g(2)/100g sln	$10^3 x_2$
323	0.158* (ref 2), 0.156* (ref 6), 0.150* (ref 13), 0.160* (ref 19), 0.156* (ref 32), 0.152* (ref 42), 0.160* (ref 61), 0.152^c (ref 102)	0.156 ± 0.003(0.003)(*R*)	6.74(*R*)
328	0.184 (ref 2), 0.173* (ref 6), 0.175 (ref 13), 0.223 (ref 19), 0.210* (ref 32), 0.201* (ref 42), 0.203^c (ref 102)	0.179 ± 0.006(0.006)(*R*)	7.76(*R*)
333	0.213* (ref 2), 0.198* (ref 6), 0.203* (ref 13), 0.223 (ref 19), 0.210* (ref 32), 0.201* (ref 42), 0.203^c (ref 102)	0.207 ± 0.008(0.008)(*R*)	8.96(*R*)
338	0.246* (ref 2), 0.230* (ref 6), 0.234* (ref 13), 0.256* (ref 19), 0.242* (ref 32), 0.226* (ref 42), 0.233^c (ref 102)	0.238 ± 0.010(0.010)(*R*)	10.0(*R*)
343	0.283* (ref 2), 0.270* (ref 6), 0.279* (ref 9), 0.272* (ref 13), 0.290* (ref 19), 0.280* (ref 32) 0.266^c (ref 102)	0.277 ± 0.008(0.008)(*R*)	11.9(*R*)

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[a] Values marked with an asterisk (*) have been graphically interpolated by the Evaluator from the authors' original data.

[b] Figures in round parentheses () are 95% confidence intervals (*t*-test). Values in square parentheses [] are averages ± σ_n of the most recent determinations (ref 58, 59, 61, 64, 68, 76, 78, 81, 87, 94, 102).

[c] Calculated from the original authors' fitting equation over the range of their experimental data.

Figure 2 plots the mean solubility values as a function of temperature. These values can be fitted to an equation of the form:

$$s(\mathrm{g(2)/100g\ sln}) = -5.6667 + 6.3536 \times 10^{-2}\, T - 2.4024 \times 10^{-4}\, T^2 + 3.0752 \times 10^{-7}\, T^3$$

(Range: T = 273 - 343 K, std. error of estimate = 0.001 g(2)/100g sln, correlation coefficient = 0.9998).

A similar expression was obtained by Hill (ref 6) by fitting his own data:

$$s(\mathrm{g(2)/100g\ sln}) = 0.03294 + 6.449 \times 10^{-4}\, t + 3.728 \times 10^{-5}\, t^2$$

(Range: t = 5 - 70°C).

Staveley *et al.* (ref 32) present an alternative equation, in terms of mole fraction, based on their data:

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2); [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

$$\log x_2 = 2.237 - (1427/T)$$

over the range T = 295 - 346 K.

Application of the van't Hoff equation to the mean values in Table 3 gives $\Delta H^{\infty}_{\mathrm{sln}}$ = 24.0 kJ mol^{-1} and $\Delta C^{\infty}_{p,\mathrm{sln}}$ = 89 J K^{-1} mol^{-1} for the dissolution of water in benzene (R^2 = 0.9995).

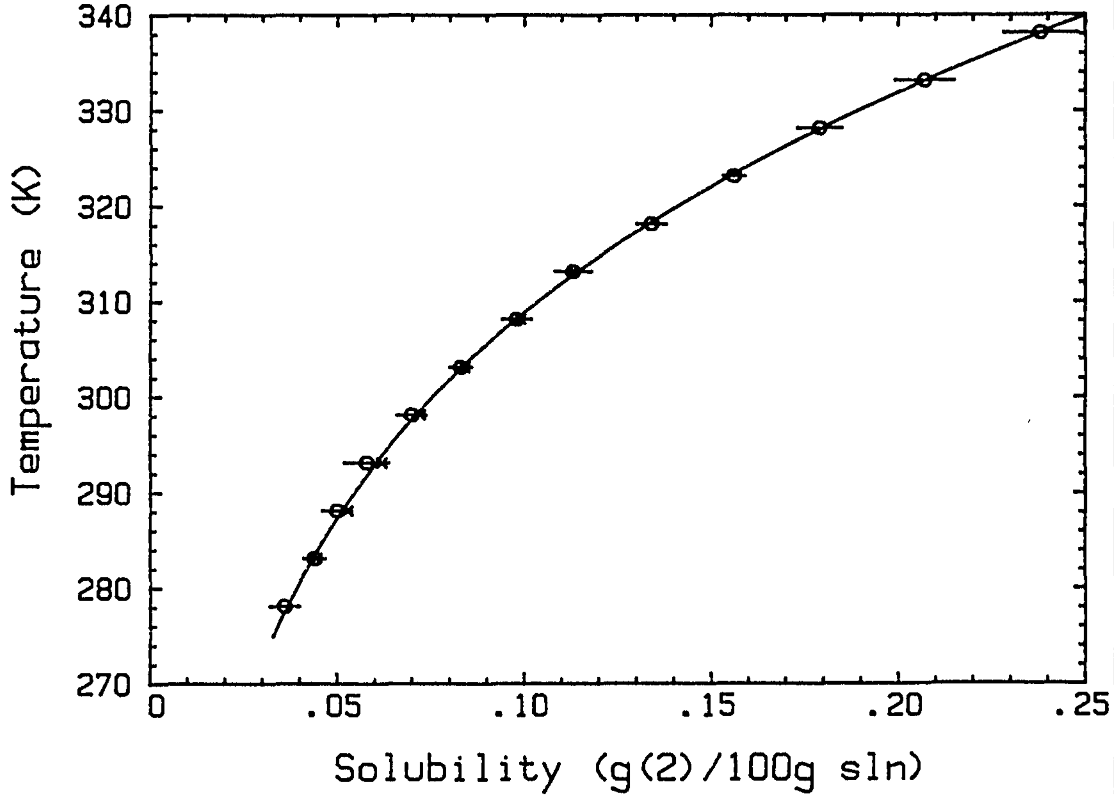

FIGURE 2. Solubility of water in benzene: average of all determinations (o); average of more recent determinations (x). Error bars represent $\pm\sigma_n$.

3. THE MUTUAL SOLUBILITIES OF BENZENE (1) AND WATER (2) AT ELEVATED PRESSURES

To clarify the relationship between the phases in equilibrium in this system it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. On such a projection, phases with the same values of pressure and temperature but different composition will be located at the same point. Benzene + water has type III phase behaviour, using Scott and von Konynenburg's classification (ref 105 106). This type of phase behaviour is characterised by two critical loci, one starting at the critical point of the least volatile component, water in the present

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

case, and eventually approaching high pressures. The other critical locus starts at the critical point of the other component and ends on a three phase (liquid-liquid-vapor) line at a critical end point. Type III phase behaviour is illustrated in Figure 3. It is important to note that the three phase line on a pressure-temperature projection corresponds to three lines on the pressure-temperature-composition diagram. In the region above the three phase line on the pressure-temperature projection, the pressure is greater than the vapor phase and a maximum of two liquid phases is possible. There may be one or two liquid phases depending on the overall composition. To the left of the critical line starting at the least volatile component it is also possible to have one or two phases present depending on the overall composition.

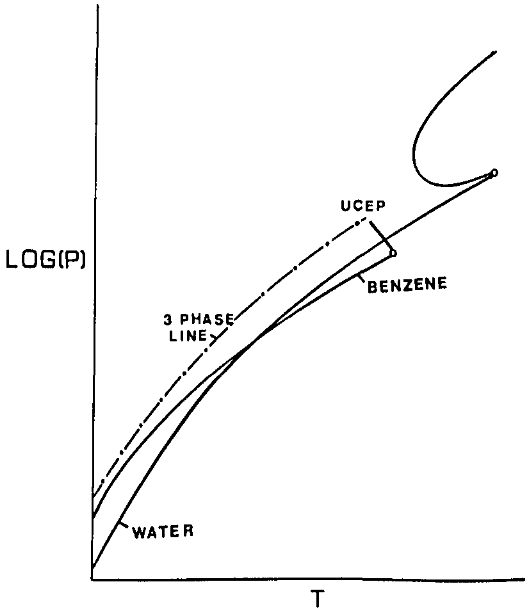

FIGURE 3. Pressure-temperature projection of the equilibrium pressure-temperature-composition surface for the benzene-water system.

Solubility data for the benzene-water system at elevated pressures have been reported in the publications listed in Table 4.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 4: Solubility Studies of the Benzene-Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Umano and Hayano (ref 38)	-[a]	459-554	(2) in (1)
Rebert and Kay (ref 44)	12-16	560-579	mutual
Kudchadker and McKetta (ref 46)	0.1-6	311-411	(1) in (2)
Guseva and Parnov (ref 49)	-[b]	426-527	(1) in (2)
Thompson and Snyder (ref 55)	7,36	311-477	mutual
Connolly (ref 57)	10-80	533-573	(1) in (2)
Alwani and Schneider (ref 63)	15-302	523-636	mutual
O'Grady (ref 65)	25	561,566	mutual
Burd and Braun (ref 67)	0.2-3	359-473	(2) in (1)
Bradley *et al.* (ref 74)	6	298-328	(1) in (2)
Filyas (ref 75)	1	568	(2) in (1)
Sultanov and Skripka (ref 79,89)	5-79	498-533	(2) in (1)
Tsonopoulos and Wilson (ref 102)	0-3[a]	377-485	mutual

a Along three phase line.
b Unspecified but presumably at pressures along the three phase line.

As Table 4 shows, almost none of the solubility data collected at elevated pressures have been obtained under comparable conditions thus making evaluation of their reliability difficult. Although some of the data are in reasonable agreement (*e.g.* the value of 22 g(1)/100g sln at 574.85 K and 14.6 MPa (ref 44) and 22.8 g(1)/100g sln at 573.15 K and 14.7 MPa (ref 57), most are not. Thus the interpolated solubilities of ref 46 and ref 55 at 311K and 5 MPa are 0.336 and 0.187 g(1)/100g sln respectively and other broadly comparable data (*e.g.* ref 55 and ref 57) are only in fair agreement. It should also be noted that the atmospheric pressure data of Kudchadker and McKetta (ref 46) are in poor agreement with the "Recommended" values in Tables 2 and 3.

Table 5 summarizes solubilities of benzene and water as a function of temperature and pressure. All values were obtained by double graphical interpolation (temperature and pressure) to produce data at convenient intervals. The interested user is referred to the original measurements in the Data Sheets for more comprehensive values. For the reasons given above all the values in Table 3 should be regarded as very tentative, subject to further investigations.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_8; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 5: Tentative Values of the Mutual Solubilities of Benzene and Water at High Pressures[a]

T/K	*p*/MPa			
	1	10	20	30
(a) Benzene (1) in water (2), g(1)/100g sln				
313	0.26[b]	0.20	0.22	0.23
373	0.40	0.41	0.50	0.56
423	1.0	1.1	1.1	1.3
473	3.0	3.3	3.5	3.2
523	6.5[c]	6.6[c]	6.9[c]	6.5[c]
(b) Water (2) in benzene (1), g(2)/100g sln				
313	0.10	0.10	0.09	0.09
373	0.60	0.60	0.55	0.55
423	1.7	1.7	1.6	1.6
473	4.5	4.4	4.4	4.2
523	-	13.2[d]	11.5[d]	10.2[d]

[a] Data from ref 55 unless otherwise indicated.
[b] Averaged value of ref 46, 55.
[c] Data from ref 57.
[d] Data from ref 79, 89.

Figure 4 plots the mutual solubilities of benzene and water at elevated temperatures and pressures. The chief effect is to make the solution composition at the (projected) upper critical solution temperature more benzene-rich. This is because the solubility of benzene in water shows a smaller dependence on pressure than the solubility of water in benzene at temperatures near the UCST.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

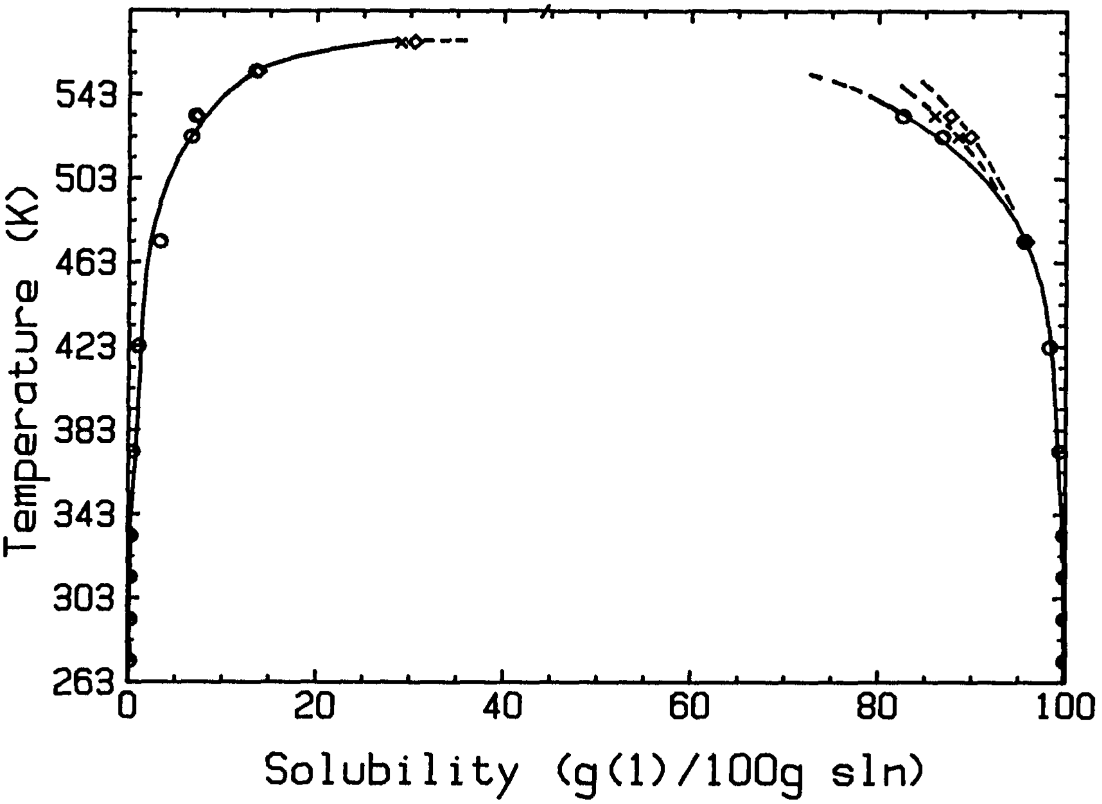

FIGURE 4. Mutual solubility of benzene (1) and water (2) at elevated temperatures and pressures: 0.1 or 10 MPa (o); 20 MPa (x); 30 MPa (◇).

A number of workers (ref 47, 49, 102) have studied the solubility of benzene in water along the three phase equilibrium locus (Figure 3). The data are summarized graphically in Figure 5 and are seen to be in only fair agreement (note that the solubility is represented logarithmically and that the data from ref 47 is only approximate, see Figure 5 caption). The interested user is referred to the relevant Data Sheets (ref 49, 102) for experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

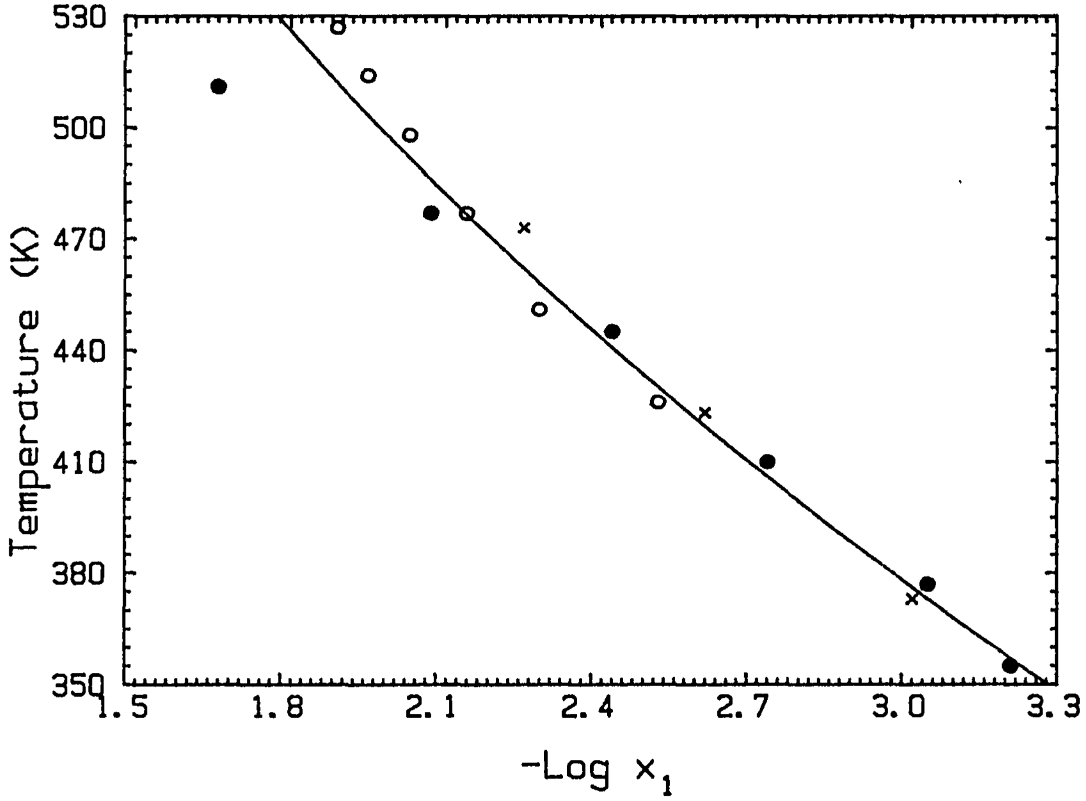

FIGURE 5. Solubility of benzene in water at three phase equilibrium pressures: ref 47 (o, data obtained graphically from ref 102); ref 49 (●); ref 102 (x).

The solubility of water in benzene along the three phase equilibrium locus has also been reported by three groups (ref 38, 47, 102). The data are summarized graphically in Figure 6 and are seen to be in reasonable agreement. Again it should be noted that the data from ref 47 are approximate only, having been obtained graphically from ref 102. The interested user is referred to the relevant Data Sheets (ref 38, 102) for experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. June 1986.

CRITICAL EVALUATION: (continued)

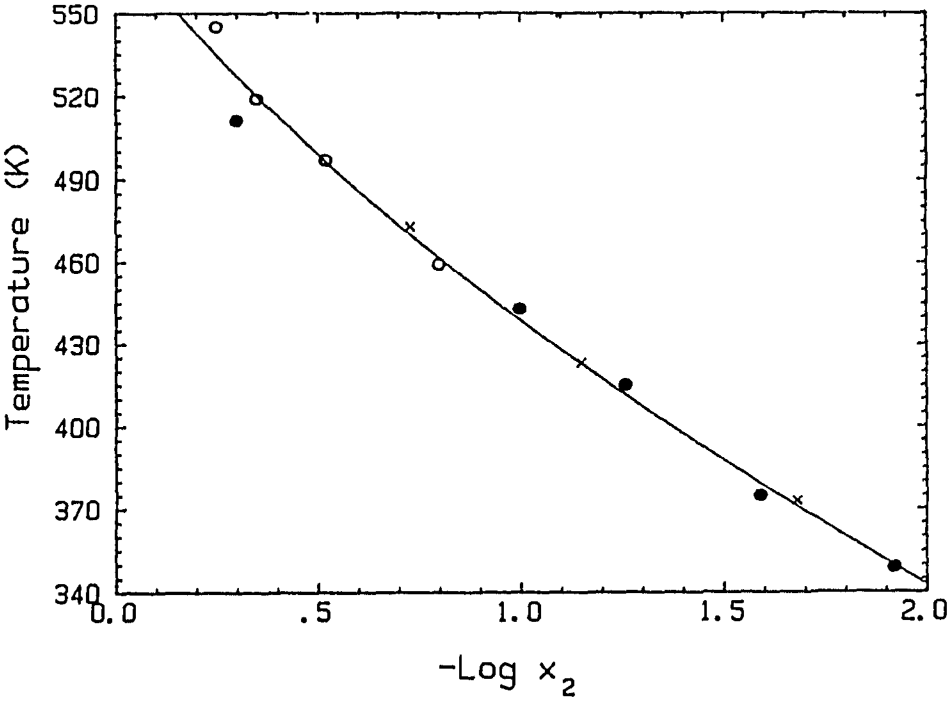

FIGURE 6. Solubility of water in benzene at three phase equilibrium pressures: ref 38 (o); ref 55 (●); ref 102 (x).

For the benzene + water system three workers have determined the temperature and pressure of the critical end point and these are given in Table 6. The values are in surprisingly good agreement.

Alwani and Schneider (ref 63) have reported detailed measurements in the high pressure region to the left of the critical line starting at the critical point of benzene (Figure 3). These data are for the one phase-two phase boundary and at the pressures and temperatures studied (Table 4), the phases are at liquid-like densities. These data are classified as Tentative as they were determined using a well-tested experimental method.

TABLE 6: Critical End Point Properties of the Benzene-Water System

Reference	*T*/K	*p*/MPa
Rebert and Kay (ref 44)	541.5	9.404
Roof (ref 70)	542.6	9.460
Scheffer (ref 108)	541.0	9.39

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

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ACKNOWLEDGEMENTS

The Evaluator thanks Dr Brian Clare for the non-linear regression analyses and graphics. Section 3 was written jointly with C. L. Young, Department of Physical Chemistry, University of Melbourne, Australia.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Herz, W.

Ber. Dtsch. Chem. Ges. 1898, *31*, 2669-72.

VARIABLES:

One temperature: 22°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 22°C was reported to be 0.082 mL(1)/100 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The composition of the saturated solution was evaluated by extrapolation of calibration density measurements (carried out on a series of synthetic solutions) to the measured density of the saturated solution. The maximum difference between the actual and the synthetic densities was a few units in the third decimal place.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) d^{22} 0.9980 g/cm^3.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Groschuff, E. von

Z. Elektrochem. 1911, *17*, 348-54.

VARIABLES:

Temperature: 3-77°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene

t/°C	g(2)/100 g sln	x_2 (compiler)
3	0.030	0.0013
23	0.061	0.0026
40	0.114	0.0049
55	0.184	0.0079
66	0.255	0.0110
77	0.337	0.0145

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In 1 dm^3 long-necked flask (1) was placed and (2) was added dropwise.

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum; stored over Na; distilled twice from K-Na alloy; m.p. 5.4°C,

(2) not specified.

ESTIMATED ERROR:

temp. ± 1-2 K

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Clifford, C.W.

Ind. Eng. Chem. 1921, *13*, 631-2.

VARIABLES:

Temperature: 21-55°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	x_2 (compiler)
21.0	0.046	0.0020
26.6	0.055	0.0024
42.0	0.088	0.0038
55.0	0.113	0.0049

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A current of air predried by calcium chloride was passed through a sample. The moisture abstracted from the sample by this air was absorbed in calcium chloride tubes. The amount of water was calculated from the weights of these tubes. This method is described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; 100 percent benzene; dehydrated with metallic sodium; purity not specified.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Clifford, C.W.; *Ind. Eng. Chem.* 1921, *13*, 628.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hill, A.E.

J. Am. Chem. Soc. 1922, *44*, 1163-93.

VARIABLES:

One temperature: 0°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 0°C was reported to be 0.153 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by compiler is 3.53×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Three determinations of freezing point of (2) saturated with (1) gave 0.037°C as the average depression.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hill, A.E.

J. Am. Chem. Soc. 1923, *45*, 1143-55.

VARIABLES:

Temperature: 5.4-69.5°C

PREPARED BY:

A. Maczynski and A. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
5.4 a)	0.034	1.5
15.0	0.054	2.3
25.0	0.073	3.2
37.5	0.115	5.0
50.0	0.156	6.7
57.5	0.185	8.0
65.0	0.230	9.9
69.5 b)	0.265	11.4

$$S = 0.03294 + 0.0006449t + 0.00003728t^2$$

(S = g(2)/100 g sln)

---

a) quadruple point

b) boiling point of 2-liquid system

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was mechanically stirred at various temperatures and, after saturation was obtained, was transferred to small cylinders, treated with weighed amounts of silver perchlorate and the solubility of the salt in the mixed solvent determined at 25°C. After a correction for the amount of (1) present in the solid phase, the original (2) content of the saturated solution could be determined from the reference curve.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; purified by recrystallization; dried over calcium chloride and finally over bright sodium wire; m.p. 54°C or higher.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Jaeger, A.

Brennst. Chem. 1923, *4*, 259.

VARIABLES:

Temperature: 100-300°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mL(1)/100 mL(2)
100	0.2
150	0.6
200	2.1
250	7.3
285	10.6
300	14.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined in sealed glass tubes.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Milligan, L.H. *J. Phys. Chem.* 1924, *28*, 494-7.
VARIABLES: One temperature: 25°C	**PREPARED BY:** G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.07 mL (1)/100 mL (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

20 cm^3 of benzene/air vapor were introduced into a glass cell, containing 120 cm^3 of air-saturated distilled water in a thermostatted water bath. The apparatus was removed from the bath and shaken for two minutes to bring about equilibrium. Benzene solubility in water was determined by analysis of the vapor by combustion in a Haldane apparatus before and after equilibration.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Barbaudy, J. *J. Chim. Phys.* 1926, *23*, 289-91.
VARIABLES: One temperature: 69.25°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 69.25°C was reported to be 0.281 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler is 6.49×10^{-4}.

The solubility of water in benzene at 69.25°C was reported to be 0.279 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by compiler is 0.0120.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sealed glass tubes were heated in a paraffinic oil bath for a long time above the cloud point and then cooled to turbidity.

SOURCE AND PURITY OF MATERIALS:

(1) Poulenc, cryoscopic grade; thiophene free; dried over $CaCl_2$ and distilled; purity not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Uspenskii, S.P.

Neft. Khoz. 1929, *11-12*, 713-7.

VARIABLES:

Temperature: 10 and 22°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
10	0.175 ± 0.001	4.04
22	0.1865 ± 0.0015	4.306

Solubility of water in benzene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
10	0.051 ± 0.0011	2.2
22	0.0662 ± 0.0008	2.86

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by Clifford's (ref 1), method. Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with $CaCl_2$ and next the adsorbed (2) was weighed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; b.p. 79.8°C at 740 mm Hg, d_4^{22} 0.8768, d_4^{10} 0.8887.

(2) not specified.

ESTIMATED ERROR:

soly. see experimental values above.

REFERENCES:

1. Clifford, C.W. *Ind. Eng. Chem.* 1921, *13*, 628.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rosenbaum, C.K.; Walton, J.H.

J. Am. Chem. Soc. 1930, *52*, 3568-73.

VARIABLES:

Temperature: 10-60°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g (1)	10^3x_2 (compiler)
10	0.0451	1.95
20	0.0573	2.48
30	0.0746	3.22
40	0.0953	4.12
50	0.1271	5.48
60	0.1637	7.05

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The organic phase was first saturated by shaking with water in a flask at a high temperature and then allowing the flask to cool in a thermostat to the desired temperature, with the resulting separation of excess water. After one day or more the solution was allowed to react with added calcium hydride in dry solvent. Hydrogen was evolved and the gas volume was read.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; reagent grade; free from thiophene;
b.p.79.6°C
m.p. 5.4°C;
used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Gross, P.M.; Saylor, J.H. *J. Am. Chem. Soc.* 1931, *53*, 1744-51.
VARIABLES:	**PREPARED BY:**
One temperature: 30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 30°C was reported to be 1.85 g(1)/kg (2) and 0.0237 mol (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.185 g(1)/100 g solution and 4.27×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions were prepared by shaking in a thermostat and were analyzed by means of an interferometer. The instrument used was a combination liquid and gas interferometer made by Zeiss.	(1) Eastman Kodak Co., best grade; distilled; m.p. 5.40°C, (2) distilled.
	ESTIMATED ERROR:
	soly. 1.0% (from values of duplicate determinations)
	REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tarassenkow, D.N.; Poloshinzewa, E.N.

Ber. Dtsch. Chem. Ges. 1932, *65B*, 184-6.

VARIABLES:

Temperature: 5-73°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
5	0.024	1.0
9.5	0.034	1.5
14.5	0.041	1.8
22.5	0.060	2.6
32	0.082	3.5
40	0.102	4.4
56	0.181	7.8
67.5	0.251	10.8
73	0.300	12.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Alexejew's method was used (ref 1). No additional details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum, CP; dried over calcium chloride and distilled from sodium; purity not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ± 0.01% (not specified).

REFERENCES:

1. Alexejew, W. *Wied. Ann. Physik* 1886, *28*, 35.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Robertson, J.B. *Sth. African J. Sci.* 1933, *30*, 187-95.
VARIABLES:	**PREPARED BY:**
One temperature: 5.4°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of water in benzene at 5.4°C was reported to be 0.035 per cent, corresponding to 0.035 g(2)/100 g sln.

The corresponding mole fraction (x_2), calculated by the compiler, is 1.5×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Moist benzene-saturated air was allowed to bubble through moist benzene in a freezing-point tube until a constant freezing point was obtained. A few drops of distilled water were then added and the solution stirred "for some time" and the freezing point re-determined. The water content of the saturated sln was calculated from the freezing point depression (relative to pure benzene) by assuming the water to be monomolecular in solution.

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaum, "pro-analysi", used without further purification.

(2) Distilled, purity not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Niini, A.

Suomen Kemistilehti A 1938, *11*, 19-20.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be 0.085 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler is 2.0×10^{-4}.

The solubility of water in benzene at 20°C was reported to be 0.059 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by compiler is 2.6×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The weight concentration was determined by combined refractometry and pycnometry.

SOURCE AND PURITY OF MATERIALS:

(1) Kahlbaums; analytical grade; dried with P_2O_5 and distilled; purity not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ± 0.005 g(2)/100 g sln (type of error not specified).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Saylor, J.H.; Stuckey, J.M.; Gross, P.M.

J. Am. Chem. Soc. 1938, *60*, 373-6.

VARIABLES:

Temperature: 30 and 35°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mol(1)/1000 g(2)	g(1)/100 g sln (compiler)	10^4x_1 (compiler)
30	0.0236	0.184	4.25
35	0.0243	0.190	4.38

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A large quantity of (1) was brought to equilibrium with a limited quantity of (2). Analyses were made by comparing the readings of the solutions in a Zeiss combination interferometer with those of known standards made by dissolving weighed quantities of (1) in known weights of (2) as described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; purified; m.p. 5.48°C

(2) distilled.

ESTIMATED ERROR:

Presumably:
temp. ± 0.01 K
soly. ± 0.005 g(1)/100 g(2)

REFERENCES:

1. Gross, P.M.; Saylor, J.H. *J. Am. Chem. Soc.* 1931, *53*, 1747.

COMPONENTS:

(1) Benzene; C_6H_6 [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Berkengeim, T.I.

Zavod. Lab. 1941, *10*, 592-4.

VARIABLES:

Temperature: 10-50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.040	1.7
20	0.053	2.3
30	0.066	2.9
40	0.084	3.6
50	0.114	4.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified;
CP reagent;
b.p. 80.4°C; used as received.

(2) not specified

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Staveley, L.A.K.; Jeffes, J.H.E.; Moy, J.A.E.

Trans. Faraday Soc. 1943, *39*, 5-13.

VARIABLES:

Temperature: 24-71°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
24.7	0.685	0.0685	2.96
41.4	1.213	0.1212	5.23
44.0	1.296	0.1294	5.88
50.4	1.619	0.1616	6.97
58.2	2.073	0.2069	8.91
58.5	2.190	0.2185	9.41
71.0	2.976	0.2967	12.74

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 50 cm^3 of (1) was introduced into a clean dry glass tube about 3.5 cm in diameter with a narrow inlet, a small amount of (2) was added from a weighted pipette, and the tube at once sealed off. It was then agitated at a sufficiently high temperature until all (2) had gone into solution, placed in a bath of water, and allowed to cool slowly. The temperature at which (1) was saturated with respect to (2) was taken to be that at which opalescence appeared.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; dried over sodium wire; distilled from sodium powder.

(2) not specified.

ESTIMATED ERROR:

temp. ± 1.5 K

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. *J. Chem. Phys.* 1947, *15*, 496-507.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	A. Maczynski and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.086 and 0.085 g(1)/100 g sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.085 g(1)/100 g sln and 2.0×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 3 K

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-43.
VARIABLES:	**PREPARED BY:**
Temperature: 10-26°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g(1)	g(2)/100 g sln (compiler)	10^3x_2 (compiler)
10	0.030	0.030	1.30
20	0.0425	0.0425	1.84
20	0.0445	0.0445	1.93
26	0.054	0.054	2.34

(at total saturation pressure of 1 atm)

The same data are reported in ref (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Air saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred into the counter by equilibration with ethanol vapor. The method is described in ref (1).

SOURCE AND PURITY OF MATERIALS:

(1) Ohio State University under an American Petroleum Institute project, purity not specified; used as received.

(2) not specified.

ESTIMATED ERROR:

soly. ± 1% (type of error not specified)

REFERENCES:

1. Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 45.

COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES: One temperature: 25.0°C (298.2K)	**PREPARED BY:** G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25.0°C was reported to be 0.16 mg (1)/100 mL (2). The solubility of (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate was also reported to be 0.37 mL (1)/100 mL sulfonate sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute measured directly in the neck of the tube from the total added.

SOURCE AND PURITY OF MATERIALS:

(1) "Highest grade commercial sample available"; no other details given.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Durand, R.

C.R. Hebd. Seances Acad. Sci. 1948, *226*, 409-10.

VARIABLES:

One temperature: 16°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 16°C was reported to be 1.65 $cm^3(1)/dm^3(2)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) distilled.

ESTIMATED ERROR:

soly. ± 0.05 $cm^3(1)/dm^3(2)$

REFERENCES:

1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* 1946, *223*, 898-900.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-77.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.174 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 4.02×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled b.p. 80°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Booth, H.S.; Everson, H.E.

Ind. Eng. Chem. 1949, *41*, 2627-8.

VARIABLES:

Temperature: 25 and 60°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mL(1)/100 mL(2)
25	0.11
60	0.19

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. Then the mixture was separated by gentle rotation. After this treatment, the volume was determined directly.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; CP or highest commercial grade; used as received.

(2) Distilled.

ESTIMATED ERROR:

temp. ± 0.1 K at 25°C
soly. ± 0.1 mL(1)/100 mL(2).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Griswold, J.; Chew, J.-N.;
Klecka, M.E.

Ind. Eng. Chem. 1950, *42*, 1246-51.

VARIABLES:

Temperature: 25 and 50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	$10^4\ x_1$ (compiler)
25	0.18	4.2
50	0.22	5.5

Solubility of water in benzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
25	0.06	2.6
50	0.15	6.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Samples of (1) or (2) were placed in glass-stoppered flasks mounted on a rotating shaft and immersed in a water bath.

Compositions were obtained by titrating a known sample, alternately adding the major and minor components from microburets until the two-phase point was found accurately. The flask was reimmersed in the bath after each titration to maintain thermal equilibrium. Finally, one drop of reagent would cause the second phase to appear or to disappear.

SOURCE AND PURITY OF MATERIALS:

(1) Koppers Co., industrial pure grade; purified by azeotropic distillation with acetone and refractionated; purity 99.7%,

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.05 K
soly. ± 0.1% (not specified)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.86 g(1) dm^{-3} sln and 0.0239 mol(1) dm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.186 g(1)/100 g sln and 4.31×10^{-4}.
The assumption that 1.00 dm^3 sln = 1.00 kg sln was used in this calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem. Soc. 1951, *73*, 1571-8.

VARIABLES:

Temperature: 0.4-42.8°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100g sln[a] (compiler)	$10^4 x_1$ (compiler)
0.4	0.174[b]	4.01
5.2	0.181	4.17
10.0	0.180	4.15
14.9	0.178	4.10
21.0	0.179	4.13
25.0	0.179[c]	4.13[c]
25.6	0.179	4.13
30.2	0.184	4.24
34.9	0.189	4.36
42.8	0.200	4.61

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Data refer to the solubility of solid (1) in (2).

[c] Given in the original paper as 1.79g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Baker and Adamson, purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. Purity was determined by refractometry (no values given).

(2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McBain, J.W.; Lissant, K.J.

J. Phys. Colloid. Chem. 1951, *55*, 665-62.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.151 g(1)/100 mL sln.

The corresponding mass percent and mole fraction solubilities, calculated by the compilers assuming a solution density of 1.00 kg dm^{-3}, are 0.151 g(1)/100 g sln and $x_1 = 3.48 \times 10^{-4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

10 mL portions of (2) are pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.

SOURCE AND PURITY OF MATERIALS:

(1) C.P. grade.

(2) distilled and boiled to remove CO_2.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Staveley, L.A.K; Johns, R.G.S.; Moore, B.C.

J. Chem. Soc. 1951, 2516-23.

VARIABLES:

Temperature: 22.7-73.2°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	10^3x_2	g(2)/100 g sln (compiler)
22.7	2.606	0.0602
30.5	3.674	0.0849
33.0	3.784	0.0875
40.6	5.041	0.1167
41.9	5.153	0.1193
45.9	6.064	0.1405
51.9	6.902	0.1600
52.2	7.078	0.1641
53.2	7.211	0.1672
54.7	7.521	0.1744
60.9	9.294	0.2158
65.3	10.50	0.2441
67.2	11.21	0.2607
73.2	13.02	0.3032

$$\log x_2 = 2.237 - 1427/(t/°C + 273.1)$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A synthetic mixture of known amounts of (2) and (1) was heated in a sealed tube until homogeneous and then the temperature of phase splitting on cooling was determined. The apparatus and procedure are described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; stored over phosphoric oxide.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K

soly. ± 0.2% (type of error not specified)

REFERENCES:

1. Staveley, Jeffes, and Moy *Trans. Faraday Soc.* 1943, *39*, 5.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Donahue, D.J.; Bartell, F.E.

J. Phys. Chem. 1952, *56*, 480-4.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be $x_1 = 4.2 \times 10^{-4}$.

The corresponding mass percent calculated by compiler is 0.182 g(1)/100 g sln.

The solubility of water in benzene at 25°C was reported to be $x_2 = 0.0031$.

The corresponding mass percent calculated by compiler is 0.072 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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 analyzed for (2) content by the Karl Fischer method and the (2)-rich phases were analyzed interferometrically.

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 K

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McDevit, W.F.; Long, F.A.

J. Am. Chem. Soc. 1952, *74*, 1773-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.775 mol(1) dm^{-3} sln.

Presumably this should be 1.775 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler assuming a solution density of 1.000 g mL^{-1} are 0.1775 g(1)/100 g sln and 4.091×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by a variation of the Euler method in which a measured excess volume of (1) is added to (2), and after equilibration, the volume of undissolved (1) is determined by measuring its length in a precision bore tube which leads from the top of the apparatus.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, reagent grade; thiophene-free; distilled; purity not specified.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.02 K

soly. ± 0.5% (from duplicate determinations)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Morrison, T.J.; Billett, F.

J. Chem. Soc. 1952, 3819-22.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.0220 mol(1)/1000 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by compilers are 0.172 g(1)/100 g sln and $x_1 = 3.96 \times 10^{-4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

After an excess of (1) had been shaken with about 1 dm^3 of (2) for about a week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.

SOURCE AND PURITY OF MATERIALS;

(1) source not specified; purest obtainable material; distilled; purity not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 0.5% (mean of large numbers of determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	McCants, J.F.; Jones, J.H.; Hopson, W.H. *Ind. Eng. Chem.* 1953, *45*, 454-6.
VARIABLES:	**PREPARED BY:**
One temperature: 100°F (311 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 100°F (311 K) was reported to be 0.5 g(1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler, is 1.2×10^{-3}.

The solubility of water in benzene at 100°F (311 K) was reported to be <0.3 g(2)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $<1.3 \times 10^{-2}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.

SOURCE AND PURITY OF MATERIALS:

(1) Baker; thiophene free; used without further purification; n_D^{20} 1.5004.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Washburn, E.R.; Hnizda, V.; Vold, R.D. *J. Am. Chem. Soc.* 1931, *53*, 3232.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hayashi, M.; Sasaki, T.

Bull. Chem. Soc. Japan 1956, *29*, 857-9.

VARIABLES:

Temperature: 20 and 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
20	0.137	3.16
25	0.180	4.16

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experiment has been described for the determination of the solubility in a ternary system (1)-(2)-Tween 80.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; shaken repeatedly with concentrated H_2SO_4, boiled with H_2O, recrystallized several times and distilled over Na metal.

(2) not specified.

ESTIMATED ERROR:

soly. more than 0.4 g(1)/100 g sln (type of error not specified).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]
(2) Sodium chloride; NaCl; [76-14-5]
(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Umano, S.; Hayano, I.
Kogyo Kagaku Zasshi 1957, *60*, 1436-7.

VARIABLES:

Temperature: 20-284°C
Concentration of NaCl

PREPARED BY:

H. Miyamoto and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of water in benzene at system pressure

Concn. NaCl[a]	t/°C	g(3)/100 g sln	$10^2 x_3$ (compilers)
0.0	281.0	28.46	63.29
	271.5	25.11	59.24
	250.1	17.22	47.41
	223.0	8.98	29.95
	186.0	4.42	16.7
9.939	78.0	0.240	0.103
	66.0	0.189	0.814
	40.0	0.0762	3.29
	20.2	0.042	1.82
10.0	284.0	27.44	62.11
	265.0	18.91	50.27
	249.0[b]	13.02	39.35
	223.0[c]	7.65	26.4
	183.5	3.70	14.3

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

At higher temperatures: (1) and the aqueous brine were placed in an autoclave, described in detail in the paper, and equilibrated by stirring. After settling, the solubility of (3) in (1) was determined volummetrically by withdrawing layers from the autoclave into a burette.

At lower temperatures: (1) and the aqueous solution were refluxed in a flask at constant temperature. After equilibration, an aliquot of the water rich layer was withdrawn and analysed argentometrically and the solubility of (3) in (1) calculated.

The solubility of NaCl in benzene was determined to be negligible in these experiments (8 x 10^{-5} mol dm^{-3} at 223°C and 54.23 atm.).

SOURCE AND PURITY OF MATERIALS:

(1) : c.p. grade, source not specified; purified by single fractional distillation.

(2) : not specified.

(3) : c.p. grade, source not specified; recrystallized.

ESTIMATED ERROR:

Not specified

REFERENCES:

(1) Benzene; C_6H_6; [71-43-2]
(2) Sodium chloride; NaCl; [76-14-5]
(3) Water; H_2O; [7732-18-5]

(continued)

Concn. NaCl[a]	t /°C	g(3)/100 g sln	10^2x_3 (compilers)
19.200	81.0	0.155	0.67
	63.0	0.079	0.34
	40.0	0.037	0.16
	21.0	0.024	0.10
20.0	280.0	17.93	48.6
	265.0	13.56	40.5
	245.0	7.96	27.3
	221.0	3.98	15.2
	178.0	1.52	6.3
20.0	277.5	15.17	43.7
	268.5	12.47	38.2
	245.5	6.69	23.7
	219.0	3.85	14.8
	178.0	1.58	6.5

---

[a] Stated as % in paper: presumably g(2)/100 g sln (compilers).
[b] Given as 294.0 in the original (corrected in personal communication by the authors to H. Miyamoto).
[c] p = 54.23 atm.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wing, J.; Johnston, W.H.

J. Am. Chem. Soc. 1957, *79*, 864-5.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0554 mL(2)/100 mL sln and 0.0635 mL(2)/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.114 g(2)/100 g sln and 4.9 x 10^{-3}. The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small amount of (2) was equilibrated with 20 mL of (1) using a Teflon stirrer in a 100 mL flask in a Sargent constant temperature bath. At the end of two hours, the mixture was poured into a test tube immersed in the bath and the organic phase separated from water by gravitation. The determination of THO in the organic phase was done by isotopic dilution with a large excess of H_2O. The tritium activities in the tritiated water samples were determined by the acetylene method described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical grade; redistilled in a column of 50 theoretical plates; purity not specified.

(2) Tracerlab, Inc., tritiated water with an activity of approximately 1 μCi/mL.

ESTIMATED ERROR:

temp. ± 0.02 K
soly. 0.9% (st. dev. from 6 determinations).

REFERENCES:

1. Wing, J; Johnson, W.H. *Science* 1955, *121*, 674.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Arnold, D.S.; Plank, C.A.; Erickson, E.E.; Pike, F.P.

Chem. Eng. Data Ser. 1958, *3*, 253-6.

VARIABLES:

Temperature: 0.4-69°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

Solid, gaseous benzene plus water and air

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
0.4	0.168	3.88
3.0	0.170	3.92
3.9	0.176	4.06
4.5	0.172	3.97

Solid, liquid, gaseous benzene plus water and air

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
4.9	0.172	3.97

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a thermostatted 3 L borosilicate glass flask (2) was saturated with (1), the water phase stirred very slowly, then the flask left quiescent, and the saturated solution sampled repeatedly and analyzed on a Beckman model DU unit until a constant benzene concentration response was achieved on successive days. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) the Barrett Division of Allied Chemical and Dye Corp., thiophene-free, 1°; water washed and distilled; for two determinations (a) thrice crystallized.

(2) distilled; electrical conductivity confirmed its high quality.

ESTIMATED ERROR:

temp. ± 0.05 K

soly. 0.0028 g(1)/100 g sln (standard deviation).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Arnold, D.S.; Plank, C.A.; Erickson, E.E.; Pike, F.P.

Chem. Eng. Data Ser. 1958, *3*, 253-6.

Solubility of benzene in water

Liquid, gaseous benzene plus water and air

t/°C	g(1)/100 g sln	$10^4 x_1$ (compiler)
5.6	0.174	4.02
6.7	0.174	4.02
9.0	0.173	3.99
12.5	0.172	3.97
15.0	0.173	3.99
20.0	0.171	3.95
20.6	0.172	3.97
24.8	0.171	3.95
24.9	0.174	4.02
27.3	0.174	4.02
30.0	0.177	4.09
30.0	0.176	4.06
35.0	0.182	4.20
39.9	0.188	4.34
45.0	0.197	4.55
45.0	0.196	4.53
49.8	0.204	4.71
54.5	0.215	4.97
59.8	0.226	5.22
64.8	0.241	5.57
69.0	0.260	5.67

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Brady, A.P.; Huff, H.

J. Phys. Chem. 1958, *62*, 644-9.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.76 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.176 g(1)/100 g sln and 4.06×10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) has been extrapolated from vapor-pressure measurements.

The vapor pressure apparatus used the same principle as that of ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly: 0.03 (standard deviation)

REFERENCES:

1. McBain, J.W.; O'Connor, J.J. *J. Am. Chem. Soc.* 1936, *58*, 2610.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pavia, R.A.

"The Solubility of Water in Benzene", M.S. Thesis, 1958, North Carolina State College, Raleigh, N.C., U.S.A.

VARIABLES:

Temperature: 9.3-65°C

PREPARED BY:

C. Tsonopoulos and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	p_1^s/mm Hg	g(2)/100 g sln[a]	$10^3\ x_2$ (compilers)
9.28	8.774	0.04117	1.783
20.00	17.535	0.05989	2.592
20.00	17.535	0.06076	2.629
30.17	32.136	0.08318	3.597
40.15	55.764	0.11216	4.845
49.97	92.37	0.15222	6.567
59.90	148.70	0.2010	8.657
65.00	187.54	0.2261	9.730

[a] Average of three separate analyses.

Results were represented with a "probable deviation of 0.8%" by the equation

$$\log_{10} (100\ s) = 0.117135 + 0.5162095 \log_{10} p_1^s + 0.0127866 (\log_{10} p_1^s)^2$$

where s is the solubility of water in benzene in g(2)/100 g sln and p_1^s is the equilibrium vapour pressure of the solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water and benzene were equilibrated in a 4-L pyrex vessel fitted with a stirrer. Equilibration typically required about 100 h of stirring. Care was taken to avoid condensation of water on the vessel lid and selective adsorption of water on the glass walls. Samples for analysis were withdrawn by air pressure. Water was determined by Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled in a tinned Barnstead still (specific conductivity 5-20 x 10^{-7} Ω^{-1}).

(2) Allied Chemical: purified by triple fractional crystallization; purity 99.99 mol %; n_D^{25} = 1.49806.

ESTIMATED ERROR:

temp. ± 0.01°C
soly. ± 1% relative; type of error not stated

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Alexander, D.W.

J. Phys. Chem 1959, *63*, 1021-2.

VARIABLES:

Temperature: 0.8 - 65.4°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100g sln	10^4x_1 (compiler)
0.8	0.184*	4.25
9.4	0.179	4.13
16.8	0.177	4.09
24.0	0.180	4.16
31.0	0.183	4.23
38.0	0.192	4.50
44.7	0.203	4.69
51.5	0.214	4.94
58.8	0.234	5.40
65.4	0.257	5.94

*supercooled liquid

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was based on that of Bohon and Claussen (1). Absorbance was determined with a Beckman model D.U. ultraviolet spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Analar benzene; shaken with mercury and purified according to the method of Mair *et al.* (2); purity not specified.

(2) not specified.

ESTIMATED ERROR:

soly. ±0.5% (type of error not specified).

REFERENCES:

1. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1517.

2. Mair, B.J.; Termini, D.J.; Willingham, C.B.; Rossini, F.D. *J. Research Natl. Bur. Standar* 1946, *37*, 229.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rebert, C.J.; Kay, W.B.

A. I. Ch. E. J. 1959, *5*, 285-9.

VARIABLES:

Temperature: 282.8-306.4°C
Pressure: 11.51-15.87 MPa

PREPARED BY:

A. Maczynski, Z. Maczynska and
A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	p/psia	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
287.5	1763	12.16	11.7	0.030
301.7	2118	14.60	22	0.061
306.4	2301	15.86	35.1	0.111
306.4*	2302	15.87	41	0.138

Solubility of water in benzene

t/°C	p/psia	p/MPa (compiler)	g(2)/100 g sln	x_2 (compiler)
282.8	1670	11.51	29.9	0.649
297.5	1992	13.73	31.6	0.667
306	2302	15.87	50.9	0.818
306.4*	2302	15.87	59	0.862

*upper critical solution temperature

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus employed was a modification of that described in refs 1 and 2 for P-T-x studies.
A schematic diagram and construction details amply reported.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, reagent grade; dried over P_2O_5 and distilled; purity not specified.

(2) freshly prepared, conductivity grade.

ESTIMATED ERROR:

soly. ± 0.022 wt. fraction
temp. ± 0.05 K
pressure ± 1 lb/sq.in.

REFERENCES:

1. Young, S. *Stoichiometry* Longmans, Green, New York, 1918, p. 122.
2. Kay, W.B. *Ind. Eng. Chem.* 1938, *30*, 450.

COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Caddock, B.D.; Davies, P.L. *J. Inst. Petrol.* 1960, *46*, 391-6.
VARIABLES: One temperature: 20°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 20°C was reported to be 52 mg(2)/100 g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.052 g(2)/100 g sln and 0.0022.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A sample of (1) was equilibrated at 20°C with an air stream containing a known amount of water vapor tagged with HTO. At equilibrium a sample of (1) was taken and its (2) content determined by liquid scintillation counting.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.01 K

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Kudchadker, A.P.; McKetta, J.J.

Petrol Refiner 1962, *41*, 191-2.

VARIABLES:

Temperature: 37.8 - 137.8°C
Pressure: 0.1 - 5.7 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°F	t/°C (compiler)	p/psia	p/MPa (compiler)	10^4x_1	g(1)/100 g sln (compiler)
100	37.8				
		15.8	0.109	1.24	0.0538
		20.2	0.139	1.32	0.0572
		37.9	0.261	1.57	0.0681
		49.2	0.339	1.66	0.0720
		97.1	0.669	2.06	0.0893
		161.35	1.112	2.61	0.113
		225.7	1.556	3.28	0.142
		244.2	1.684	3.43	0.149
		308.2	2.125	4.01	0.174
		373.7	2.577	4.84	0.201
		406.3	2.801	4.98	0.216
		486.4	3.354	5.78	0.250
		554.8	3.825	6.41	0.277
		635.2	4.380	6.84	0.296
		743.23	5.124	7.87	0.340
		822.7	5.672	8.5	0.38

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental apparatus and analytical technique are described in ref 1. The equilibrium apparatus consisted of a jacketed cell with an internal heating coil. The mixing of the contents of the cell was achieved by a rocking mechanism.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co., purity 99.0 mole percent; used as received.

(2) distilled and boiled to remove any dissolved gases.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Davis, J.E., The Solubility of Methane and Ethylene in Water, M.S. Thesis, the University of Texas, Austin, Tex., 1959.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Kudchadker, A.P.; McKetta, J.J.
(2) Water; H_2O; [7732-18-5]	*Petrol Refiner* 1962, *41*, 191-2.

Solubility of benzene in water

t/°F	t/°C (compiler)	p/psia	p/MPa (compiler)	10^4x_1	g(1)/100 g sln (compiler)
160	71.1	19.8	0.137	1.75	0.0758
		17.7	0.122	1.91	0.0828
		23.8	0.164	1.88	0.0815
		27.5	0.190	2.01	0.0871
		37.6	0.259	2.24	0.0971
		74.0	0.510	2.81	0.1218
		209.8	1.447	4.80	0.2078
		260.2	1.794	5.71	0.2471
		314.3	2.167	6.39	0.2765
		390.6	2.693	7.69	0.3327
		449.1	3.096	8.58	0.3710
		509.8	3.536	10.00	0.4326
		607.2	4.186	12.23	0.5283
220	104.4	29.4	0.203	2.35	0.1018
		36.25	0.250	2.93	0.1270
		46.2	0.319	3.50	0.1516
		49.9	0.344	3.80	0.1646
		84.8	0.585	4.89	0.2127
		165.2	1.139	7.68	0.332
		195.0	1.344	8.49	0.367
		204.6	1.411	9.39	0.406
		218.2	1.504	9.40	0.406
		259.3	1.788	10.75	0.465
		283.1	1.952	11.62	0.502
		327.8	2.260	13.28	0.573
		372.6	2.569	14.68	0.633
		447.5	3.085	16.85	0.727
		548.2	3.780	21.49	0.925
280	137.8	61.3	0.423	3.92	0.170
		76.2	0.525	5.84	0.253
		78.5	0.541	6.10	0.264
		103.7	0.715	7.78	0.337
		112.0	0.772	8.11	0.351
		114.9	0.792	8.28	0.358
		137.5	0.948	9.0	0.389
		170.0	1.172	10.55	0.456
		195.2	1.346	11.59	0.501
		265.1	1.766	14.28	0.616
		316.2	2.180	16.22	0.700
		325.1	2.241	16.98	0.732
		356.2	2.456	18.39	0.793
		402.6	2.776	20.20	0.870
		462.5	3.189	23.0	0.990

(continued)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Kudchadker, A.P.; McKetta, J.J.
(2) Water; H_2O; [7732-18-5]	*Petrol. Refiner* 1962, *41*, 191-2

Author's smoothed values

p/psia		10^4x_1		
	100°F	160°F	220°F	280°F
14.7	1.18	1.56		
20.0	1.33	1.80	1.01	
40.0	1.58	2.22	3.16	
60.0	1.75	2.58	4.16	3.52
80.0	1.92	2.89	4.88	6.20
100.0	2.10	3.17	5.61	7.53
150.0	2.58	3.89	7.18	9.71
200.0	3.03	4.60	8.61	11.82
250.0	3.50	5.52	10.61	13.74
300.0	3.98	6.24	12.32	15.80
350.0	4.41	7.20	14.03	17.84
400.0	4.85	8.15	15.80	20.00
450.0	5.30	9.05	17.61	22.38
500.0	5.77	10.00	19.56	
550.0	6.21	11.06	21.54	
600.0	6.68	12.01		
650.0	7.13			
700.0	7.54			
750.0	7.94			
800.0	8.35			

Author's smoothed values calculated by compiler

p/MPa		g(1)/100 g sln		
	37.8°C	71.1°C	104.4°C	137.8°C
0.101	0.0512	0.0676	-	-
0.138	0.0577	0.0780	0.0438	-
0.276	0.0685	0.0962	0.1369	-
0.414	0.0758	0.1109	0.1802	0.1525
0.552	0.0832	0.1252	0.2113	0.2683
0.689	0.0910	0.1373	0.2428	0.3258
1.034	0.1118	0.1685	0.3107	0.4198
1.379	0.1313	0.1992	0.3723	0.5106
1.724	0.1516	0.2390	0.4585	0.5975
2.068	0.1724	0.2701	0.5321	0.6817
2.413	0.1910	0.3115	0.6057	0.7691
2.758	0.210	0.3525	0.6817	0.8615
3.103	0.229	0.3913	0.7593	0.9634
3.447	0.250	0.4323	0.8428	-
3.792	0.269	0.4779	0.9275	-
4.137	0.289	0.5188	-	-
4.482	0.308	-	-	-
4.826	0.326	-	-	-
5.171	0.343	-	-	-
5.551	0.361	-	-	-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Franks, F.; Gent, M.; Johnson, H.H. *J. Chem. Soc.* 1963, 2716-23.
VARIABLES:	**PREPARED BY:**
Temperature: 17-63°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

T/K	10^4x_1	g(1)/100 g sln (compiler)
290.2	3.95	0.171
295.2	3.97	0.172
299.2	3.99	0.173
302.2	4.02	0.174
305.2	4.12	0.178
308.2	4.20	0.182
313.7	4.39	0.190
315.2	4.40	0.191
317.2	4.45	0.193
319.2	4.57	0.198
324.2	4.78	0.207
329.2	5.03	0.218
334.2	5.31	0.230
336.2	5.42	0.235

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorbance of saturated solutions of (2) in (1) were measured directly at 254 nm on a Unicam S.P. 500 spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; thiophene-free; recrystallized twice from ethanol, washed, filtered through silica gel and distilled.

(2) deionized and doubly distilled from alkaline potassium permanganate and aqueous phosphoric acid.

ESTIMATED ERROR:

temp. ± 0.05 K
absorbance ± 0.5%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76-9.
VARIABLES:	**PREPARED BY:**
Temperature: 153-254°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	$10^3\ x_1$ (compiler)
153	1.283	2.978
178	1.913	5.044
204	2.902	6.844
225	3.790	9.000
241	4.471	10.67
254	5.073	12.17

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; n_D^{20} 1.5011,

(2) doubly distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Jones, J.R.; Monk, C.B.

J. Chem. Soc. 1963, 2633-5.

VARIABLES:

Temperature: 25-35°C

PREPARED BY:

A. Maczynski, Z. Maczynska and
A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	10^4 mL(2)/mL(1)
25	5.7
30	6.5
35	7.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a thermostatted glass-stoppered flask 10-25 mL(1) was shaken for min 4 hrs with tritiated water (a few mL of HTO equivalent to ca. 2 mCi/mL) and decanted. A 5-mL aliquot was reshaken for 4 hrs with 5 mL H_2O in a 10-mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quenching effects (due to solvent) on the scintillator.

SOURCE AND PURITY OF MATERIALS:

(1) 'AnalaR' grade repurified by conventional methods ref 1.

(2) not specified.

ESTIMATED ERROR:

soly. 5% ± 1%
(average deviation)

REFERENCES:

1. Vogel 'Practical Organic Chemistry', Longmans, Green and Co., London, 1956.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McAuliffe, C.

Nature (London) 1963, *200*, 1092-3.
J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.1780 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers is 4.11×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer.
A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+%; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 0.0045 (standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schatzberg, P.J.

J. Phys. Chem. 1963, *67*, 776-9.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski, Z. Maczynska and
A. Szafranski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 20°C was reported to be 532 mg(2)/kg(1).

The corresponding mass percent and mole fraction calculated by the compilers are 0.0532 g(2)/100 g sln and 2.30×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a serum cap-sealed 4-oz. brown glass bottle immersed in a water bath, (1) was saturated with (2) at 20 ± 0.02°C for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe pushed about 2/3 of the way into the hydrocarbon liquid. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a dead-stop end-point using a Beckman KF3 automatic titrimeter with a 5-mL microburet.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson, Coleman and Bell Chromatoquality reagent, 99+ mole%; used as received.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02 K
soly. ± 3 mg(2)/kg(1) (type of error not specified).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Udovenko, V.V.; Aleksandrova, L.P.

Zh. Fiz. Khim. 1963, *37*, 52-6.

VARIABLES:

Temperature: 20-79.5°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
20.0	0.210	4.85
30.0	0.227	5.24
40.5	0.248	5.73
44.5	0.259	5.98
56.5	0.288	6.65
60.0	0.300	6.93
65.0	0.319	7.37
79.5	0.373	8.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The polythermic method of Alekseev was used.
No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; dried over metallic sodium, and distilled;

n_D^{20} 1.5013; d_4^{30} 0.8661.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Hoegfeldt, E.; Bolander, B. *Ark. Kemi* 1964, *21*, 161-86.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene was reported to be 0.032 mol(2) dm^{-3} sln at 25°C.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.066 g(2)/100 g sln and 2.9×10^{-3}.

The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration in ref 1, 2.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, 0.04% of toluene; purity 99.6%; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.3 K
soly. ± 0.001 mol(2) dm^{-3} sln
(type of error not specified)

REFERENCES:

1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. *J. Chem. Soc.* 1961, *90*.
2. Johansson, A. *Sv. Papperstidn.* 1947, *11B*, 124.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Thompson, W.H.; Snyder, J.R.

J. Chem. Eng. Data 1964, *9*, 516-20.

VARIABLES:

Temperature: 37.9-204.3°C
Pressure: 7 and 34.6 MPa

PREPARED BY:

A. Maczynski, Z. Maczynska and
A. Szafranski

EXPERIMENTAL VALUES:

Mutual solubility of benzene and water at 1000 psig (7 MPa compiler)

t/°F	*t*/°C (compiler)	10^4x_2 (1)-rich phase	10^4x_1 (2)-rich phase	g(2)/100 g sln (compiler) (1)-rich phase	g(1)/100 g sln (compiler) (2)-rich phase
99.9	37.7	41.6	4.33	0.0962	0.187
99.9	37.7	41.8	4.61	0.0967	0.200
100.1	37.8	46.6	4.54	0.1078	0.197
100.3	37.9	48.7	4.34	0.1127	0.188
101.0	38.3	42.1	4.60	0.0974	0.199
101.5	38.6	43.3	-	0.1002	-
160.3	71.2	124	6.63	0.289	0.287
218.0	103.3	-	9.84	-	0.425
219.0	103.8	274	8.56	0.645	0.370
280.0	137.8	558	-	1.344	-
280.3	137.9	-	14.3	-	0.617
281.0	138.3	-	18.6	-	0.802
339.3	170.7	-	41.6(a)	-	1.780
339.3	170.7	-	42.7(a)	-	1.826
340.0	171.1	1000	44.2(a)	2.498	1.889
340.3	171.3	-	46.5(a)	-	1.986
341.0	171.7	-	36.0(a)	-	1.543
396.3	202.4	-	85.3	-	3.60
397.3	202.9	1770	-	4.724	-
398.0	203.3	-	94.2(a)	-	3.96
399.0	203.9	-	72.6	-	3.07
399.7	204.3	-	81.0	-	3.42

(a) results known to be high due to a high analytical blank

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 70 mL each of (1) and (2) were placed in a high-pressure equilibrium cell. The cell was installed in the phase-contacting equipment, pressurized with nitrogen, heated and kept horizontal with no agitation for min. 24 hr, then rotated and kept vertical for 3 hr to ensure complete phase separation. Each phase was sampled (20 mL) and the sample volume measured under the experimental conditions. The (1)-rich phase was analyzed for (2) by the Karl Fischer method and the (2)-rich phase for (1) via combustion at 1450-1500°F over CuO, absorption of CO_2 and back-titration of NaOH.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade, 99+ mole%; used as received.

(2) distilled and redistilled in the absence of carbon dioxide.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Thompson, W.H.; Snyder, J.R.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1964, *9*, 516-20.

Mutual solubility of benzene and water at 500 psig (34.6 MPa compiler)

t/°F	t/°C (compiler)	10^4x_2 (1)-rich phase	10^4x_1 (2)-rich phase	g(2)/100 g sln (compiler) (1)-rich phase	g(1)/100 g sln (compiler) (2)-rich phase
100.3	37.9	38.1	5.61	0.0881	0.243
159.7	70.9	-	8.95	-	0.387
160.3	71.3	110	-	0.256	-
161.0	71.7	105	-	0.244	-
219.7	104.3	-	14.1	-	0.609
220.7	104.8	263	-	0.619	-
279.3	137.4	505	22.8	1.211	0.981
339.3	170.7	959	43.1	2.387	1.843
400.7	204.8	1530	98.3	3.998	4.13
459.7	237.6	4320	248	14.92	9.93
460.7	238.1	4600	265	16.42	10.56

Author's smoothed values of the mutual solubility of benzene and water at 1000 psig (7 MPa)

t/°F	t/°C	10^4x_2 (1)-rich phase	10^4x_1 (2)-rich phase	g(2)/100 g sln (1)-rich phase	g(1)/100 g sln (2)-rich phase
100	38	42.3	4.46	0.0978	0.193
160	71	121	6.65	0.282	0.288
220	104	274	10.1	0.645	0.436
280	138	558	18.6	1.34	0.801
340	171	1000	36.0	2.50	1.54
400	204	1780	82.0	4.75	3.46

Author's smoothed values of the mutual solubility of benzene and water at 5000 psig (34.6 MPa)

t/°F	t/°C	10^4x_2 (1)-rich phase	10^4x_1 (2)-rich phase	g(2)/100 g sln (1)-rich phase	g(1)/100 g sln (2)-rich phase
100	38	38.1	5.61	0.0880	0.243
160	71	106	9.05	0.246	0.392
220	104	245	14.1	0.575	0.608
280	138	500	22.8	1.20	0.980
340	171	905	43.0	2.24	1.84
400	204	1620	98.0	4.45	4.11
460	238	4500	255	15.90	10.20

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 0-50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
0	0.03996	1.730
10	0.0446	1.93
20	0.0582	2.52
30	0.0749	3.24
40	0.0948	4.10
50	0.1177	5.09

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. 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:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Connolly, J.F.

J. Chem. Eng. Data 1966, *11*, 13-6.

VARIABLES:

Temperature: 260-300°C

Pressure: 100-800 atm

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	*p*/atm	*p*/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
260	100	10.1	7.1	0.0173
	250	25.3	7.3	0.0178
	500	50.7	7.2	0.0176
	800	81.1	6.6	0.0160
281	150	15.2	13.7	0.0353
	250	25.3	13.8	0.0356
	500	50.7	13.3	0.0342
	600	60.8	12.7	0.0325
287.5	165	16.7	17.2	0.0457
	195	19.8	18.1	0.0485
	320	32.4	18.1	0.0485
	380	38.5	17.3	0.0460
	735	74.5	13.9	0.0359
295	135	13.7	18.2	0.0488
	160	16.2	22.8	0.0638
	185	18.7	27.0	0.0786
	210	21.3	31.3	0.0951
	225	22.8	34.0	0.1062
	230	23.3	35.3	0.1117
	240	24.3	35.5	0.1126
	250	25.3	35.3	0.1117
	265	26.8	34.0	0.1062

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small droplet of a second phase appeared at the top of the cell. Then mercury was injected to change pressure, more (1) was injected and the measurement was repeated.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips reagent grade; better than 99.8%; used as received.

(2) distilled and deaerated.

ESTIMATED ERROR:

temp. ± 0.02 K

pressure ± 2 atm.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Connolly, J.F.

J. Chem. Eng. Data 1966, *11*, 13-6.

Solubility of benzene in water

t/°C	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
295	290	29.4	31.3	0.0951
	350	35.5	27.0	0.0786
	450	45.6	22.9	0.0641
	690	69.9	18.2	0.0488
300	145	14.7	22.8	0.0638
	155	15.7	27.3	0.0797
	160	16.2	30.9	0.0935
	160	16.2	34.3	0.1074
	165	16.7	37.5	0.1216
	165	16.7	40.0	0.1332
	160	16.2	43.0	0.1482
	160	16.2	46.1	0.1647
	490	49.6	56.0	0.2269
	480	48.6	52.5	0.2031
	470	47.6	49.5	0.1843
	470	47.6	46.1	0.1647
	470	47.6	43.0	0.1482
	470	47.6	40.0	0.1332
	480	48.6	37.5	0.1216
	490	49.6	34.3	0.1074
	505	51.2	31.0	0.0939
	555	56.2	27.3	0.0797
	665	67.4	22.9	0.0641

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Johnson, J.R.; Christian, S.D.;
Affsprung, H.E.

J. Chem. Soc. A. 1966, 77-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0349 mol(2)/dm^3 sln.
The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g(2)/100 g sln and 3.11×10^{-3}.
The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus described in ref 1 was used without modification. Samples were equilibrated in a constant-temperature water-bath maintained at 25 ± 0.1°C. Water solubilities were determined by using a Beckman Model KF-3 Aquameter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; certified or reagent grade; distilled through a 30-plate Oldershaw column.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 0.0005 mol(2)dm^3 sln
(type of error not specified)

REFERENCES:

1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. *J. Chem. Educ.* 1963, *40*, 419.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Masterton, W.L.; Gendrano, M.C.

J. Phys. Chem. 1966, *70*, 2895-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0347 mol(2) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0715 g(2)/100 g sln and 3.09×10^{-3}. The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibration of (1) and (2) was allowed to take place for at least 2 days. The organic phase was analyzed for water by the Karl Fischer method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; free from thiophene; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.05 K
soly. 0.0002 mol(2) dm^{-3} (mean deviation from duplicate determinations)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Moule, D.C.; Thurston, W.M.

Can. J. Chem. 1966, *44*, 1361-7.

VARIABLES:

Temperature: 9.44-49.45°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	10^3x_2 (compiler)
9.44	442.5	0.0443	1.92
14.98	530.2	0.0530	2.30
20.10	639.2	0.0639	2.77
24.54	726.0	0.0726	3.14
29.52	848.0	0.0848	3.67
34.88	1017.1	0.102	4.40
40.06	1177.8	0.117	5.09
43.78	1333.7	0.133	5.76
49.45	1570.6	0.157	6.78

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A method based on an isotope dilution procedure was used. This method involves the exchange of the water present in the sample with D_2O determined by infrared difference spectroscopy.

SOURCE AND PURITY OF MATERIALS:

(1) Fischer Certified reagent grade; distilled twice and dried over molecular sieve (Linde No. 4A).

(2) from Ottawa River (0.0146 mole % D_2O; distilled from alkaline permanganate).

ESTIMATED ERROR:

temp. ± 0.05 K

soly. ± 0.8% (mean of three determinations)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Taha, A.A.; Grigsby, R.D.; Johnson, J.R.; Christian, S.D.; Affsprung, H.E.

J. Chem. Educ. 1966, *43*, 432-5.

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported as 0.022 mol/L sln. The corresponding mass per cent and mole fraction solubility, x_1, calculated by the compiler are, assuming a solution density of 1.00 kg L^{-1}, 0.16 g(1)/100 g sln and 4.0×10^{-4} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility of (1) in (2) was determined from vapor pressure measurements. 190 mL of pure water were placed in a glass manometric apparatus of known vapor volume. The apparatus is described in detail in the paper. The apparatus was evacuated, benzene added (probably as a liquid), and the pressure measured.

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not specified.

(2) Pure; purity not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Alwani, Z.; Schneider, G.M.

Ber. Bunsenges. Phys. Chem. 1969, *73*, 294-301.

VARIABLES:

Critical temperature and pressure

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

Values of Critical Temperatures and Pressures

T/°C	T/K	P/bar
339,5	612.7	2000
329,7	602.9	1600
320,2	593.4	1200
309,5	582.7	800
297,1	570.3	400
294,2	567.4	200
297,4	570.6	170
304,9	578.1	154
325,4	598.6	171
363,0	636.2	210

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Steel optical cell in large aluminum block furnace. Cell contents stirred by magnetically operated stirrer. Pressure measured using a movable piston and Boardon gauge. Temperature measured using a steel-sheathed thermocouple. Components charged into cell and one phase-two phase boundaries observed visually. Critical properties determined from boundary envelopes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical grade product fractionally distilled, purity 99.9 mole per cent.

(2) Distilled and degassed.

ESTIMATED ERROR:

$\delta T/K = 0.4$
$\delta P/P = \pm 0.02$ (estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Gregory, M.D.; Christian, S.D.; Affsprung, H.E. *J. Phys. Chem.* 1967, *71*, 2283-9.
VARIABLES: One temperature: 35°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 35°C was reported to be 0.0465 mol(2) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0970 g(2)/100 g sln and 4.19×10^{-3}.

The assumption that 1 dm^3 sln = 863 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A solution of (2) in (1) was obtained using solute isopiestic equilibrator described in ref 1. Water concentration was determined with a Beckman KF-3 aquameter by the Karl Fischer analysis.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, reagent grade; fractionally distilled using a 30-plate Oldershaw,

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.05 K

REFERENCES:

1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Warley, J.D. *J. Chem. Educ.* 1963, *40*, 419.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

O'Grady, T.M.

J. Chem. Eng. Data 1967, *12*, 9-12.

VARIABLES:

Temperature: 288 and 293°C
Pressure: 3600 psig (24.9 MPa)

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°F	t/°C	p/psig	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
550	288	3600	24.9	19.0	0.0513
560	293	3600	24.9	26.3	0.0751

Solubility of water in benzene

t/°F	t/°C	p/psig	p/MPa (compiler)	g(1)/100 g sln	x_2 (compiler)
550	288	3600	24.9	32.6	0.677
560	293	3600	24.9	41.0	0.751

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Measured amounts of (1) and (2) of known composition were pumped into the extractor and mixed for 1 or 2 hours. The phases were allowed to settle for about 2 hours; then the contents were slowly (1.5 mL per minute) displaced at constant pressure with mercury. The product was collected in 2-5 mL cuts in burets with 0.1 mL subdivisions. The (1) - (2) composition could be read directly.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips research grade; less than 0.2% impurities; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°F
pressure ± 10 psi
soly. ± 0.02 mL(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Worley, J.D. *Can. J. Chem.* 1967, *45*, 2465-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.17 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.217 g(1)/100 g sln and 5.01 x 10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The isotopic solute transfer technique of Christian *et al.* (refs 1, 2), was used.

This method consists of vapor phase equilibrations of water with solutions of benzene-dinonylphthalate in closed containers. The benzene absorbance was measured at 254 nm with a Cary 14 spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; reagent grade; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.2 K

REFERENCES:

1. Christian, S.D. *et al.* *J. Chem. Educ.* 1963, *40*, 419.
2. Christian, S.D.; Affsprung, H.E.; Johnson, J.R. *J. Chem. Soc.* 1963, 1896.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Burd, S.D.Jr.; Braun, W.G.

Proc. Div. Refining., Am. Petrol. Inst. 1968, *48*, 464-76.

VARIABLES:

Temperature: 359 - 473 K

Pressure: 0.17 - 2.76 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x_2 (compiler)
25	0.17	187	359	0.33	0.014
50	0.34	233	385	0.63	0.027
100	0.69	283	413	1.08	0.045
150	1.03	321	434	1.54	0.064
200	1.38	337	443	1.75	0.072
250	1.72	356	453	2.08	0.084
300	2.07	371	461	2.25	0.091
350	2.41	385	469	2.60	0.104
400	2.76	392	473	2.80	0.111

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were carried out in the autoclave for vapor-liquid equilibrium determination. The solubility points were obtained by incremental addition of (2) followed by stirring, settling, sampling and analysis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. The samples were analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99.0% by glc; used as received.

(2) distilled

ESTIMATED ERROR:

temp. ± 0.5°F.

soly. ± 0.004 g(2)/100 g sln.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Roddy, J.W.; Coleman, C.F.

Talanta 1968, *15*,1281-6.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be $x_2 = 3.23 \times 10^{-3}$ and 0.0363 mol(2) dm^{-3} sln.
The corresponding mass percent value calculated by the compilers is 0.0747 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A method for measuring the solubility of (2) in (1) was based on the use of tritium tracer to monitor the recovery of (2) in a conventional gravimetric method and to measure tritium distribution between the aqueous and the organic phases.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; thiophene free reagent; recrystallized three times.

(2) HTO at 5 Ci/mL, New England Corp.; diluted to about 1 mCi/mL.

ESTIMATED ERROR:

soly. better than 1%
(type of error not specified).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Corby, T.C.; Elworthy, P.H.

J. Pharm. Pharmacol. 1971, *23 suppl.* 39 S-48 S.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be 0.0218 mol dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.170 g(1)/100 g sln and 3.9×10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small excess of (1) was equilibrated with (2) by shaking at 20°C until saturation was attained. The saturated aqueous phase was analysed by ultraviolet spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

(1) W. Jarvie Ltd., cyrstalizable; distilled before use; n_D^{18} 1.5028.

(2) distilled once from glass.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Pierotti, R.A.; Liabastre, A.A.

"Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 p.

VARIABLES:

Temperature: 278.26-318.36 K

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benzene in water

T/K	g(1)/100 g sln	10^3x_1
278.26	0.2071 ± 0.0052	0.4776
288.06	0.2078 ± 0.0055	0.4792
293.06	0.2085 ± 0.0040	0.4809
298.16	0.2088 ± 0.0038	0.4815
308.26	0.2102 ± 0.0046	0.4848
318.86	0.2300 ± 0.0054	0.5304

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

10 mL of (2) were placed along with 4-10 drops of (1) in 10 ml serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson, Coleman & Bell; Chromatoquality; 99+mole%; used as received.

(2) laboratory distilled water.

ESTIMATED ERROR:

soly.: standard deviation from at least 15 measurements are given above.

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Ben-Naim, A.; Wilf, J.; Yaacobi, M. *J. Phys. Chem.* 1973, *77*, 95-102.
VARIABLES:	**PREPARED BY:**
Temperature: 10-50°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water is expressed in terms of the standard free energy of solution; $\Delta\mu_s^\circ$, determined as:

$$\Delta\mu_s^\circ = \lim_{\rho_s \to 0} [-RT\ \ell n(\rho_s^\ell/\rho_s^g)_{eq}]$$

where $(\rho_s^\ell/\rho_s^g)_{eq}$ is the Ostwald absorption coefficient and ρ_s^ℓ and ρ_s^g are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, $\Delta\mu_s^\circ$ was fitted to a second degree polynomial of the form:

$$\Delta\mu_s^\circ = -9536.2 + 37.122\ t - 0.02666\ t^2$$

where t is in °C ($10 < t < 50$°C) and $\Delta\mu_s^\circ$ is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined spectroscopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for *ca.* 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at λ_{max} with a Model 450 Perkin-Elmer spectrophotometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three compartment cell, details of which are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; puriss, 99.94%, used as received.

(2) Distilled water, further distilled from alk. $KMnO_4$ and acid $K_2Cr_2O_7$; κ, 0.8×10^{-6} S cm^{-1}.

ESTIMATED ERROR:

Temperature: ±0.05 K

Solubility: std. dev. in $\Delta\mu_s^\circ$, 8.788 cal/mol

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Bradley, R.S.; Dew, M.J.; Munro, D.C. *High Temp. High Press.* 1973, *5* 169-76.
VARIABLES:	PREPARED BY:
Temperature: 25-55°C Pressure: 1-1200 bar	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	p/bar[b]	mol/L sln	g(1)/100g sln[a] (compiler)	$10^4 x_1$[a] (compiler)
25	1	0.0234	0.183	4.21
45	1	0.0277	0.216	4.99
55	1	0.0305	0.238	5.49
45	625	0.0268	0.209	4.82
55	625	0.0326	0.254	5.87

[a] Assuming a solution density of 1.00kg/L at all temperatures and pressures.

[b] 1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of (1) in aqueous solutions of $AgNO_3$ and KNO_3 at various temperatures and pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) at room temperature and pressure was determined in a stoppered 1mm silica cuvette placed in a Unicam SP500 spectrophotometer and stirred magnetically. Measurements were made until a constant concentration was reached. The value was cross-checked against a 2-L sample of saturated solution which had been equilibrated for some months.

Solubilities at higher temperatures and pressures were similarly determined in a special cell fitted into the spectrophotometer. Many details of the apparatus are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) A.R. grade, thiophene-free, no further details given.

(2) Distilled, air-free

ESTIMATED ERROR:

Not specified

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Filyas, Yu.I.

Sb. Nauch. Tr. Vses. Neftegazov. Nauch.-Issled. Inst. 1973, *45*, 68-70.

VARIABLES:

One temperature: 295°C
One pressure: 10 atm

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 295°C and 10 atm was reported to be 0.318 g(2)/g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 24.1 g(2)/100 g sln and 0.580 at 1.01 MPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing is specified in the paper

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Karisson, R.

J. Chem. Eng. Data 1973, *18*, 290-2.

VARIABLES:

Temperature: 14-35°C

PREPARED BY:

A. Maczynski, Z. Maczynska
and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	mg(2)/kg(1)	10^2 g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
14.97	533.0	5.33	2.31
17.94	591.3	5.91	2.56
20.05	631.4	6.31	3.74
22.95	686.7	6.87	2.98
24.90	724.8	7.24	3.14
27.97	803.2	8.03	3.14
29.95	853.5	8.53	3.70
31.96	915.8	9.16	3.97
35.06	1021.1	10.21	4.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The determination of the solubility of (2) in (1) was based on an accurate method for determining small amounts of water via coulometrically generated iodine at a controlled potential in a Karl Fischer reagent as described in ref(1,2). Two 100-mL Erlenmeyer flasks, each containing 10 mL of (2) and 40 mL of (1), were placed in a water bath. The temperatures were measured with a platinum resistance thermometer. When equilibrium was reached, samples were withdrawn from the benzene phase with a dried Agla microsyringe and immediately added through a membrane to the electrolysis cell.

SOURCE AND PURITY OF MATERIALS:

(1) Fisher Scientific Co., thiophene-free; twice recrystallized.

(2) twice distilled.

ESTIMATED ERROR:

temp. ± 0.3 K
soly. ± 0.3% (type of error not specified).

REFERENCES:

1. Karisson, R. *Talanta* 1972, *19*, 1639.
2. Karisson, R.; Karrman, K.J. *Talanta* 1951, *18*, 459.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Leinonen, P.J.; Mackay, D.

Can. J. Chem. Eng. 1973, *51*, 230-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and
A. Szafranski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1765 mg(1) dm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.1765 g(1)/100 g sln and 4.07 x 10^{-4}.
The compiler's calculation assumes a solution density of 1.000 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was equilibrated at 25 ± 0.1°C for a minimum of 12 hrs in a 200-mL Teflon-stoppered vessel (25 cm long and 3.5 cm across) with gentle shaking, allowed to settle for 6 hrs and tested for the absence of emulsion (Tyndall effect). The aqueous and organic phases were analyzed by glc (with internal standardization) on a Hewlett-Packard Model 700 instrument equipped with a 15% SE-30 on 60/80 mesh acid-washed (CH3)$_2$Cl$_2$Si-treated Chromosorb P column (steel capillary 10 ft x 0.125 inch). The (1) in the aqueous phase was extracted into 5 ml of heptane and the extract analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.
research grade, 99+ mole%;
used as received.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. 30 mg(1) dm^{-3} (two standard deviations)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10^4x_1 (compiler)
0† (a)	1678 (c)	0.167	3.87
25 (b)	1755 (c)	0.175	4.05

Solubility of water in benzene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	10^3x_2 (compiler)
0‡ (a)	302 (d)	0.030	1.31
25 (b)	692 (e)	0.069	2.99

†Benzene was at supercooled liquid state.
‡Solubility in supercooled liquid.
[a-e] see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

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% (from two or three determinations)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Brown, R.L.; Wasik, S.P.

J. Res. Natl. Bur. Stds. A. 1974, *78*, 453-60.

VARIABLES:

Temperature: 4.5-20.1°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of Benzene in Water

t/°C	g(1)/100 g sln		10^4 x_1 (compiler)
4.5	0.184	0.0033	4.25
6.3	0.185	0.0033	4.27
7.1	0.181	0.0055	4.18
9.0	0.181	0.0034	4.18
11.8	0.177	0.0041	4.09
12.1	0.177	0.0035	4.09
15.1	0.179	0.0038	4.14
17.9	0.179	0.0038	4.14
20.1	0.176	0.0032	4.07

[a] Errors given as standard deviations.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 cm^3 of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 mole per cent purity; source and methods of purification not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.01 K

Solubility: see Table above

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Goldman, S.

Can. J. Chem. 1974, *52*, 1668-80.

VARIABLES:

Temperature: 10-40°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	mol(2) dm^{-3} sln	g(2)/100 g sln (compiler)	$10^3\ x_2$ (compiler)
10	0.02171	0.0440	1.91
15	0.02561	0.0522	2.26
20	0.03017	0.0618	2.67
25	0.03518	0.0725	3.14
30	0.03950	0.0820	3.55
35	0.04690	0.0979	4.23
40	0.05243	0.1101	4.76

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 175-mL milk-dilution bottle fitted with a bakelite screw cap and a Teflon insert and rotated end-over-end at 20 min^{-1}, (1) was equilibrated with an excess of (2) at 25 ± 0.02°C, sampled (5 mL ± 0.2%) with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.

SOURCE AND PURITY OF MATERIALS:

(1) certified grade; washed successively with conc. H_2SO_4, H_2O, 1N NaOH, H_2O, dried with silica gel, and distilled; d_4^{25} 0.87365,

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.02 K
soly. 0.00039 (st. dev.)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Vodnye. Resursy. 1975, *2*, 170-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.000 mg(1) cm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.1000 g (1)/100 g sln and 2.305×10^{-4}.
The compiler's calculation assumes a solution density of 1.000 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by glc.
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.

SOURCE AND PURITY OF MATERIALS:

(1) described in ref 1.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K

REFERENCES:

1. Kresnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

Can. J. Chem. Eng. 1975, *53*, 239-41.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.7795 g(1) dm^{-3}.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.178 g(1)/100 g sln and 4.11×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility of (1) in (2) was determined by gas chromatography. The gas chromatograph was Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector. Many details were given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co., research grade; 99.9+%; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 0.0164 g(1) dm^3

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Sada, E.; Kito, S.; Ito, Y. *J. Chem. Eng. Data* 1975, *20*, 373-5.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.0403 mL(1)/1000 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sudan IV was used to dye (1). The experimental apparatus and procedure used in this work were similar to those of Sobotka and Khan (ref 1). To make the measurements more accurate, the apparatus used consisted of a 1-liter dissolution flask and a 2-mL microburet. The scale was calibrated in advance by use of mercury. The dissolution flask was immersed in a water bath controlled thermostatically at 25°C. To avoid condensation of (1) from the gas phase, the temperature of gas phase in the dissolution flask was kept 1°C higher than that of the liquid phase. The dissolution flask and the microburet were connected tightly.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; reagent grade; used as received; purity not specified.

(2) pure.

ESTIMATED ERROR:

temp. ± 0.01 K

soly. less than 0.008 mL(1)/1000 mL sln (type of error not specified)

REFERENCES:

1. Sobotka, H.; Kahn, J. *J. Am. Chem. Soc.* 1948, *53*, 2935.

COMPONENTS:

(1) Benzene; C_6H_6; [77-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S.

Zh. Fiz. Khim. 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 438-76.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be $x_1 = 4 \times 10^{-4}$.

The corresponding mass percent calculated by the compiler is 0.17 g(1)/100 g sln.

The solubility of water in benzene at 20°C was reported to be $x_2 = 0.0026$.

The corresponding mass percent calculated by the compiler is 0.060 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; pure or analytical reagent grade; purity <99.9%.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* 1976, *54*, 3909-16.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0349 mol(2) dm^{-3} sln. The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g(2)/100 g sln and 3.11×10^{-3}.

The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was submerged up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days.
The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.

SOURCE AND PURITY OF MATERIALS:

(1) Fisher B-245; purified by double crystallization; d_4^{25} 0.87378.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. 0.0002 mol(2) dm^{-3} sln (standard deviation from 5 determinations).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C and at system pressure was reported to be 1740 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.174 g(1)/100 g sln and 4.01×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. ± 17 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water, H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

VARIABLES:

Temperature: 225-260°C
Pressure: 4.7-78.5 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
225	48	4.7	0.256	7.35
	100	9.8	0.250	7.14
	150	14.7	0.242	6.86
	200	19.6	0.228	6.37
	300	29.4	0.227	6.34
	400	39.2	0.217	6.01
	500	49.0	0.209	5.74
	600	58.8	0.200	5.45
	700	68.6	0.191	5.16
	800	78.5	0.183	4.91
250	75	7.4	0.410	13.81
	100	9.8	0.399	13.27
	150	14.7	0.378	12.29
	200	19.6	0.361	11.52
	300	29.4	0.332	10.28
	400	39.2	0.314	9.55
	500	49.0	0.312	9.47
	600	58.8	0.291	8.64
	700	68.6	0.280	8.23
	800	78.5	0.270	7.86

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical reagent grade; purity not specified; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Prom.* 1971, *4*, 6.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
260	84.5	8.3	0.491	18.19
	100	9.8	0.479	17.49
	150	14.7	0.442	15.44
	200	19.6	0.416	14.10
	300	29.4	0.381	12.43
	400	39.2	0.363	11.61
	500	49.0	0.352	11.13
	600	58.8	0.342	10.70
	700	68.6	0.332	10.28
	800	78.5	0.321	9.83

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* 1978, *51*, 957-8.
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.82 g(1)dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.084 g(1)/100 g sln and 1.94 x 10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 200-500 mL(2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc). was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	soly. 0.01 g (1)dm^{-3} sln (standard deviation from 6 determinations).
	REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1740.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.174 g(1)/100 g sln and 4.02×10^{-4}.

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.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The 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.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 35.0 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. <u>1978</u>, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1791 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 0.1791 g(1)/100 g sln and 4.130×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05 K
soly. ± 10 mg(1)/100 kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* <u>1975</u>, *13*, 535.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Singh, R.P.; Sah, R.

Indian J. Chem. 1978, *16A*, 692-4.

VARIABLES:

One temperature: 303.15 K

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 303.15 K was reported to be 0.064 g(2)/mol(1).

The corresponding mass percent and mole fraction, x_2, values calculated by compiler are 0.082 g(2)/100 g sln and 0.0035.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titrations were carried out in well stoppered volumetric flasks in order to check for loss due to vaporization. Shaking after each addition of water was done in an ultrasonic shaker for at least 30 min. The contents were equilibrated in a thermostat. The final end point was determined when a second phase appeared and the volume of the water added was noted. Each titration was repeated at least three times to check the reproducibility of the results.

SOURCE AND PURITY OF MATERIALS:

(1) BDH, analar quality; purified; purity not specified.

(2) conductivity water.

ESTIMATED ERROR:

temp. ± 0.05 K

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bittrich, H.J.; Gedan, H.; Feix, G.

Z. Phys. Chem., Leipzig 1979, *260* 1009-13.

VARIABLES:

Temperature: 20 - 40°C

PREPARED BY:

A. Maczynski and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln	10^4x_1 (compiler)
20	1790	0.1790	4.133
40	2025	0.2025	4.676
60	2442	0.2442	5.641

Solubility of water in benzene

t/°C	mg(2)/kg(2)	g(2)/100 g sln	10^3x_2 (compiler)
20	586	0.0586	2.54
40	712	0.0712	3.08
60	860	0.0860	3.72

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was shaken at a specified temperature and then thermostatted for 48 h. The equilibrated phases were sampled and analyzed by flame-ionization glc using 3-m steel columns of 10% SE 30-on-Chromaton N (90°C) and 1.5 g + 10% SE 30-on-Chromaton N (120°C) for (1) and (2), respectively.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; distilled and crystallized; glc pure.

(2) not specified.

ESTIMATED ERROR:

soly. ± 5% (type of error not specified).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water was reported to be 2.24×10^{-2} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction (x_1) solubilities, calculated by the compiler, are 0.175 g(1)/100 g sln and 4.05×10^{-4} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of ^{14}C-labelled benzene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) ^{14}C-labelled benzene: New England Nuclear, used without further purification.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2 K

Solubility: ±0.7% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schwarz, F. P.

Anal. Chem. 1980, *52*, 10-15.

VARIABLES:

One temperature: 23.5°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benzene in water at 23.5°C

g(1)/100 g sln	10^4x_1 (compiler)
0.188 ± 0.005*a	4.34
0.188 ± 0.009 b	4.34
0.182 ± 0.007 c	4.20
0.193 ± 0.011 d	4.45
0.190 ± 0.007 e	4.38

*values determined for different masses of (1) coated into the inert support. a: 0.014; b: 0.0154; c: 0.0124; d:0.0464; e: 0.0526 g/cm

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) spectral grade used without further purification

(2) distilled

ESTIMATED ERROR:

temp. ± 1.5°C

soly. 4% (average std. dev.)

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Chem. Lett. 1981, 225-8.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/L	g(1)/100 g sln[a]	10^4x_1[a]
15	1.54 ± 0.04	0.154	3.56
25	1.61 ± 0.09	0.161	3.72
35	1.76 ± 0.06	0.177	4.09
45	1.85 ± 0.11	0.187	4.32

[a] Assuming the solution density to be that of pure water at the same temperature (ref. 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

SOURCE AND PURITY OF MATERIALS:

(1) analytical reagent grade used as purchased.

(2) redistilled.

ESTIMATED ERROR:

soly. : given above

REFERENCES:

1. CRC Handbook of Chemistry and Physics, R.C. weast, Editor, CRC Press, Florida, 63rd edn., 1982, pF-11.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55* , 1054-62.

VARIABLES:

Temperature: 5-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	10^4 x_1 (compiler)[a]
5	20.7	0.162	3.73
15	20.2 ± 0.3	0.158	3.65
25	20.7[b] ± 0.1	0.162	3.74
35	21.8 ± 0.6	0.171	3.94
45	22.8 ± 0.5	0.180	4.15

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

[b] No error estimate given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 99.5%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.01°C.

REFERENCES:

1. Kell, G.S.
J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
Deguchi, Y.; Nagai, H.
Chem. Lett. 1981, 225-8.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tsonopoulos, C.; Wilson, G.M.
A. I. Ch. E. J. 1983, *29*, 990-9.

VARIABLES:

Temperature: 313-473 K
Pressure: 0.03-3.0 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water

T/K	p^a/MPa	$10^3\ x_1$	g(1)/100 g sln (compiler)
313.15	0.03054	0.4435	0.192
373.15	0.2758	0.949	0.412
423.15	1.0549	2.42	1.05
473.15	3.020	5.40	2.34

The solubility of water in benzene

T/K	p^a/MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
313.15	0.03054	0.471,0.501	0.112[b]
373.15	0.2758	1.81,2.08	0.448[b]
423.15	1.0549	7.13	1.64
473.15	3.020	18.5	4.26

a Absolute pressure
b Average value

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:

(1) No details given

(2) No details given

ESTIMATED ERROR:

soly. ± 5% relative; repeatability of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

(continued)

The three phase critical point was reported to be 541.7K, 9.42 MPa and $x_1 = 2.528 \times 10^{-2}$ (10.1 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-542K, *viz.*

$$\ln x_1 = -170.04018 + 6922.912/T + 24.398795 \ln T$$

$$\ln x_2 = -1.64055 - 2029.41/T + 0.00900544\ T$$

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Arakawa, S.;
Araki, M.; Deguchi, T.
Bull. Chem. Soc. Jpn. 1984, *57*,
1539-44.

VARIABLES:

One Temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.07 x 10^{-2} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 0.162 g(1)/100 g sln, x_1 = 3.73 x 10^{-4}, calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade source and purity not stated, used without further purification.

(2) Deionized and redistilled; no further details given.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Water-d_2; D_2O; [7789-20-0]

ORIGINAL MEASUREMENTS:

Brollos, K.; Peter, K.; Schneider, G. M.

Ber. Bunsenges. Phys. Chem. 1970, *74*, 682-6.

VARIABLES:

Pressure and temperature on one phase-two phase boundary.

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
339.1	2445	0.25	56.5
337.5	2300		
333.4	2000		
328.0	1750		
323.9	1530		
314.9	1100		
308.4	840		
303.8	655		
300.1	490		
295.6	220		
326.1	170		
315.9	158		
355.2	2855	0.546	82.4
351.0	2600		
348.2	2450		
342.4	2095		
337.9	1850		
332.4	1585		
330.4	1480		
324.9	1300		
319.6	1100		
311.8	790		

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Measurements were made in a steel optical cell within an aluminum block furnace. The cell contents were stirred magnetically. Pressure was measured using a movable piston and Bourdon gauge. Temperature was measured with a steel-sheathed thermocouple. Components were charged into the cell and the transition from one phase to two phases was observed visually.

SOURCE AND PURITY OF MATERIALS:

1. Merck sample, purity 99.9 mole per cent.
2. Isotopic purity 99.7 mole per cent.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$
$\delta P/P = \pm 0.01$
(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water-d_2; D_2O; [7789-20-0]	Brollos, K.; Peter, K.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* 1970, *74*, 682-6.

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
303.4	521	0.546	82.4
297.0	300		
296.2	250		
300.2	181		
312.2	166		
325.2	182		
330.3	2750	0.755	92.3
327.4	2600		
322.9	2300		
318.9	2000		
310.0	1500		
313.1	1700		
304.4	1200		
298.9	990		
296.4	840		
288.1	540		
281.0	290		
275.4	168		

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Deuterium oxide (heavy water); D_2O; [7789-20-0]

ORIGINAL MEASUREMENTS:

Ben-Naim, A.; Wilf, J.; Yaacobi, M.

J. Phys. Chem. 1973, *77*, 95-102.

VARIABLES:

Temperature: 10-50°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in heavy water is reported in terms of the standard free energy of solution, $_s$, determined as:

$$\Delta\mu_s = \lim_{\rho_s \to 0} [-RT\ \ell n(\rho_s^\ell/\rho_s^g)_{eq}]$$

where $(\rho_s^\ell/\rho_s^g)_{eq}$ is the Ostwald absorption coefficient and ρ_s^ℓ and ρ_s^g are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, $\Delta\mu_s^\circ$ was fitted to a second degree polynomial of the form:

$$\Delta\mu_s^\circ = -10657.5 + 44.618\ t - 0.03864\ t^2$$

where t is in °C ($10 < t < 50$°C) and $\Delta\mu_s^\circ$ is in cal/mol (1 cal = 4.187 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined spectroscopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for *ca.* 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at λ_{max} with a Model 450 Perkin-Elmer spectrophotometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three compartment cell, details of which are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, puriss, 99.94%, used as received.

(2) Fluka, 99.75%, used as received.

ESTIMATED ERROR:

Temperature: 0.05°C

Solubility: std. dev. in $\Delta\mu_s^\circ$, 15.103 cal/mol.

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Deuterium oxide (heavy water); D_2O; [7789-20-0]

ORIGINAL MEASUREMENTS:

Backx, P.; Goldman, S.

J. Phys. Chem. 1981, *85*, 2975-9.

VARIABLES:

Temperature: 283-313 K

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of deuterium oxide in benzene

T/K	$10^3 x_2$	std. dev.	10^3 g(2)/100 g sln (compiler)
283	1.70	0.03	0.436
288	1.91	0.03	0.490
293	2.17	0.04	0.557
298	2.68	0.06	0.689
303	3.02	0.04	0.776
308	3.56	0.04	0.915
313	4.12	0.08	1.057

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 175-ml milk-dilution bottle fitted with a Bakelite screw cap and a Teflon insert and rotated end-over-end, (1) was equilibrated with an excess of (2), sampled with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.

SOURCE AND PURITY OF MATERIALS:

(1) certified grade; washed successfully with conc. H_2SO_4, H_2O, 1 N NaOH, again H_2O, dried with silica gel, and distilled; d^{25} 0.87365.

(2) obtained from the manufacturer; minimum isotopic purity of 99.7 atom % D.

ESTIMATED ERROR:

Temp. ± 0.01 K
Std. dev. of soly calcd from 25-36 determinations reported above.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of benzene (1) in seawater (2) at 298 K has been reported by the following workers:

Authors	Method	Salinity g salts/kg sln	g(1)/100 g sln
Mackay and Shiu (ref 2)	GLC	35	0.1340
Price (ref 3)	GLC	34.472	0.1391
May *et al.* (ref 4)	HPLC	35	0.1365

These three determinations made by two methods agree within their experimental error of 8 to 10%. Each group of workers has also determined the solubility of benzene in pure water and obtained results within the same error of the value recommended in this volume. Therefore, the mean of the reported values, 0.135 g(1)/100 g sln, is accepted as the recommended value at the indicated temperature and salinity. These studies measured solubility over a range of salinities. Mackay and Shiu and May *et al.* reported their data in terms of the Setschenow equation. Their values of K_S (0.1836 and 0.175 L/mol) indicate the same (within experimental error) dependence of solubility on salinity and may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

Brown *et al.* (ref 1) determined the solubility of benzene in seawater at a salinity of 34.42 g salts/kg sln over the temperature range 273 to 293 K. Linear extrapolation by the evaluator of these results to 298 K gives a value of 0.127 g(1)/100 g sln. This suggests that the results of Brown *et al.* may be slightly low.

SOLUBILITY OF BENZENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	35	0.136

Since the solubility of seawater (1) and benzene (2) has been reported only by Umano and Hayano (ref 5), no critical evaluation is possible. The interested reader is referred to the relevant data sheet which is included with the preceeding benzene-water system.

REFERENCES

1. Brown, R.L.; Wasik, S.P.; *J. Res. Natl. Bur. Stds.* A. 1974, *78*, 453-60.
2. Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* 1975, *53*, 239-42.
3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
4. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
5. Umano, S.; Hayano, I.; *Kogyo Kagaku Zasshi* 1957, *60*, 1436-7.

COMPONENTS:

(1) Benzene; C_6H_6; [71-42-2]

(2) Artificial seawater

ORIGINAL MEASUREMENTS:

Brown, R.L.; Wasik, S.P.

J. Res. Natl. Bur. Stds. A. 1974, *78*, 453-60.

VARIABLES:

Temperature: 0-20°C

Salinity: 34.42 g salts/kg sln

PREPARED BY:

G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of benzene in artificial seawater

t/°C	g(1)/100 g sln[a]	$10^4\ x_1$(compiler)
0.19	0.1323 (0.0017)	3.129
5.32	0.1376 (0.0022)	3.255
10.05	0.1347 (0.0023)	3.186
14.96	0.1318 (0.0025)	3.117
20.04	0.1296 (0.0022)	3.065

[a] numbers in parentheses are standard deviations from 4 observations

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 cm^3 of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 mole per cent purity; source and methods of purification not specified.

(2) Prepared according to ref. 1. Purity not specified.

ESTIMATED ERROR:

Temperature: ±0.01 K

Solubility: see Table above

REFERENCES:

1. Sverdrup, H.U.; Johnson, M.W.; Fleming, R.H.; The Oceans 1942, Prentice-Hall, Englewood Cliffs, New Jersey p186.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Sodium chloride; NaCl;
[7647-14-5]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

Can. J. Chem. Eng. 1975, *53*, 239-42.

VARIABLES:

One temperature: 25°C

Salinity: 0-200 g(2)/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where, S_o is the solubility of benzene in water (mg/L)
S is the solubility of benzene in solution (mg/L)
K_s is the Setschenow constant (L /mol)
C_s is the concentration of sodium chloride (L/mol)

evaluating the equation for S over the range of C_s 0-4 mol/L, $K_s = 0.1836 \pm 0.0072$ (standard error) with $S_o = 1779.5 \pm 16.4$.

The corresponding mass percent and mole fraction, x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1340 g(1)/100 g sln and 3.227×10^{-4} assuming a solution density of 1.025 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility was determined by vapor phase extraction and gas chromatographic analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.

SOURCE AND PURITY OF MATERIALS:

(1) research grade, 99.9+%, from Phillips Petroleum Co.

(2) and (3) not specified

ESTIMATED ERROR:

temp. ± 0.1 K
soly. 95% confidence limit is about 8%

REFERENCES:

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Sodium chloride; NaCl; [7647-14-5]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

Salinity: 1-360 g(2)/kg sln

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Benzene in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction $10^4 x_1$ (compilers)
1.002	0.1718	3.96
10.000	0.1628	3.78
34.472[a]	0.1391	3.28
50.030	0.1194	2.85
125.100	0.0593	1.48
199.900	0.0388	1.01
279.800	0.0214	0.581
358.700	0.0134	0.378

[a] Artificial seawater, composition not specified but probably similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) commercial, 99 + % pure

ESTIMATED ERROR:

Temperature ± 1 K

Solubility ± 10 relative %

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Benzene; C_6H_6; [71-43-2]

(2) Sodium Chloride; NaCl; [7647-14-5]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of benzene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, K_s = 0.175 with S_o = 1791.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1365 g(1)/100 g sln and 3.22×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05 K

K_s ± 0.006

S_o ± 10

REFERENCES: