IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 10. C_{11} and C_{12} Hydrocarbons with Water

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The mutual solubilities and related liquid–liquid equilibria of C_{11} and C_{12} hydrocarbons with water and heavy water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 24 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 12 systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of all the experimental data for a given series of aliphatic and aromatic hydrocarbons was used.
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Key words: C_{11} and C_{12} hydrocarbons; critical evaluation; liquid–liquid equilibria; solubilities; water.

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*A Critical Evaluation is prepared for this system.

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1. Preface

1.1. Scope of this Volume

This paper is Part 10 of a revised and updated version of an earlier compilation and evaluation of the mutual solubility of water and hydrocarbon compounds containing five or more carbon atoms.[1,2] This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations reported solubility values are characterized as ''Recommended, Tentative, Doubtful, or Rejected,'' based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3–8]

Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value, at given temperature, differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

For one system, acenaphthalene in water, the smoothing equations used for the systems were not applicable because of insufficient data on solubility trends for this aromatic system. Consequently this system was evaluated without the use of calculated reference values. In this system, Recommended values are those supported by two or more independent measurements in agreement with one another. Tentative values are consistent with Recommended values at another temperature and Doubtful values are not conisistent with Recommended values.

The solubilities of the higher n-alkanes were measured mostly at 298 K. It was found that these solubilitites can be described by the following equation:

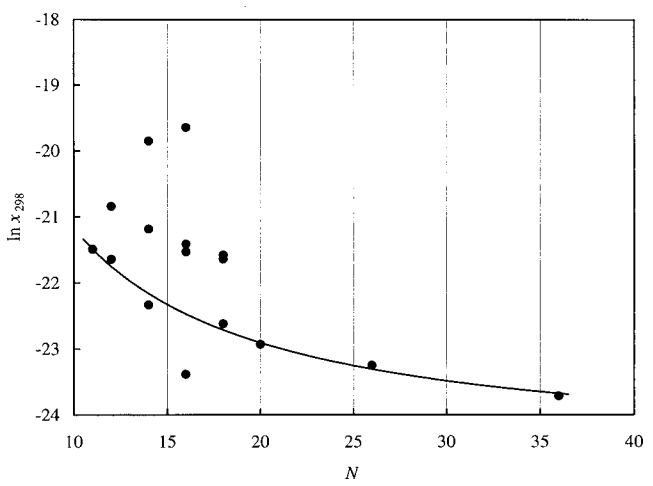

FIG. 1. Logarithm of mole fraction of C_{11}–C_{36} alkanes in water at 298 K ($\ln x_{298}$) vs number of carbon atoms of the alkanes (N).

$$\ln x_{298} = -24.63 + 34.61/N \tag{1}$$

where x_{298} is mole fraction of the given n-alkane at 298 K and N is number of carbon atoms of the alkane. The validity of Eq. (1) is illustrated by Fig. 1.

The points shown in Fig. 1 form two distinct curves with three outliers. To choose between the two curves, it is necessary to take into account the point for undecane. This point is well established, because it fits the smoothing equation for lower alkanes as presented by Maczynski and co-workers.[3,4,5,7] The points for the higher alkanes shown in Fig. 1 should be consistent with the point for undecane. This constraint is met by Eq. (1).

The solubilities of water in the higher n-alkanes at 298 K were calculated using liquid–liquid equilibria data in the same way as described by Maczynski and co-workers.[3–7] The solubilities obtained with Eq. (1) were used as the input data for these calculations.

Alkylnaphthalenes were smoothed with the same equation as those used for alkylbenzenes but supplemented with an additional term, $g(T)$

$$\ln x_1 = \ln_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)] + g(T), \tag{2}$$

where x_1 is mole fraction of the hydrocarbon in water at temperature T, whereas D, $\ln x_{1,\min}$, and $T_{\min}$ are adjustable parameters. Equation (2) is supplemented with the term $g(T)$ in order to meet the constraint that the derivative $\partial x_1/\partial T$ go to infinity as it approaches the two phase critical point of solubility (T_{2c}). The following empirical equation was used for $g(T)$:

$$g(T) = 0.36 \ln(T_{2c} - T)/(T_{2c} - T_{\min}). \tag{3}$$

Equation (2) approximates very well the solubilities of methylnaphthalene and ethylnaphthalene up to T_{2c}. For both systems $T_{\min} = 265$ K was used. This is consistent with the tendency observed for previously investigated solubilities of

hydrocarbons in water: *n*-alkanes (T_{min}=306 K); cycloalkanes (T_{min}=298 K); alkylbenzenes (T_{min}=290 K).

As in the previously investigated types of systems, it was assumed that both $\ln x_{1,min}$ and D are linearly dependent on excluded volume (b). Fitting the experimental solubilities for 1-methylnaphthalene, 2-methylnaphthalene, 1-ethylnaphthalene, 1,3-dimethylnaphthalene, and 1,4-dimethylnaphthalene gives:

$$\ln x_{1,min} = -5.46 - 0.0475b, \quad (4)$$

$$D = 30.90 + 0.0611b, \quad (5)$$

where, as previously, the excluded volume of the hydrocarbon (in cm^3) is calculated from its critical temperature, T_c, and critical pressure, P_c

$$b = 0.08664RT_c/P_c. \quad (6)$$

In order to test the accuracy of Eqs. (2)–(5), more experimental data are necessary. Nevertheless these equations are useful for the estimation of the alkylnaphtalenes solubility when measurements are not available.

For five isomers of dimethylnaphthalene only one or two measurements at 298 K are reported. They can be compared to the solubility of ethylnaphthalene, which is well established by measurements from four independent sources. Solubility of similar hydrocarbons at the same temperature depends only on their excluded volumes, which are almost the same for the alkylnaphthalenes mentioned. Hence, the corresponding solubilities should be approximately the same. This is true for ethylnaphthalene, 1,3-dimethylnaphthalene, and 1,4-dimethylnaphthalene. Three other dimethylnaphthalenes disagree with them and with each other.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, and the scope of the Solubility Data Series can be found in Part 1 (Goral *et al.*[7]). The derivation of the smoothing equations used to calculate reference values for undecane and alkylbenzenes can be found in Parts 1 and 2.[7,8]

1.2. References for the Preface

[1] D. Shaw, Editor, *IUPAC Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[2] D. Shaw, Editor, *IUPAC Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).
[3] A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, Monatshefte für Chemie **134**, 633 (2003).
[4] A. Maczynski, B. Wisniewska-Goclowska, and M. Goral, Recommended Liquid-Liquid Equilibrium Data, Part 1: Binary C_5–C_{11} Alkane—Water Systems, J. Phys. Chem. Ref. Data **33**, 549 (2004).
[5] M. Goral, B. Wisniewska-Goclowska, and A. Maczynski, Recommended Liquid-Liquid Equilibrium Data, Part 2: Binary Unsaturated Hydrocarbon—Water Systems, J. Phys. Chem. Ref. Data **33**, 579 (2004).
[6] M. Goral, B. Wisniewska-Goclowska, and A. Maczynski, Recommended Liquid-Liquid Equilibrium Data, Part 3: Binary Alkylbenzene—Water Systems, J. Phys. Chem. Ref. Data **33**(4), 1159 (2004).
[7] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 1. C_5 Hydrocarbons with Water, J. Phys. Chem. Ref. Data **34**(2), 441 (2005).
[8] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 2. Benzene with Water and Heavy Water, J. Phys. Chem. Ref. Data **34**(2), 477 (2005).

2. C_{11} and C_{12} Hydrocarbons with Water

2.1. 1-Methylnaphthalene+Water

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 1-Methylnphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Christensen and Paulaitis[1]	573 (9200 kPa)	Mackay and Shiu[5]	298
Economou *et al.*[2]	311–589 (4895–11 273 kPa)	Schwarz and Wasik[6]	283–298
Eganhouse and Calder[3]	298	Schwarz[7]	282–305

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 10 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)] + 0.36\ln(T_{2c} - T)/(T_{2c} - T_{\min}), \quad (1)$$

where: $\ln x_{1,\min} = -12.83$; $D = 40.38$; $T_{\min} = 265$ K; $T_{2c} = 589.4$ K.

Equation (1) is based on all available solubility data of 1-methylnaphthalene in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 1.

All the experimental and reference data are listed in Table 2 and shown in Fig. 2.

Critical Evaluation of the Solubility of Water (2) in 1-Methylnaphthalene (1)

The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Christensen and Paulaitis[1]	573 (9200 kPa)	Englin *et al.*[4]	273–323
Economou *et al.*[2]	311–589 (4895–11 273 kPa)		

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.081$; $d_2 = -5.252$; $d_3 = -1.857$; $d_4 = 2.407$; $T_r = T/589.5$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1-methylnaphthalene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 3 and shown in Fig. 3. The data of Englin *et al.*[4] at 323 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

High Pressure Solubility of 1-Methylnaphthalene (1) in Water (2)

The experimental high pressure solubility for (1) in (2), investigated by Christensen and Paulaitis[1] at 573 K and 9474–10 305 kPa, has not been critically evaluated because the developed method is not applied for such data.

References:

[1]S. P. Christensen and M. E. Paulaitis, Fluid Phase Equilib. **71**, 63 (1992).
[2]I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
[3]R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[4]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[5]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[6]F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data **22**, 270 (1977).
[7]F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).

TABLE 1. The data categories for solubility of 1-methlynaphthalene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
281.8		Schwarz[7]	
283.2		Schwarz and Wasik[6]	
287.2	Schwarz and Wasik,[6] Schwarz[7]		
290.3		Schwarz[7]	
293.2	Schwarz and Wasik,[6] Schwarz[7]		
296.2		Schwarz[7]	
298.2	Eganhouse and Calder,[3] Mackay and Shiu,[5] Schwarz and Wasik,[6] Schwarz[7]		
299.3		Schwarz[7]	
302.4		Schwarz[7]	
304.9		Schwarz[7]	
310.9		Economou *et al.*[2]	
366.5		Economou *et al.*[2]	
422.0		Economou *et al.*[2]	
478.0		Economou *et al.*[2]	
533.5		Economou *et al.*[2]	
550.5		Economou *et al.*[2]	
573.1			Christensen and Paulaitis[1]
589.4		Economou *et al.*[2]	

TABLE 2. Experimental values for solubility of 1-methylnaphthalene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
281.8		$2.52 \cdot 10^{-6}$ (T; Ref. 7)	$3.0 \cdot 10^{-6}$
283.2		$2.90 \cdot 10^{-6}$ (T; Ref. 6)	$3.0 \cdot 10^{-6}$
287.2		$3.60 \cdot 10^{-6}$ (R; Ref. 6), $2.86 \cdot 10^{-6}$ (R; Ref. 7)	$3.1 \cdot 10^{-6}$
290.3		$2.90 \cdot 10^{-6}$ (T; Ref. 7)	$3.2 \cdot 10^{-6}$
293.2		$3.60 \cdot 10^{-6}$ (R; Ref. 6), $3.21 \cdot 10^{-6}$ (R; Ref. 7)	$3.4 \cdot 10^{-6}$
296.2		$3.49 \cdot 10^{-6}$ (T; Ref. 7)	$3.5 \cdot 10^{-6}$
298.2		$3.27 \cdot 10^{-6}$ (R; Ref. 3), $3.55 \cdot 10^{-6}$ (R; Ref. 5), $3.80 \cdot 10^{-6}$ (R; Ref. 6), $3.80 \cdot 10^{-6}$ (R; Ref. 7)	$3.6 \cdot 10^{-6}$
299.3		$3.85 \cdot 10^{-6}$ (T; Ref. 7)	$3.7 \cdot 10^{-6}$
302.4		$4.21 \cdot 10^{-6}$ (T; Ref. 7)	$3.9 \cdot 10^{-6}$
304.9		$4.59 \cdot 10^{-6}$ (T; Ref. 7)	$4.0 \cdot 10^{-6}$
310.9		$4.30 \cdot 10^{-6}$ (T; Ref. 2)	$4.5 \cdot 10^{-6}$
366.5		$1.80 \cdot 10^{-5}$ (T; Ref. 2)	$1.7 \cdot 10^{-5}$
422.0		$1.10 \cdot 10^{-4}$ (T; Ref. 2)	$8.6 \cdot 10^{-5}$
478.0		$5.60 \cdot 10^{-4}$ (T; Ref. 2)	$4.7 \cdot 10^{-4}$
533.5	4895 (Ref. 2)	$3.10 \cdot 10^{-3}$ (T; Ref. 2)	$2.7 \cdot 10^{-3}$
550.5	6412 (Ref. 2)	$4.90 \cdot 10^{-3}$ (T; Ref. 2)	$4.8 \cdot 10^{-3}$
573.1	9200 (Ref. 1)	$5.20 \cdot 10^{-2}$ (D; Ref. 1)	$1.2 \cdot 10^{-2}$
589.4	11 273 (Ref. 2)	$7.80 \cdot 10^{-2}$ (T; Ref. 2)	$1.1 \cdot 10^{-1}$

TABLE 3. Experimental values for solubility of water (2) in 1-methlynaphthalene (1)

T/K	P/kPa	Experimental values x_2 (T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2		$1.59 \cdot 10^{-3}$ (T; Ref. 4)	$1.7 \cdot 10^{-3}$
283.2		$2.22 \cdot 10^{-3}$ (T; Ref. 4)	$2.5 \cdot 10^{-3}$
293.2		$2.97 \cdot 10^{-3}$ (T; Ref. 4)	$3.5 \cdot 10^{-3}$
303.2		$3.82 \cdot 10^{-3}$ (T; Ref. 4)	$4.8 \cdot 10^{-3}$
310.9		$5.15 \cdot 10^{-3}$ (T; Ref. 2)	$6.1 \cdot 10^{-3}$
313.2		$4.87 \cdot 10^{-3}$ (T; Ref. 4)	$6.5 \cdot 10^{-3}$
323.2		$5.97 \cdot 10^{-3}$ (D; Ref. 4)	$8.7 \cdot 10^{-3}$
366.5		$2.23 \cdot 10^{-2}$ (T; Ref. 2)	$2.4 \cdot 10^{-2}$
422.0		$6.57 \cdot 10^{-2}$ (T; Ref. 2)	$6.7 \cdot 10^{-2}$
478.0		$1.48 \cdot 10^{-1}$ (T; Ref. 2)	$1.5 \cdot 10^{-1}$
533.5	4895 (Ref. 2)	$3.63 \cdot 10^{-1}$ (T; Ref. 2)	$2.9 \cdot 10^{-1}$
550.5	6412 (Ref. 2)	$4.43 \cdot 10^{-1}$ (T; Ref. 2)	$3.5 \cdot 10^{-1}$
573.1	9200 (Ref. 1)	$6.25 \cdot 10^{-1}$ (T; Ref. 1)	$4.8 \cdot 10^{-1}$
589.4	11 273 (Ref. 2)	$9.22 \cdot 10^{-1}$ (T; Ref. 2)	$8.3 \cdot 10^{-1}$

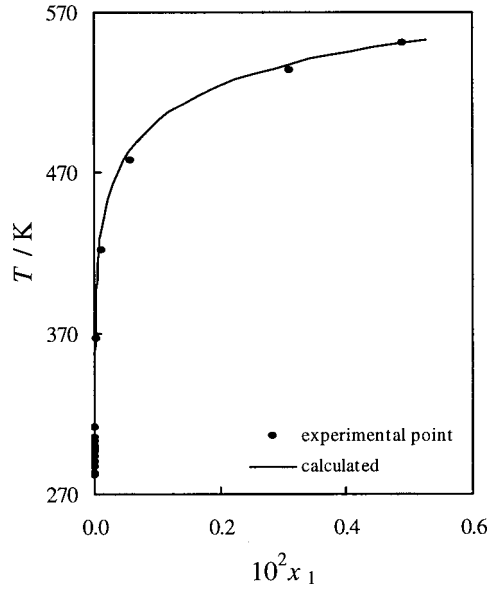

FIG. 2. All the solubility data for 1-methylnaphthalene (1) in water (2) below 570 K.

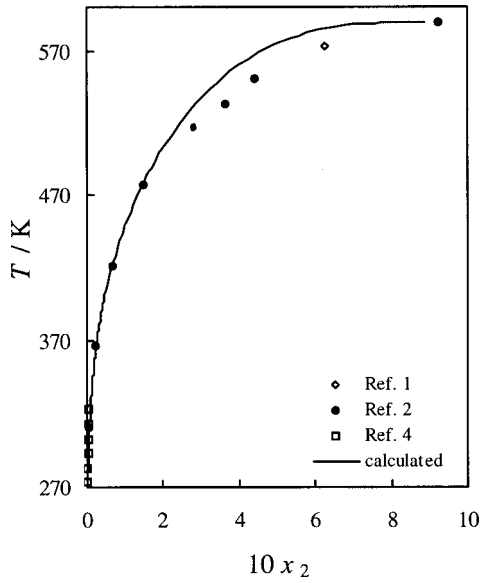

FIG. 3. All the solubility data for water (2) in 1-methylnaphthalene (1).

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. P. Christensen and M. E. Paulaitis, Fluid Phase Equilib. **71**, 63 (1992).

Variables:
One temperature: 299.9 °C
Pressure: 88.4–101.7 atm

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1-methylnaphthalene and water

t/°C	P/atm	g (1)/100 g sln (compilers)	x_1
299.9	88.4[a]	—	—
	90.8	30.2	0.052
	93.5	30.2	0.052
	101.7	30.2	0.052

Solubility of water in 1-methylnaphthalene

t/°C	P/atm	g (2)/100 g sln (compilers)	x_2
299.9	90.8	17.4	0.625
	93.5	16.7	0.612
	101.7	15.4	0.589

[a]Three phase pressure.

Auxiliary Information

Method/Apparatus/Procedure:
A flow technique was used. The apparatus contained a high-pressure view cell (60 mL volume), was equipped with sapphire windows, and was placed in a nitrogen bath, Thies and Paulatis.[1] The system pressure was measured to within ±0.1 atm with a Heise bourdon-tube gauge (Gregory Model CM). The temperature was measured with platinum resistance thermometer (Burns Engineering Co.) to within ±0.1 °C. Equilibrium phase compositions were measured with a Perkin-Elmer gas chromatograph (Model 3920 B) equipped with a Porapak P column and a thermal conductivity detector.

Source and Purity of Materials:
(1) Aldrich and Eastman Kodak Co.; purity >98%; used as received.
(2) Distilled and de-ionized.

Estimated Error:
Temperature: ±0.1 °C.
Pressure: ±0.1 atm.

References:
[1]M. C. Thies and M. E. Paulaitis, J. Chem. Eng. Data **29**, 438 (1984).

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:
Temperature: 310.93–589.43 K
Pressure: 4.895–11.273 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1-methylnaphthalene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^2 \cdot x_1$
310.93	—	0.00339	0.00043
366.48	—	0.0142	0.0018
422.04	—	0.087	0.011
477.98	—	0.440	0.056
533.54	4.895	2.40	0.31
550.48	6.412	3.74	0.49
589.43[a]	11.273	40.04	7.8

Solubility of water in 1-methylnaphthalene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
310.93	—	0.0657	0.00516
366.48	—	0.288	0.00223
422.04	—	0.883	0.00657
477.98	—	2.15	0.148
533.54	4.895	6.73	0.363
550.48	6.412	9.15	0.443
589.43[a]	11.273	59.96	0.922

[a]Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of hydrocarbon in water was measured by glc, while that of water in hydrocarbon by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:
(1) Eastman Kodak; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:
Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:
[1]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2]J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3]C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of 1-methylnaphthalene in water at 25 °C was reported to be 25.8 mg (1)/kg (2) and $1.81 \cdot 10^{-4}$ mol (l)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.58 \cdot 10^{-3}$ g (1)/100 g sln and $3.27 \cdot 10^{-6}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:
(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: ±1.2 mg (1)/kg (2) (from eight determinations).

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 0–50 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in 1-methylnaphthalene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
0	1.59	0.0202
10	2.22	0.0282
20	2.97	0.0377
30	3.82	0.0485
40	4.87	0.0619
50	5.97	0.0760

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h 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.

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 1-methylnaphthalene in water at 25 °C was reported to be 28.5 mg (1)/L sln and $x_1 = 3.55 \cdot 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00285 g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Drowman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:
(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:
Solubility: ±0.3 mg (1)/L sln (maximum deviations from several determinations).

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).

Variables:
Temperature: 8.6–31.7 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 1-methylnaphthalene in water

t/°C	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot$ g (1)/100 g sln (compiler)	$10^4 \cdot$ mol (1)/L
8.6	2.52	1.99	1.40±0.03
14.0	2.86	2.26	1.59±0.03
17.1	2.90	2.29	1.61±0.03
20.0	3.21	2.53	1.78±0.02
23.0	3.49	2.76	1.94±0.02
25.0	3.80	3.00	2.11±0.07
26.1	3.85	3.04	2.14±0.02
29.2	4.21	3.33	2.34±0.05
31.7	4.59	3.27	2.55±0.04

Auxiliary Information

Method/Apparatus/Procedure:
Two methods were used: At 25 °C the solubility of (1) in (2) was determined from ultraviolet (UV) absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry, and placed in the fluorimeter.

Source and Purity of Materials:
(1) Source not specified; better than 99.9 mole %, by glc; used as received.
(2) Distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: see above.

Components:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data **22**, 270 (1977).

Variables:
Temperature: 10–25 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 1-methylnaphthalene in water

t/°C	$10^6 \cdot x_1$ (compiler)	$10^3 \cdot$ g (1)/100 g sln (compiler)	$10^4 \cdot$ mol (1)/L
10	2.9	2.3	1.6
14	3.6	2.8	2.0
20	3.6	2.8	2.0
25	3.8	3.0	2.1

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) is too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

Source and Purity of Materials:
(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole %.
(2) Distilled from $KMnO_4$ and passed through a Sephadex column.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: $\pm 2 \cdot 10^{-5}$ mol (1)/L.

2.2. 2-Methylnaphthalene+Water

Components:
(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 2-Methylnaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Eganhouse and Calder[1] and Mackay and Shiu[2] at 298 K.

As indicated in the preface to Part 10, solubility of 2-methylnaphthalene in water should be almost the same as solubility of 1-methylnaphthalene in water, which is well established and used as the reference data.

Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 4. All the data are in good agreement (within 30% relative standard derivation) with each other and with the reference data and are Recommended.

References:
[1]R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[2]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 4. Experimental values for solubility of 2-methylnaphthalene (1) in water (2)

T/K	Experimental values x_1 (R=recommended)	Reference values $x_1 \pm 30\%$
298.2	$3.12 \cdot 10^{-6}$ (R; Ref. 1), $3.22 \cdot 10^{-6}$ (R; Ref. 2)	$3.6 \cdot 10^{-6}$

Components:	Original Measurements:
(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of 2-methylnaphthalene in water at 25 °C was reported to be 24.6 mg (1)/kg (2) and $1.72 \cdot 10^{-4}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.46 \cdot 10^{-3}$ g (1)/100 g sln and $3.12 \cdot 10^{-6}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±0.5 mg (1)/kg (2) (from eight determinations).

Components:	Original Measurements:
(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 2-methylnaphthalene in water at 25 °C was reported to be 25.4 mg (1)/L sln and $x_1 = 3.22 \cdot 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00254 g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigourously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.2 mg (1)/L sln (maximum deviation from several determinations).

2.3. 2-Ethyl-1,3,5-trimethylbenzene+Water

Components:
(1) 2-Ethyl-1,3,5-trimethylbenzene; $C_{11}H_{16}$; [3982-67-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 20–40 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in 2-ethyl-1,3,5-trimethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
20	2.13	0.0259
30	2.87	0.0350
40	3.78	0.0461

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h 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.

2.4. Pentylbenzene+Water

Components:
(1) Pentylbenzene; $C_{11}H_{16}$; [538-68-1]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of Pentylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Owens *et al.*[1] at 280–318 K and Tewari *et al.*[2] at 298 K.

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where: $\ln x_{1,\min} = -14.49$; $D = 58.35$; $T_{\min} = 290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 5 and shown in Fig. 4. The data of Owens *et al.*[1] and Tewari *et al.*[2] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).
[2]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

TABLE 5. Experimental values for solubility of pentylbenzene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$
280.2	$4.23 \cdot 10^{-7}$ (T; Ref. 1)	$5.3 \cdot 10^{-7}$
283.2	$3.86 \cdot 10^{-7}$ (T; Ref. 1)	$5.2 \cdot 10^{-7}$
285.7	$4.19 \cdot 10^{-7}$ (T; Ref. 1)	$5.1 \cdot 10^{-7}$
288.2	$3.88 \cdot 10^{-7}$ (T; Ref. 1)	$5.1 \cdot 10^{-7}$
290.7	$4.17 \cdot 10^{-7}$ (T; Ref. 1)	$5.1 \cdot 10^{-7}$
293.2	$3.87 \cdot 10^{-7}$ (T; Ref. 1)	$5.1 \cdot 10^{-7}$
298.2	$4.11 \cdot 10^{-7}$ (R; Ref. 1), $4.68 \cdot 10^{-7}$ (R; Ref. 2)	$5.2 \cdot 10^{-7}$
303.2	$4.40 \cdot 10^{-7}$ (T; Ref. 1)	$5.4 \cdot 10^{-7}$
308.2	$4.79 \cdot 10^{-7}$ (T; Ref. 1)	$5.6 \cdot 10^{-7}$
313.2	$5.21 \cdot 10^{-7}$ (T; Ref. 1)	$6.0 \cdot 10^{-7}$
318.2	$5.75 \cdot 10^{-7}$ (T; Ref. 1)	$6.4 \cdot 10^{-7}$

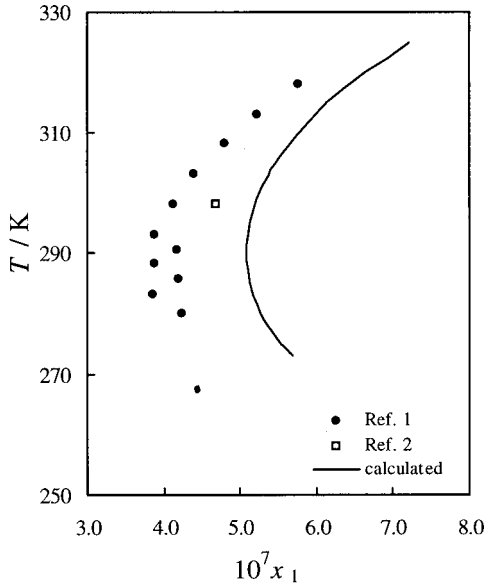

FIG. 4. All the solubility data for pentylbenzene (1) in water (2).

Components:	**Original Measurements:**
(1) Pentylbenzene; $C_{11}H_{16}$; [538-68-1] (2) Water; H_2O; [7732-18-5]	J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).
Variables:	**Prepared By:**
Temperature: 7.0–45.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of pentylbenzene in water

t/°C	$10^5 \cdot$ mol (1)/L sln	$10^4 \cdot$ g (1)/100 g sln (compilers)	$10^7 \cdot x_1$ (compilers)
7.0	2.348±0.131	3.481	4.230
10.0	2.144±0.278	3.179	3.864
12.5	2.323±0.147	3.445	4.187
15.0	2.153±0.005	3.195	3.882
17.5	2.311±0.083	3.430	4.168
20.0	2.142±0.053	3.181	3.866
25.0	2.276±0.102	3.384	4.112
30.0	2.433±0.042	3.623	4.402
35.0	2.642±0.045	3.940	4.788
40.0	2.868±0.030	4.285	5.207
45.0	3.163±0.053	4.735	5.754

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined by the technique reported in May *et al.*[1] and DeVoe *et al.*[2] and an automated coupled-column liquid chromatographic apparatus, described in Owens.[3] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. A known volume of the saturated solution was passed through a small extractor column filled with reverse phase packing where the solute was removed quantitatively. The extracted solute was then eluted with a water–methanol mixture, separated from impurities on an HPLC analytical column, and analyzed by UV spectrophotometry at 254 nm. The standard deviation of the peak area for the known solution was $<2.4\%$. 3–6 measurements at each temperature were made.

Source and Purity of Materials:

(1) Albany Internationals Chemicals Division; used as received; purity >99% by glc.
(2) HPCL grade.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: as above.

References:

[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[3]J. W. Owens, T. J. Buckley, and H. DeVoe, J. Res. Natl. Bur. Stand. (USA) **90**, 41 (1985).

Components:
(1) Pentylbenzene; $C_{11}H_{16}$; [538-68-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of pentylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$2.59 \cdot 10^{-5}$	$3.85 \cdot 10^{-4}$	$4.68 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with an organic liquid by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:
(1) Source not specified; purity >99 mole % checked by high-temperature glc.
(2) Source not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:
[1]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

2.5. *tert*-Pentylbenzene+Water

Components:
(1) *tert*-Pentylbenzene; $C_{11}H_{16}$; [2049-95-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility if *tert*-pentylbenzene in water at 25 °C was reported to be 0.00105 g (1)/100 g sln.
The corresponding mole fraction (x_1) calculated by the compilers is $1.27 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h 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. white label; fractionally distilled; boiling point range 188.0–189.0 °C.
(2) Not specified.

Estimated Error:
Not specified.

2.6. 2-Methyldecalin+Water

Components:
(1) 2-Methyldecalin; $C_{11}H_{20}$; [2958-76-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **3**, C-61 (1958).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 2-methyl–C^{14} decalin in water at 25 °C was reported to be $40.6 \cdot 10^{-9}$ g (1)/g (2).

The corresponding mass percentage and mole fraction (x_1), calculated by the compiler, are $4.06 \cdot 10^{-6}$ g (1)/100 g sln and $4.82 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
Carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)–(2) dispersion has been described in Baker.[1] A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

Source and Purity of Materials:
(1) Nuclear Instrument and Chemical Corporation; used as received.
(2) Distilled.

Estimated Error:
Solubility: 20% (standard deviation from 17 replicate runs).

References:
[1]E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **1**, 2, 5 (1956).

2.7. Hexylcyclopentane+Water

Components:
(1) Hexylcyclopentane; $C_{11}H_{22}$; [4457-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 10–30 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in hexylcyclopentane

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
10	4.45	0.0052
20	7.19	0.0084
30	12.07	0.0141

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h 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.

2.8. Undecane+Water

Components:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of Undecane (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed:

Author (s)	T/K	Author (s)	T/K
Krasnoshchekova and Gubergrits[1]	298	Schatzberg[3]	298
McAuliffe[2]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + (\Delta_{s\ \ln} C_p / R)[T_{\min}/T - \ln(T_{\min}/T) - 1], \quad (1)$$

where: $\ln x_{1,\min} = -21.68$; $\Delta_{sln} C_p / R = 89.7$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 6. All the data are in good agreement with the reference data and are Tentative.

Critical Evaluation of the Solubility of Water (2) in Undecane (1)

The experimental solubility data for (1) in (2) have been investigated by Schatzberg[2] at 298 and 313 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 1 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.104$; $d_2 = -5.430$; $d_3 = -0.984$; $d_4 = -2.656$; $T_r = T/582.6$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of undecane in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 7. All the data are in good agreement with the reference data and are Tentative.

References:

[1]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
[2]C. McAuliffe, Science **163**, 478 (1969).
[3]P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).

TABLE 6. Experimental values for solubility of undecane (1) in water (2)

T/K	Experimental values x_1 (T=tentative)	Reference values $x_1 \pm 30\%$
298.2	$4.1 \cdot 10^{-10}$ (T; Ref. 1), $5.07 \cdot 10^{-10}$ (T; Ref. 2)	$4.8 \cdot 10^{-10}$

TABLE 7. Experimental values for solubility of water (2) in undecane (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
298.2	$6.0 \cdot 10^{-4}$ (T; Ref. 3)	$6.4 \cdot 10^{-4}$
313.2	$1.13 \cdot 10^{-3}$ (T; Ref. 3)	$1.2 \cdot 10^{-4}$

Components:	Original Measurements:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of undecane in water at 25 °C was reported to be $x_1 = 4.10 \cdot 10^{-10}$.

The corresponding mass percent calculated by the compiler is $3.6 \cdot 10^{-7}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10–12 h. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20 mL aliquots were introduced into 40 mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.	(1) Source not specified; CP reagent; purity not specified. (2) Distilled. **Estimated Error:** Not specified.

Components:	Original Measurements:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, Science **163**, 478 (1969).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Values

The solubility of undecane in water at 25 °C was reported to be 0.0044 mg (1)/kg (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $4.4 \cdot 10^{-7}$ g (1)/100 g sln and $5.07 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 min. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(1) Not specified. (2) Distilled. **Estimated Error:** Solubility: ±0.0018 mg (1)/kg (2).

Components:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).

Variables:
Temperature: 25 and 40 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of water in undecane

t/°C	$10^4 \cdot x_2$	mg (2)/kg sln
25	6.0	69[a]
40	11.3	130[b]

[a,b]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20 mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. 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.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; research grade; 99.33 mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220–340 nm spectral range.
(2) Distilled and de-ionized.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: (a) 0%–6%; (b) 0%–2% (deviations from the mean).

2.9. Acenaphthylene+Water

Components:
(1) Acenaphthylene; $C_{12}H_8$; [208-96-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

Variables:
One temperature: 25 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of acenaphthylene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	4.16±0.57	$4.17 \cdot 10^{-4}$	$4.87 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as auxiliary property at adsorption measurements. The mean value of three determinations was reported.

Source and Purity of Materials:
(1) Source not specified (Aldrich or Eastman Kodak); purity >98%; used as received.
(2) De-ionized, purified on activated carbon bed from Continenetal water Co.; pH in the range 6.8–7.2

Estimated Error:
See above.

2.10. Acenaphthene+Water

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of Acenaphthene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Banerjee *et al.*[1]	298	Rossi and Thomas[5]	298
Eganhouse and Calder[2]	298	Vesala[6]	298
Haines and Sandler[3]	298	Walters and Luthy[7]	298
Mackay and Shiu[4]	298	Wauchope and Getzen[8]	273–348

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic system. All experimental data are listed in Table 8 and shown in Fig. 5. At 298 K the data of Eganhouse and Calder,[2] Haines and Sandler,[3] Mackay and Shiu,[4] and Wauchope and Getzen[8] are in good agreement and are Recommended. From these data the mean value was calculated. As shown in Fig. 5, the data of Banerjee *et al.*[1] appear to be high and Doubtful. The data of Rossi and Thomas[5] seem to be low and Doubtful. All the remaining data of Vesala,[6] Walters and Luthy,[7] and Wauchope and Getzen[8] at other temperatures are consistent with the mean value at 298 K and are Tentative.

References:

[1]S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
[2]R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[3]R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).
[4]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[5]S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
[6]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[7]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[8]R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

TABLE 8. Experimental values for solubility of acenaphthene (1) in water (2)

T/K	Experimental values x_1 (R=Recommended, T=Tentative, D=Doubtful)	Mean value
273.2	$1.69\cdot10^{-7}$ (T; Ref. 8)	
295.2	$4.04\cdot10^{-7}$ (T; Ref. 8)	
298.0	$4.20\cdot10^{-7}$ (T; Ref. 6), $4.87\cdot10^{-7}$ (T; Ref. 7)	
298.2	$8.6\cdot10^{-7}$ (D; Ref. 1), $4.05\cdot10^{-7}$ (R; Ref. 2), $4.53\cdot10^{-7}$ (R; Ref. 3), $4.59\cdot10^{-7}$ (R; Ref. 4), $1.6\cdot10^{-8}$ (D; Ref. 5), $4.53\cdot10^{-7}$ (R; Ref. 8)	$4.4\cdot10^{-7}$
303.2	$5.61\cdot10^{-7}$ (T; Ref. 8)	
307.7	$6.81\cdot10^{-7}$ (T; Ref. 8)	
312.5	$8.04\cdot10^{-7}$ (T; Ref. 8)	
317.9	$1.07\cdot10^{-6}$ (T; Ref. 8)	
323.2	$1.39\cdot10^{-6}$ (T; Ref. 8)	
323.3	$1.39\cdot10^{-6}$ (T; Ref. 8)	
328.8	$1.82\cdot10^{-6}$ (T; Ref. 8)	
337.7	$2.84\cdot10^{-6}$ (T; Ref. 8)	
338.4	$2.94\cdot10^{-6}$ (T; Ref. 8)	
343.0	$3.75\cdot10^{-6}$ (T; Ref. 8)	
345.1	$4.19\cdot10^{-6}$ (T; Ref. 8)	
346.6	$4.56\cdot10^{-6}$ (T; Ref. 8)	
347.9	$4.88\cdot10^{-6}$ (T; Ref. 8)	
348.2	$4.97\cdot10^{-6}$ (T; Ref. 8)	

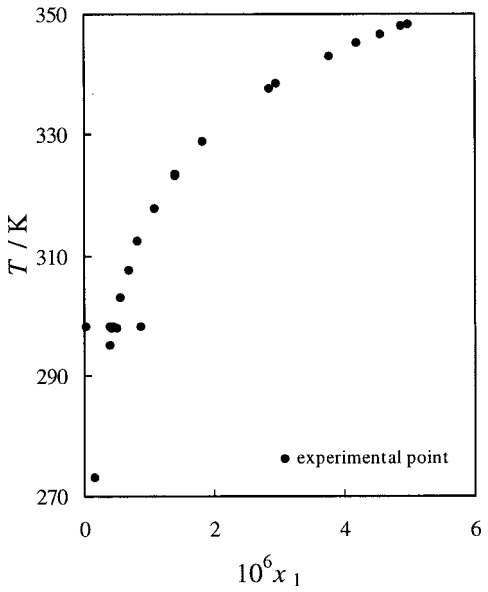

FIG. 5. All the solubility data for acenaphthene (1) in water (2).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Values

The solubility of acenaphthene in water was reported to be $4.78 \cdot 10^{-5}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass percent and mole fraction (x_1) solubilities, calculated by the compiler, are $7.3 \cdot 10^{-4}$ g (1)/100 g sln and $8.60 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of acenaphthene 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-labeled: New England Nuclear, purity not specified.
(2) Distilled.

Estimated Error:

Temperature: ±0.2 °C.
Solubility: ±4.1% relative (representing 1 standard deviation).

Components:	Original Measurements:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of acenaphthene in water at 25 °C was reported to be 3.47 mg (1)/kg (2) and $2.2 \cdot 10^{-5}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $3.47 \cdot 10^{-4}$ g (1)/100 g sln and $4.05 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±0.06 mg (1)/kg (2) (from eight determinations).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of acenaphthene in water

t/°C	g (1)/100 g sln (compilers)	x_1
25.0	$3.88 \cdot 10^{-4}$	$4.53 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equipment consisted of an 1800 mL Pyrex flask, a heating/stirring plate, and a cooling jacket. 50 mg (1) and about 1800 mL (2) were mixed at 30 °C for at least 4 days, and equilibrated at 25 °C for 2 days. Samples were analyzed by the high performance liquid chromatograph. Analysis details are reported in the paper. The mean of seven separate experiments is reported. (Confirmatory analyses were made after 2 days of additional mixing.)

Source and Purity of Materials:

(1) Aldrich Chemicals Co.; purity 99 mass %; used as received.
(2) Distilled and de-ionized water.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 2% (reproducibility).

Components:	**Original Measurements:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of acenaphthene in water at 25 °C was reported to be 3.93 mg (1)/L sln and $x_1 = 4.59 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $3.93 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.014 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of acenaphthene in distilled water at 25 °C was reported to be 2.42 μg/g, corresponding to a mole fraction, x_1 , of $1.6 \cdot 10^{-8}$.

The corresponding mass per cent calculated by the compiler is $2.42 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

Flasks containing 500 mL of water and (1) were placed in a constant temperature (±0.1 °C) gyrotary shaker (200 rpm) for at least 24 h. Following a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass–wool plug into a separatory funnel. Acenaphthene was isolated from solution by triplicate extraction with 10 mL of hexane, which recovered over 99% of hydrocarbon as determined in experiments with spiked solutions. Acenaphthene levels in concentrated extracts were determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m×0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally determined by ultraviolet spectrophotometry. Agreement was typically within 2%. Further details are given in the paper.

Source and Purity of Materials:

(1) Aldrich; 99.9% purity; recrystallized twice from distilled MeOH.
(2) Doubly distilled in all-glass apparatus; free of trace organics.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±0.02 μg/g (standard deviation for six determinations).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of acenaphthene in water

T/K	mol (1)/g (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(2.33 \pm 0.03) \cdot 10^{-8}$	$3.60 \cdot 10^{-6}$	$4.20 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibration was carried out in a modified vessel, Franks *et al.*,[1] equipped with a magnetic stirrer. The temperature of the water bath was maintained within ±0.05 K. Equilibrium was obtained after several days and then samples were analyzed by spectrophotometry. At least five parallel determinations were performed.

Source and Purity of Materials:

(1) Commercial analytical grade reagent; purity >99% by glc; twice recrystallized.
(2) Distilled water passed through an Amberlite CG 120+CG 400 ion-exchange column.

Estimated Error:

Temperature: ±0.05 K.
Solubility: as above.

References:

[1]F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

Variables:
One temperature: 25 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of acenaphthene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	4.16±0.57	$4.17 \cdot 10^{-4}$	$4.87 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as auxiliary property at adsorption measurements. The mean value of three determinations was reported.

Source and Purity of Materials:
(1) Source not specified (Aldrich or Eastman Kodak); purity >98%; used as received.
(2) De-ionized, purified on avtivated carbon bed from Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

Components:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

Variables:
Temperature: 0–75 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of acenaphthene in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2) experiment	mg (1)/kg (2) smoothed with (standard deviation)
0.0	1.69	1.45	—	1.45(0.04)
22.0	4.04	3.46	3.57	3.46
25.0	4.53	3.88	—	3.88(0.07)
30.0	5.61	4.80	4.76, 4.60, 4.72	4.80
34.5	6.81	5.83	6.00, 5.68, 5.73	5.83
39.3	8.4	7.2	6.8, 7.1, 70	7.2
44.7	10.7	9.2	9.4, 9.4, 9.3	9.2
50.0	13.9	11.9	—	11.9(0.1)
50.1	13.9	11.9	12.5, 12.4, 12.4	11.9
55.6	18.2	15.6	15.8, 16.3, 15.9	15.6
64.5	28.4	24.3	25.9, 27.8	24.3
65.2	29.4	25.2	23.7, 23.4, 22.8	25.2
69.8	37.5	32.1	30.1, 34.3, 33.6	32.1
71.9	41.9	35.9	35.2	35.9
73.4	45.6	39.0	39.1, 40.1	39.0
74.7	48.8	41.8	40.8, 39.3	41.8
75.0	49.7	42.5	—	42.5(0.7)

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 20 g of (1) was placed in each of three 250 mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from 1 to 3 weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1–0.2 g of samples followed by serial dilution in calibrated glassware.

Source and Purity of Materials:
(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.
(2) Distilled and de-ionized.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: see experimental values above.

2.11. Biphenyl+Water

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of Biphenyl (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Akiyoshi *et al.*[1]	298	Janado *et al.*[8]	298
Andrews and Keefer[2]	298	Mackay and Shiu[9]	298
Banerjee[3]	298	Miller *et al.*[10]	298
Bohon and Claussen[5]	274–316	Vesala[11]	298
Coyle *et al.*[6]	295	Wauchope and Getzen[12]	273–338
Eganhouse and Calder[7]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{1,\min} = -15.317$; $D = 76.654$; $T_{\min} = 245$ K.

The parameters $\ln x_{\min,1}$ and D were individually adjusted to solubility of biphenyl. Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 9 and shown in Fig. 6. All the data at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

Rejected and Inaccessible Data

The data reported by Ben-Naim and Wilf[4] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1] *M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn.* **60**, 3935 (1987).
[2] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[3] S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
[4] A. Ben-Naim and J. Wilf, J. Phys. Chem. **77**, 95 (1973).
[5] R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[6] G. T. Coyle, T. C. Harmon, and I. H. Suffet, Environ. Sci. Technol. **31**, 384 (1997).
[7] R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[8] M. Janado, Y. Yano, Y. Doi, and H. Sakamoto, J. Solution Chem. **12**, 741 (1983).
[9] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[10] M. M. Miller, S. Ghodbane, S. P. Wasik, Y. B. Tewari, and D. E. Martire, J. Chem. Eng. Data **29**, 184 (1984).
[11] A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[12] R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

TABLE 9. Experimental values for solubility of biphenyl (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative)	Reference values $x_1 \pm 30\%$
273.2	$3.081 \cdot 10^{-7}$ (T; Ref. 12)	$3.4 \cdot 10^{-7}$
295.0	$8.183 \cdot 10^{-7}$ (T; Ref. 6)	$7.2 \cdot 10^{-7}$
297.8	$8.126 \cdot 10^{-7}$ (T; Ref. 12)	$8.0 \cdot 10^{-7}$
298.0	$8.847 \cdot 10^{-7}$ (T; Ref. 11)	$8.1 \cdot 10^{-7}$
298.2	$8.257 \cdot 10^{-7}$ (R; Ref. 1), $6.897 \cdot 10^{-7}$ (R; Ref. 2), $7.050 \cdot 10^{-7}$ (R; Ref. 3), $8.698 \cdot 10^{-7}$ (R; Ref. 5), $8.698 \cdot 10^{-7}$ (R; Ref. 7), $8.777 \cdot 10^{-7}$ (R; Ref. 8), $8.151 \cdot 10^{-7}$ (R; Ref. 9), $7.862 \cdot 10^{-7}$ (R; Ref. 10), $8.274 \cdot 10^{-7}$ (R; Ref. 12)	$8.2 \cdot 10^{-7}$
303.1	$1.020 \cdot 10^{-6}$ (T; Ref. 12)	$1.0 \cdot 10^{-6}$
303.5	$1.040 \cdot 10^{-6}$ (T; Ref. 12)	$1.0 \cdot 10^{-6}$
311.6	$1.481 \cdot 10^{-6}$ (T; Ref. 12)	$1.5 \cdot 10^{-6}$
313.3	$1.610 \cdot 10^{-6}$ (T; Ref. 12)	$1.6 \cdot 10^{-6}$
320.7	$2.281 \cdot 10^{-6}$ (T; Ref. 12)	$2.3 \cdot 10^{-6}$
323.2	$2.569 \cdot 10^{-6}$ (T; Ref. 12)	$2.6 \cdot 10^{-6}$
323.3	$2.579 \cdot 10^{-6}$ (T; Ref. 12)	$2.6 \cdot 10^{-6}$
323.4	$2.590 \cdot 10^{-6}$ (T; Ref. 12)	$2.6 \cdot 10^{-6}$
327.9	$3.240 \cdot 10^{-6}$ (T; Ref. 12)	$3.3 \cdot 10^{-6}$
332.4	$4.069 \cdot 10^{-6}$ (T; Ref. 12)	$4.1 \cdot 10^{-6}$
333.7	$4.351 \cdot 10^{-6}$ (T; Ref. 12)	$4.4 \cdot 10^{-6}$
337.7	$5.358 \cdot 10^{-6}$ (T; Ref. 12)	$5.4 \cdot 10^{-6}$

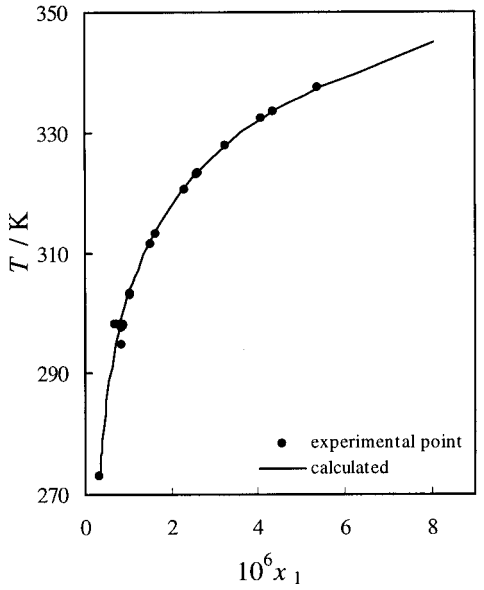

FIG. 6. All the solubility data for biphenyl (1) in water (2).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn. **60**, 3935 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of biphenyl in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(4.57 \pm 0.05) \cdot 10^{-5}$	$7.07 \cdot 10^{-4}$	$8.26 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Aqueous solutions saturated with vapor of (1) were prepared in the apparatus described in Sanemasa *et al.*[1] Samples were extracted with $CHCl_3$, dehydratted, and (1) was determined with a Hitachi 100-50 spectrophotometer. Details of equilibrations and sampling were described in the paper. Measurements were repeated at least four times and the average was taken as the solubility.

Source and Purity of Materials:
(1) Wako Pure and Nakarai Chemicals Co.; analytical grade, purity 98%; used as received.
(2) Distilled and de-ionized water.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: as above.

References:
[1] I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of biphenyl in water at 25 °C was reported to be $5.94 \cdot 10^{-4}$ g (1)/100 g sln.
The corresponding mole fraction (x_1), calculated by the compilers, is $6.9 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h 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; melting point 70.0–70.5 °C; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
Variables:	**Prepared By:**
Temperature: 0.4–42.8 °C	G. T. Hefter

Experimental Values

Solubility of biphenyl in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln[a] (compiler)
0.4	3.30	2.83
2.4	3.47	2.97
5.2	3.94	3.38
7.6	4.25	3.64
10.0	4.74	4.06
12.6	5.35	4.58
14.9	5.96	5.11
15.9	6.15	5.27
25.0	8.73[b]	7.48[b]
25.6	9.08	7.78
30.1	11.2	9.64
30.4	11.2	9.58
33.3	12.8	11.0
34.9	13.9	11.9
36.0	14.6	12.5
42.8	20.1	17.2

[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)/100 g sln by assuming a solution density of 1.00 kg/L.

[b]Given in the paper as $7.48 \cdot 10^{-3}$ g (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 24 h, and then allowed to settle for at least another 24 h. 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 absorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:

(1) Matheson Co., purified by recrystallization from absolute methanol.
(2) Air-free conductivity water, no further details given.

Estimated Error:

Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Values

The solubility of biphenyl in water was reported to be $3.91 \cdot 10^{-5}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass percent and mole fraction (x_1) solubilities, calculated by the compiler, are $6.03 \cdot 10^{-4}$ g (1)/100 g sln and $7.05 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of biphenyl 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 high-performance liquid chromatography using a Waters M6000A instrument fitted with a μC_{18} Bondapak column. The mobile phase was a mixture of methanol/water or acenotrile/water. 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) Aldrich; purity not specified.
(2) Distilled.

Estimated Error:

Temperature: ±0.2 °C.
Solubility: ±6.0% relative (representing 1 standard deviation).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	G. T. Coyle, T. C. Harmon, and I. H. Suffet, Environ. Sci. Technol. **31**, 384 (1997).
Variables:	**Prepared By:**
One temperature: 22 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of biphenyl in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
22	6.99	$7.00 \cdot 10^{-4}$	$8.18 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

The generator column technique was used. The dynamic coupled column liquid chromatography method, described in May *et al.*,[1] was based on generating saturated solutions by pumping water through a column packed with glass beads that were previously coated with component (1). The concentration of (1) in the effluent of the generator column was measured by standard HPCL techniques with a UV detector (Hewlett Packard Model 1050). The mean of three measurements is reported.

Source and Purity of Materials:

(1) Sigma Chemicals; purity 98%; used as received.
(2) Not specified.

Estimated Error:

Temperature: ± 1 °C.
Solubility: 5.4% (relative standard deviation).

References:

[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of biphenyl in water at 25 °C was reported to be 3.47 mg (1)/kg (2) and $4.8 \cdot 10^{-5}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $7.45 \cdot 10^{-4}$ g(1)/100 g sln and $8.70 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen, and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ± 0.5 °C.
Solubility: ± 0.06 mg (1)/kg (2) (from eight determinations).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Janado, Y. Yano, Y. Doi, and H. Sakamoto, J. Solution Chem. **12**, 741 (1983).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of biphenyl in water

t/°C	mg (1)/L (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	7.49	$7.52 \cdot 10^{-4}$	$7.87 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. About 10 g of water with an excess of 1,1′-biphenyl was placed in a thermostat, stirred for 6 h, gently shaken for another 18 h, and next allowed to stand for separation for the next 6 h. A portion of a clear solution was placed in a 1.5 mL vial containing a weighed amount of *n*-hexane. After extracting into *n*-hexane, biphenyl was determined by spectrophotometry.

Source and Purity of Materials:
(1) Nakarai Chemicals Ltd.; analytical grade; used as received.
(2) Glass redistilled water.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: <1.0% (average deviation from the mean).

Components:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of biphenyl in water at 25 °C was reported to be 7.0 mg (1)/L sln and $x_1 = 8.15 \cdot 10^{-7}$.
The corresponding mass percent calculated by the compiler is $7.0 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:
(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:
Solubility: ±0.06 mg (1)/L sln (maximum deviation from several determinations).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	M. M. Miller, S. Ghodbane, S. P. Wasik, Y. B. Tewari, and D. E. Martire, J. Chem. Eng. Data **29**, 184 (1984).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of biphenyl in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(4.35 \pm 0.14) \cdot 10^{-5}$	$6.73 \cdot 10^{-4}$	$7.86 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

A modified generator column coupled with a high pressure chromatography, described in detail in Tewari *et al.*,[1] were used.

Source and Purity of Materials:

(1) Ultra Scientific, Inc.; used as received.
(2) Distilled water.

Estimated Error:

Solubility: as above (standard deviation of three replicate measurements).

Refernces:

[1]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
Variables:	**Prepared By:**
One temperature: 298.15 K	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of biphenyl in water

T/K	mol (1)/g (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(4.91 \pm 0.04) \cdot 10^{-8}$	$7.58 \cdot 10^{-6}$	$8.85 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibration was carried out in a modified vessel (Franks *et al.*)[1] equipped with a magnetic stirrer. The temperature of the water bath was maintained within ±0.05 K. Equilibrium was obtained after several days and then samples were analyzed by spectrophotometry. At least five parallel determinations were performed.

Source and Purity of Materials:

(1) Commercial analytical grade reagent; purity >99% by glc; twice recrystallized.
(2) Distilled water passed through an Amberlite CG 120+CG 400 ion-exchange column.

Estimated Error:

Temperature: ±0.05 K.
Solubility: as above.

References:

[1]F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

Components:	**Original Measurements:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).
Variables:	**Prepared By:**
Temperature: 0–64.5 °C	A. Maczynski

Experimental Values

Solubility of biphenyl in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2) experiment	mg (1)/kg (2) smoothed with (standard deviation)
0.0	3.08	2.64	—	2.64(0.07)
24.6	8.13	6.96	7.13, 7.29, 7.35	6.96
25.0	8.27	7.08	—	7.08(0.09)
29.9	10.2	8.73	8.77, 8.64, 8.95	8.73
30.3	10.4	8.88	8.55, 8.54, 8.48	8.88
38.4	14.8	12.7	13.2, 13.3, 13.5	12.7
40.1	16.1	13.8	13.1, 13.4, 13.4	13.8
47.5	22.8	19.5	18.8, 19.0, 18.7	19.5
50.0	25.7	22.0	—	22.0(0.2)
50.1	25.8	22.1	20.6, 21.6, 21.8	22.1
50.2	29.9	22.2	20.7, 21.8	22.2
54.7	32.4	27.7	28.3, 28.8, 28.8	27.7
59.2	40.7	34.8	36.4, 36.3, 36.0	34.8
60.5	43.5	37.2	40.4	37.2
64.5	53.6	45.9	43.7, 44.7, 46.6	45.9

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 20 g of (1) was placed in each of three 250 mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from 1 to 3 weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1–0.2 g of samples followed by serial dilution in calibrated glassware.

Source and Purity of Materials:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.
(2) Distilled and de-ionized.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: see experimental values above.

2.12. 1,3-Dimethylnaphthalene+Water

Components:	**Original Measurements:**
(1) 1,3-Dimethylnaphthalene; $C_{12}H_{12}$; [575-41-7] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 1,3-dimethylnaphthalene in water at 25 °C was reported to be 8.0 mg (1)/L sln and $x_1 = 9.2 \cdot 10^{-7}$.
The corresponding mass percent calculated by the compiler is $8.0 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.5 mg (1)/L sln (maximum deviation from several determinations).

2.13. 1,4-Dimethylnaphthalene+Water

Components:
(1) 1,4-Dimethylnaphthalene; $C_{12}H_{12}$; [571-58-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 1,4-dimethylnaphthalene in water at 25 °C was reported to be 11.4 mg (1)/L sln and $x_1 = 1.31 \cdot 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00114 g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:
(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:
Solubility: ±0.1 mg (1)/L sln (maximum deviation from several determinations).

2.14. 1,5-Dimethylnaphthalene+Water

Components:
(1) 1,5-Dimethylnaphthalene; $C_{12}H_{12}$; [571-61-9]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 1,5-Dimethylnaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Eganhouse and Calder[1] and Mackay and Shiu[2] at 298 K.

As indicated in the preface to Part 10, solubility of 1,5-dimethylnaphthalene in water should be almost the same as solubility of 1-ethylnaphtalene in water, which is well established and used as the reference data.

Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 10. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:
[1] *R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta* **40**, 555 (1976).
[2] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 10. Experimental values for solubility of 1,5-dimethylnaphthalene (1) in water (2)

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$3.158 \cdot 10^{-7}$ (D; Ref. 1), $3.77 \cdot 10^{-7}$ (D; Ref. 2)	$1.1 \cdot 10^{-6}$

Components:	Original Measurements:
(1) 1,5-Dimethylnaphthalene; $C_{12}H_{12}$; [571-61-9] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of 1.5-dimethylnaphthalene in water at 25 °C was reported to be 2.74 mg (1)/kg (2) and $1.8 \cdot 10^{-5}$ mol (1)/L (2).
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $2.74 \cdot 10^{-4}$ g (1)/100 g sln and $8.70 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen, and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±0.1 mg (1)/kg (2) (from eight determinations).

Components:	Original Measurements:
(1) 1,5-Dimethylnaphthalene; $C_{12}H_{12}$; [571-61-9] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 1,5-dimethylnaphthalene in water at 25 °C was reported to be 3.38 mg (1)/L sln and $x_1 = 3.77 \cdot 10^{-7}$.
The corresponding mass percent calculated by the compiler is $3.38 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.04 mg (1)/L sln (maximum deviation from several determinations).

2.15. 2,3-Dimethylnaphthalene+Water

Components:
(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 2,3-Dimethylnaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Eganhouse and Calder[1] and Mackay and Shiu[2] at 298 K.

As indicated in the preface to Part 10, solubility of 2,3-dimethylnaphthalene in water should be almost the same as solubility of 1-ethylnaphthalene in water, which is well established and used as the reference data.

Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 11. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:
[1]R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[2]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 11. Experimental values for solubility of 2,3-dimethylnaphthalene (1) in water (2)

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$2.29 \cdot 10^{-7}$ (D; Ref. 1), $3.47 \cdot 10^{-7}$ (D; Ref. 2)	$1.1 \cdot 10^{-6}$

Components:
(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of 2,3-dimethylnaphthalene in water at 25 °C was reported to be 1.99 mg (1)/kg (2) and $1.3 \cdot 10^{-5}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.99 \cdot 10^{-4}$ g(1)/100 g sln and $2.29 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:
(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: ±0.02 mg (1)/kg (2) (from eight determinations).

Components:	Original Measurements:
(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 2,3-dimethylnaphthalene in water at 25 °C was reported to be 3.0 mg (1)/L sln and $x_1 = 3.47 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $3.0 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.01 mg (1)/L sln (maximum deviation from several determinations).

2.16. 2,6-Dimethylnaphthalene+Water

Components:	Evaluators:
(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 2,6-Dimethylnaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Eganhouse and Calder[1] and Mackay and Shiu[2] at 298 K.

As indicated in the preface to Part 10, solubility of 2,6-dimethylnaphthalene in water should be almost the same as solubility of 1-ethylnaphthalene in water, which is well established and used as the reference data.

Comparison between the reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 12. All the data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

References:

[1] *R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta* **40**, 555 (1976).
[2] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 12. Experimental values for solubility of 2,6-dimethylnaphthalene (1) in water (2)

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$1.499 \cdot 10^{-7}$ (D; Ref. 1), $2.331 \cdot 10^{-7}$ (D; Ref. 2)	$1.1 \cdot 10^{-6}$

Components:	Original Measurements:
(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of 2,6-dimethylnaphthalene in water at 25 °C was reported to be 1.30 mg (1)/kg (2) and $8.3 \cdot 10^{-6}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.30 \cdot 10^{-4}$ g (1)/100 g sln and $1.50 \cdot 10^{-}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±0.04 mg (1)/kg (2) (from eight determinations).

Components:	Original Measurements:
(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 2,6-dimethylnaphthalene in water at 25 °C was reported to be 2.0 mg (1)/L sln and $x_1 = 2.33 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $2.0 \cdot 10^{-4}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:

Solubility: ±0.02 mg (1)/L sln (maximum deviation from several determinations).

2.17. 1-Ethylnaphthalene+Water

Components:
(1) 1-Ethylnaphthalene
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of 1-Ethylnaphthalene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Economou *et al.*[1]	311–589 (467–12 238 kPa)	Schwarz and Wasik[3]	283–298
Mackay and Shiu[2]	298	Schwarz[4]	282–305

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 10 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)] + 0.36\ln(T_{2c}-T)/(T_{2c}-T_{\min}), \quad (1)$$

where $\ln x_{1,\min} = -14.01$; $D = 41.90$; $T_{\min} = 265$ K; $T_{2c} = 594.4$ K.

Equation (1) is based on all available solubility data of 1-ethylnaphthalene in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 13 and shown in Fig. 7. The data of Mackay and Shiu[2] at 298 K, and Schwarz and Wasik,[3] and Schwarz[4] at 287, 293, and 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. The data of Economou *et al.*[1] at 594 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful. All the remaining data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

Critical Evaluation of the Solubility of Water (2) in 1-Ethylnaphthalene (1)

The experimental solubility data for (2) in (1) have been investigated by Economou *et al.*[1] at 311–589 K and 467–12 238 kPa.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.076$; $d_2 = -5.418$; $d_3 = -1.985$; $d_4 = 3.117$; $T_r = T/594.6$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1-ethylnaphthalene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 14 and shown in Fig. 8. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

References:

[1] *I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J.* **43**, 535 (1997).
[2] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[3] F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data **22**, 270 (1977).
[4] F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).

TABLE 13. Experimental values for solubility of 1-ethylnaphthalene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
281.8		$9.40\cdot10^{-7}$ (T; Ref. 4)	$9.0\cdot10^{-7}$
283.2		$9.40\cdot10^{-7}$ (T; Ref. 3)	$9.1\cdot10^{-7}$
284.3		$9.40\cdot10^{-7}$ (T; Ref. 4)	$9.2\cdot10^{-7}$
287.2		$9.40\cdot10^{-7}$ (R; Ref. 3), $9.50\cdot10^{-7}$ (R; Ref. 4)	$9.6\cdot10^{-7}$
290.3		$9.90\cdot10^{-7}$ (T; Ref. 4)	$9.9\cdot10^{-7}$
293.2		$1.15\cdot10^{-6}$ (R; Ref. 3), $9.70\cdot10^{-7}$ (R; Ref. 4)	$1.0\cdot10^{-6}$
296.2		$9.90\cdot10^{-7}$ (T; Ref. 4)	$1.1\cdot10^{-6}$
298.2		$1.24\cdot10^{-6}$ (R; Ref. 2), $1.15\cdot10^{-6}$ (R; Ref. 3), $1.15\cdot10^{-6}$ (R; Ref. 4)	$1.1\cdot10^{-6}$
299.3		$1.13\cdot10^{-6}$ (T; Ref. 4)	$1.1\cdot10^{-6}$
304.9		$1.35\cdot10^{-6}$ (T; Ref. 4)	$1.3\cdot10^{-6}$
310.9		$1.30\cdot10^{-6}$ (T; Ref. 1)	$1.4\cdot10^{-6}$
366.5		$5.50\cdot10^{-6}$ (T; Ref. 1)	$5.5\cdot10^{-6}$
422.0	467 (Ref. 1)	$2.40\cdot10^{-5}$ (T; Ref. 1)	$2.9\cdot10^{-5}$
477.6	1733 (Ref. 1)	$1.50\cdot10^{-4}$ (T; Ref. 1)	$1.7\cdot10^{-4}$
533.2	4833 (Ref. 1)	$8.40\cdot10^{-4}$ (T; Ref. 1)	$1.0\cdot10^{-3}$
549.8	6343 (Ref. 1)	$1.49\cdot10^{-3}$ (T; Ref. 1)	$1.8\cdot10^{-3}$
594.4	12 238 (Ref. 1)	$7.30\cdot10^{-2}$ (D; Ref. 1)	$4.7\cdot10^{-2}$

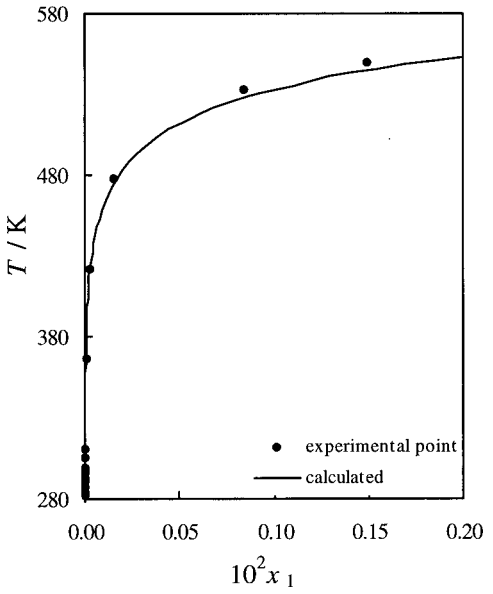

FIG. 7. All the solubility data for 1-ethylnaphthalene (1) in water (2) below 550 K.

TABLE 14. Experimental values for solubility of water (2) in 1-ethylnaphthalene (1)

T/K	P/kPa	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
310.9		$4.91 \cdot 10^{-3}$ (T; Ref. 1)	$6.2 \cdot 10^{-3}$
366.5		$2.12 \cdot 10^{-2}$ (T; Ref. 1)	$2.5 \cdot 10^{-2}$
422.0	467 (Ref. 1)	$6.23 \cdot 10^{-2}$ (T; Ref. 1)	$6.7 \cdot 10^{-2}$
477.6	1733 (Ref. 1)	$1.51 \cdot 10^{-1}$ (T; Ref. 1)	$1.4 \cdot 10^{-1}$
533.2	4833 (Ref. 1)	$3.25 \cdot 10^{-1}$ (T; Ref. 1)	$2.7 \cdot 10^{-1}$
549.8	6343 (Ref. 1)	$4.07 \cdot 10^{-1}$ (T; Ref. 1)	$3.3 \cdot 10^{-1}$
594.4	12 238 (Ref. 1)	$9.27 \cdot 10^{-1}$ (T; Ref. 1)	$8.2 \cdot 10^{-1}$

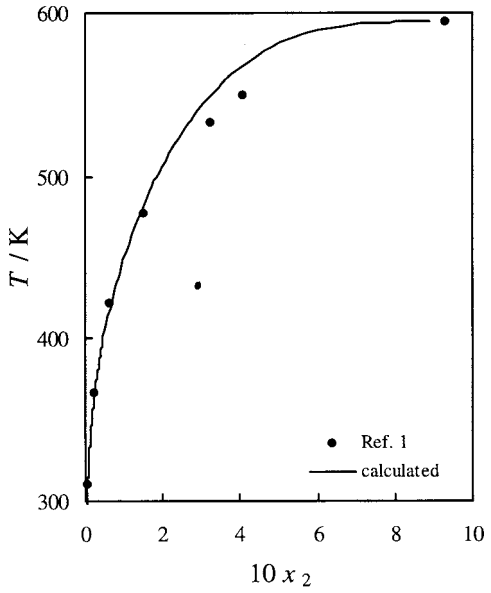

FIG. 8. All the solubility data for water (2) in 1-ethylnaphthalene (1).

Components:
(1) 1-Ethylnaphtalene; $C_{12}H_{12}$; [1127-76-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:
Temperature: 310.93–594.43 K
Pressure: 0.4668–12.238 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1-ethylnaphthalene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^2 \cdot x_1$
310.93	—	0.00113	0.00013
366.48	—	0.00477	0.00055
422.04	0.4668	0.0208	0.0024
477.59	1.7326	0.130	0.015
533.15	4.833	0.724	0.084
549.82	6.343	1.278	0.149
594.43[a]	12.238	40.58	7.3

Solubility of water in 1-ethylnaphthalene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
310.93	—	0.0569	0.00491
366.48	—	0.249	0.0212
422.04	0.4668	0.760	0.0623
477.59	1.7326	2.01	0.151
533.15	4.833	5.26	0.325
549.82	6.343	7.33	0.407
594.43[a]	12.238	59.42	0.927

[a]Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of hydrocarbon in water was measured by glc, while that of water in hydrocarbon by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:
(1) Pfaltz and Bauer; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:
Temperature: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:
[1]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2]J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3]C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

Components:
(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 1-ethylnaphthalene in water at 25 °C was reported to be 10.7 mg (1)/L sln and $x_1 = 1.24 \cdot 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00107 g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently settled at 25 °C for at least 48 h. Then the saturated solution was decanted and filtered and 50–100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 h, the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

Source and Purity of Materials:
(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.
(2) Doubly distilled.

Estimated Error:
Solubility: ±0.3 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data **22**, 270 (1977).

Variables:
Temperature: 10–25 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 1-ethylnaphthalene in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	$10^5 \cdot$ mol (1)/L
10	9.4	8.1	5.2±0.2
14	9.4	8.1	5.2±0.1
20	11.5	10.0	6.4±0.1
25	11.5	10.0	6.4±0.1

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) is too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

Source and Purity of Materials:
(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole %.
(2) Distilled from $KMnO_4$ and passed though a Sephadex column.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: see above.

Components:	Original Measurements:
(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
Variables:	**Prepared By:**
Temperature: 8.6–31.7 °C	A. Maczynski

Experimental Values

Solubility of 1-ethylnaphthalene in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	$10^6 \cdot$ mol (1)/L
8.6	9.4	8.1	5.2 ± 0.3
11.1	9.4	8.1	5.2 ± 0.2
14.0	9.5	8.3	5.3 ± 0.1
17.1	9.9	8.6	5.5 ± 0.1
20.0	9.7	8.4	5.4 ± 0.1
23.0	9.9	8.6	5.5 ± 0.1
25.0	11.5	10.0	6.4 ± 0.1
26.1	11.3	9.8	6.3 ± 0.1
31.7	13.5	11.7	7.5 ± 0.2

Auxiliary Information

Method/Apparatus/Procedure:

Two methods were used: At 25 °C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry, and placed in the fluorimeter.

Source and Purity of Materials:

(1) Source not specified; better than 99.9 mole %, by glc; used as received.
(2) Distilled over $KMnO^4$ and NaOH and passed through a Sephadex column.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: see above.

2.18. 2-Ethylnaphthalene+Water

Components:	Original Measurements:
(1) 2-Ethylnaphthalene; $C_{12}H_{12}$; [939-27-5] (2) Water; H_2O; [7732-18-5]	R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski

Experimental Values

The solubility of 2-ethylnaphthalene in water at 25 °C was reported to be 8.00 mg (1)/kg (2) and $5.1 \cdot 10^{-5}$ mol (1)/L (2).
The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $8.00 \cdot 10^{-4}$ g (1)/100 g sln and $9.22 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation)+24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

Source and Purity of Materials:

(1) Source not specified; analytical grade; used as received; no impurities by glc.
(2) Doubly distilled; free of trace organics.

Estimated Error:

Temperature: ± 0.5 °C.
Solubility: ± 0.1 mg (1)/kg (2) (from eight determinations).

2.19. 2-Allyl-1,3,5-trimethylbenzene+Water

Components:
(1) 2-Allyl-1,3,5-trimethylbenzene; $C_{12}H_{16}$; [4810-05-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 20–40 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2-allyl-1,3,5-trimethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
20	1.15	0.0246
30	1.54	0.0331
40	2.04	0.0438

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h 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.

2.20. 1,4-Diisopropylbenzene+Water

Components:
(1) 1,4-Diisopropylbenzene; $C_{12}H_{18}$; [100-18-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:
Temperature: 310.93–589.98 K
Pressure: 0.4757–12.445 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 1,4-diisopropylbenzene in water

T/K	P/MPa	g (1)/100 g sln (compilers)	$10^4 x_1$
310.93	—	0.000333	0.0037
366.48	—	0.00108	0.012
422.04	0.4757	0.00667	0.074
477.59	1.7995	0.0522	0.58
533.15	5.081	0.404	4.5
549.82	7.460	0.636	7.1
549.82	7.460	0.636	7.1

Solubility of water in 1,4-diisopropylbenzene

T/K	P/MPa	g (2)/100 g sln (compilers)	x_2
310.93	—	0.0384	0.00345
366.48	—	0.1768	0.00157
422.04	0.4757	0.704	0.00600
477.59	1.7995	2.18	0.167
533.15	5.081	5.97	0.364
549.82	7.460	8.70	0.462
589.98[a]	12.445	35.64	0.833

[a]Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of hydrocarbon in water was measured by glc, while that of water in hydrocarbon by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:
(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:
Tempertaure: ±0.6 K at critical end point.[a]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[a]
Pressure: 1% and ±0.04 MPa at critical end point.[a]

References:
[1]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2]J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3]C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

2.21. Hexylbenzene+Water

Components:
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.

Critical Evaluation of the Solubility of Hexylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Krasnoshchekova and Gubergrits[1]	298	Owens *et al.*[3]	280–318
May *et al.*[2]	378–302	Tewari *et al.*[4]	298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{1,\min} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where: $\ln x_{1,\min} = -16.16$; $D = 65.42$; $T_{\min} = 290$ K.

Equation (1) is based on all available solubility data of aromatic hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 15.

All the experimental and reference data are listed in Table 16 and shown in Fig. 9.

References:

[1]*R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy* **2**, 170 (1975).
[2]W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. M. Brown-Thomas, and R. N. Goldberg, J. Chem. Eng. Data **28**, 197 (1983).
[3]J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).
[4]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

TABLE 15. The data categories for solubility of hexylbenzene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
278.2		May *et al.*[2]	
279.2		May *et al.*[2]	
280.2		Owens *et al.*[3]	
281.2		May *et al.*[2]	
282.2		May *et al.*[2]	
283.2	May *et al.*,[2] Owens *et al.*[3]		
284.2		May *et al.*[2]	
285.2		May *et al.*[2]	
286.2		May *et al.*[2]	
287.2		May *et al.*[2]	
288.2	May *et al.*,[2] Owens *et al.*[3]		
289.2		May *et al.*[2]	
290.2		May *et al.*[2]	
291.2		May *et al.*[2]	
292.2		May *et al.*[2]	
293.2	May *et al.*,[2] Owens *et al.*[3]		
294.2		May *et al.*[2]	
295.2		May *et al.*[2]	
296.2		May *et al.*[2]	
297.2		May *et al.*[2]	
298.2	May *et al.*,[2] Owens *et al.*,[3] Tewari *et al.*[4]		Krasnoshchekova and Gubergrits[1]
299.2		May *et al.*[2]	
300.2		May *et al.*[2]	
302.2		May *et al.*[2]	
303.2		Owens *et al.*[3]	
308.2		Owens *et al.*[3]	
313.2		Owens *et al.*[3]	
318.2		Owens *et al.*[3]	

TABLE 16. Experimental values for solubility of hexylbenzene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
278.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$1.0 \cdot 10^{-7}$
279.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$1.0 \cdot 10^{-7}$
280.2	$9.26 \cdot 10^{-8}$ (T; Ref. 3)	$1.0 \cdot 10^{-7}$
281.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$9.9 \cdot 10^{-8}$
282.2	$1.01 \cdot 10^{-7}$ (T; Ref. 2)	$9.8 \cdot 10^{-8}$
283.2	$1.00 \cdot 10^{-7}$ (R; Ref. 2), $9.28 \cdot 10^{-8}$ (R; Ref. 3)	$9.8 \cdot 10^{-8}$
284.2	$1.03 \cdot 10^{-7}$ (T; Ref. 2)	$9.7 \cdot 10^{-8}$
285.2	$1.03 \cdot 10^{-7}$ (T; Ref. 2)	$9.7 \cdot 10^{-8}$
286.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
287.2	$1.03 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
288.2	$1.01 \cdot 10^{-7}$ (R; Ref. 2), $9.18 \cdot 10^{-8}$ (R; Ref. 3)	$9.6 \cdot 10^{-8}$
289.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
290.2	$1.01 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
291.2	$1.02 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
292.2	$1.05 \cdot 10^{-7}$ (T; Ref. 2)	$9.6 \cdot 10^{-8}$
293.2	$1.05 \cdot 10^{-7}$ (R; Ref. 2), $1.06 \cdot 10^{-7}$ (R; Ref. 3)	$9.6 \cdot 10^{-8}$
294.2	$1.06 \cdot 10^{-7}$ (T; Ref. 2)	$9.7 \cdot 10^{-8}$
295.2	$1.06 \cdot 10^{-7}$ (T; Ref. 2)	$9.7 \cdot 10^{-8}$
296.2	$1.09 \cdot 10^{-7}$ (T; Ref. 2)	$9.7 \cdot 10^{-8}$
297.2	$1.10 \cdot 10^{-7}$ (T; Ref. 2)	$9.8 \cdot 10^{-8}$
298.2	$2.40 \cdot 10^{-7}$ (D; Ref. 1), $1.11 \cdot 10^{-7}$ (R; Ref. 2), $1.01 \cdot 10^{-7}$ (R; Ref. 3), $1.13 \cdot 10^{-7}$ (R; Ref. 4)	$9.8 \cdot 10^{-8}$
299.2	$1.11 \cdot 10^{-7}$ (T; Ref. 2)	$9.9 \cdot 10^{-8}$
300.2	$1.12 \cdot 10^{-7}$ (T; Ref. 2)	$1.0 \cdot 10^{-7}$
302.2	$1.13 \cdot 10^{-7}$ (T; Ref. 2)	$1.0 \cdot 10^{-7}$
303.2	$1.11 \cdot 10^{-7}$ (T; Ref. 3)	$1.0 \cdot 10^{-7}$
308.2	$1.19 \cdot 10^{-7}$ (T; Ref. 3)	$1.1 \cdot 10^{-7}$
313.2	$1.20 \cdot 10^{-7}$ (T; Ref. 3)	$1.2 \cdot 10^{-7}$
318.2	$1.45 \cdot 10^{-7}$ (T; Ref. 3)	$1.3 \cdot 10^{-7}$

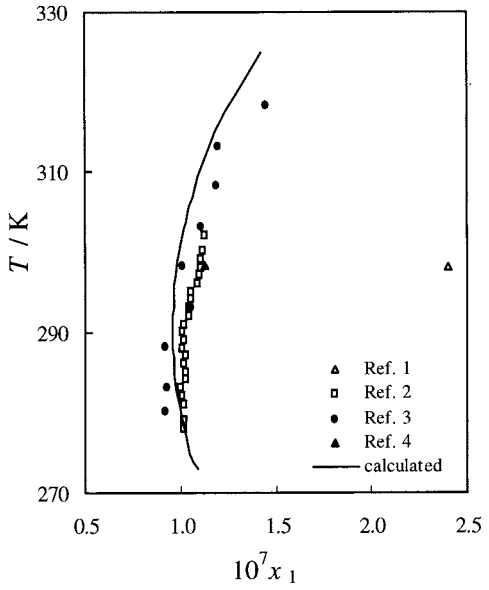

FIG. 9. All the solubility data for hexylbenzene (1) in water (2).

Components:
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of 1-hexylbenzene in water at 25 °C was reported to be 0.0021 mg (1)/mL sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00021 g (1)/100 g sln and $2.4 \cdot 10^{-7}$. The assumption that 1.00 L sln=1.00 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. A Czech-made Chom-2 chomatograph was used, equipped with a 5% Apiezon L/Chomosorb G column operated at 90–140 °C.

Source and Purity of Materials:
(1) Described in Krasnoshchekova and Gubergrits.[1]
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.

References:
[1]R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Components:
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. M. Brown-Thomas, and R. N. Goldberg, J. Chem. Eng. Data **28**, 197 (1983).

Variables:
Temperatures: 278.15–302.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of hexylbenzene in water

T/K	$10^4 \cdot$ g (1)/100 g sln (compilers)	$10^7 \cdot x_1$
278.15	0.9205	1.022
279.15	0.9205	1.022
281.15	0.9187	1.020
282.15	0.9052	1.005
283.15	0.9034	1.003
284.15	0.9268	1.029
285.15	0.9295	1.032
286.15	0.9187	1.020
287.15	0.9241	1.026
288.15	0.9070	1.007
289.15	0.9178	1.019
290.15	0.9088	1.009
291.15	0.9205	1.022
292.15	0.9422	1.046
293.15	0.9485	1.053
294.15	0.9548	1.060
295.15	0.9521	1.057
296.15	0.9818	1.090
297.15	0.9944	1.104
298.15	0.9980	1.108
299.15	0.9980	1.108
300.15	1.0115	1.123
302.15	1.0151	1.127

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by an automated coupled-column liquid chromatographic apparatus; technique and apparatus were reported in May *et al.*[1] and Tewari *et al.*[2] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. The HPLC method and UV detection were used for analysis.

Source and Purity of Materials:
(1) Source not specified; purity >99 mole % by glc.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 K (Tewari *et al.*[2]).

References:
[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Components:
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).

Variables:
Temperature: 7.0–45.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of hexylbenzene in water

t/°C	$10^6 \cdot$ mol (1)/L sln	$10^4 \cdot$ g (1)/100 g sln (compilers)	$10^7 \cdot x_1$ (compilers)
7.0	5.14±0.15	0.834	0.926
10.0	5.15±0.24	0.836	0.928
15.0	5.09±0.24	0.826	0.918
20.0	5.86±0.18	0.953	1.058
25.0	5.56±0.11	0.905	1.005
30.0	6.14±0.34	1.001	1.111
35.0	6.59±0.15	1.076	1.194
40.0	6.59±0.55	1.078	1.196
45.0	8.00±0.23	1.311	1.455

Auxiliary Information

Method/Apparatus/Procedure:
Solubility was determined by the technique reported in May *et al.*[1] and DeVoe *et al.*[2] and an automated coupled-column liquid chromatographic apparatus, described in Owens *et al.*[3] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. A known volume of the saturated solution was passed through a small extractor column filled with reverse phase packing where the solute was removed quantitatively. The extracted solute was then eluted with a water–methanol mixture, separated from impurities on an HPLC analytical column, and analyzed by UV spectrophotometry at 254 nm. The standard deviation of the peak area for the known solution was $<2.4\%$. 2–3 measurements at each temperature were made.

Source and Purity of Materials:
(1) Albany Internationals Chemicals Division; used as received; purity >99% by glc.
(2) HPCL grade.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: as above.

References:
[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[3]J. W. Owens, T. J. Buckley, and H. DeVoe, J. Res. Natl. Bur. Stand. (USA) **90**, 41 (1985).

Components:
(1) Hexylbenzene; $C_{12}H_{18}$; [1077-16-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of hexylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$6.27 \cdot 10^{-6}$	$1.020 \cdot 10^{-4}$	$1.133 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with an organic liquid by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hpcl. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:
(1) Source not specified; purity >99 mole % checked by high-temperature glc.
(2) Source not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:
[1]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

2.22. 2-Propyl-1,3,5-trimethylbenzene+Water

Components:	**Original Measurements:**
(1) 2-Propyl-1,3,5-trimethylbenzene; $C_{12}H_{18}$; [4810-04-2]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
(2) Water; H_2O; [7732-18-5]	
Variables:	**Prepared By:**
Temperature: 20–40 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 2-propyl-1,3,5-trimethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
20	2.29	0.0255
30	3.08	0.0343
40	4.09	0.0455

Auxiliary Information

Method/Apparatus/Procedure:

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

2.23. Dodecane+Water

Components:	**Evaluators:**
(1) Dodecane; $C_{12}H_{26}$; [112-40-3]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, April, 2004.
(2) Water; H_2O; [7732-18-5]	

Critical Evaluation of the Solubility of Dodecane (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by Franks[1] and Sutton and Calder[4] at 298 K.

Reference solubility data for (1) in (2) at 298 K were obtained by the Evaluators using the procedures described in the Preface to Part 10 and expressed by the equation:

$$\ln x_1 = -24.63 + 34.61/N, \quad (1)$$

where N is a number of carbon atoms in n-alkane.

Equation (1) is based on all available solubility data of C_{10}–C_{36} n-alkanes in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to categories.

All the experimental and reference data are listed in Table 17. The data of Sutton and Calder[4] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Franks[1] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in Dodecane (1)

The experimental solubility data for (2) in (1) have been investigated by Schatzberg[2] at 298 and 313 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using LLE calculations described in the Preface to Part 1. The input data for these calculations at 298 K was the solubility of dodecane in water calculated with Eq. (1). The input solubility at 313 K was estimated with corrected equation used for lower alkanes.

Comparison between the reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 18. The data of Schatzberg[2] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

High Pressure Solubility of Dodecane (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Stevenson *et al.*[3] at 604–633 K and 13 890–24 920 kPa have not been critically evaluated because the developed method is not applied for such data

References:

[1] *F. Franks, Nature (London)* **210**, 87 (1966).
[2] P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
[3] R. L. Stevenson, D. S. LaBracio, T. A. Beaton, and M. C. Thies, Fluid Phase Equilib. **93**, 317 (1994).
[4] C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

TABLE 17. Experimental values for solubility of dodecane (1) in water (2)

T/K	Experimental values x_1 (T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$8.9 \cdot 10^{-10}$ (D; Franks[1]), $4.0 \cdot 10^{-10}$ (T; Sutton and Calder[4])	$3.6 \cdot 10^{-10}$

TABLE 18. Experimental values for solubility of water (2) in dodecane (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
298.2	$6.1 \cdot 10^{-4}$ (T; Schatzberg[2])	$7.5 \cdot 10^{-4}$
313.2	$1.2 \cdot 10^{-3}$ (T; Schatzberg[2])	$1.4 \cdot 10^{-3}$

Components:
(1) Dodecane; $C_{12}H_{26}$; [112-40-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).

Variables:
Temperature: 25 and 40 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of water in dodecane

t/°C	$10^4 \cdot x_2$	mg (2)/kg sln
25	6.1	65[a]
40	12.0	127[b]

[a]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water bath for 7 days. A 20 mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized the 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.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade; 99+mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220–340 nm spectral range.
(2) Distilled and de-ionized.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: (a) 0%–6%; (b) 0%–2% (deviations from the mean).

Components:
(1) Dodecane; $C_{12}H_{26}$; [112-40-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. Franks, Nature (London) **210**, 87 (1966).

Variables:
One temperature: 25 °C

Prepared By:
F. Kapuku

Experimental Values

The solubility of dodecane in water at 25 °C was reported to be in mole fraction $x_1 = 8.9 \cdot 10^{-10}$.
The corresponding mass percent calculated by the compiler is $8.42 \cdot 10^{-7}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
The analysis was performed by glc. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by Drierite. The (1) concentrations were obtained from the peak areas, after initial calibrations.

Source and Purity of Materials:
(1) Fluka; purum grade; purity >97% (chromatographic analysis).
(2) Not specified.

Estimated Error:
Solubility: ±12%.

Components:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. L. Stevenson, D. S. LaBracio, T. A. Beaton, and M. C. Thies, Fluid Phase Equilib. **93**, 317 (1994).

Variables:

Temperature: 603.6 and 633.0 K
Pressure: 138.9–249.2 bar

Prepared By:

A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Mutual solubility of dodecane in water

T/K	P/bar	g (1)/100 g sln (compilers)	x_1
603.6	138.9	0.94	0.0010
	138.9	0.66	0.0007
	145.8	1.12	0.0012
	145.8	1.12	0.0012
	152.7	1.31	0.0014
	159.6	1.22	0.0013
	173.4	1.31	0.0014
	173.4	1.31	0.0014
	187.2	1.22	0.0013
	201.0	1.22	0.0013
633.0	234.1[a]	21.41	0.0280
	238.9	14.34	0.0174
	238.9	15.97	0.0197
	249.2	11.91	0.0141

Mutual solubility of water in dodecane

T/K	P/bar	g (2)/100 g sln (compilers)	x_2
603.6	138.9	72.48	0.9614
	138.9	72.16	0.9608
	145.8	54.95	0.9202
	145.8	55.63	0.9222
	152.7	39.78	0.862
	159.6	30.53	0.806
	173.4	24.09	0.750
	173.4	24.18	0.751
	187.2	20.97	0.715
	201.0	18.77	0.686
633.0	234.1[a]	78.59	0.9720
	238.9	73.13	0.9626
	238.9	72.27	0.9610
	249.2	61.99	0.9391

[a]Liquid–liquid critical point.

Auxiliary Information

Method/Apparatus/Procedure:

The flow apparatus for the high temperature experiments was used. The streams of both components were combined, mixed, preheated, and pumped into the stainless equilibrium cell of volume 10 cm^3 with two transparent sapphire windows. Pressure was measured with a Heise–Bourdon tube gauge. Details of the apparatus and procedure were described in the paper. The both phases were sampled, cooled, homogenized with 1-propanol, and analyzed by glc (Hewlett Packard 5710 A, 2 m column packed with Chromosorb 102, thermal conductivity detector, intergrator Hewlett Packard 21MX).

Source and Purity of Materials:

(1) Aldrich Chemicals Co.; stated purity >99%; purity checked by glc >99.5%; used as received.
(2) Distilled and de-ionized water.

Estimated Error:

Temperature: ±0.1 K.
Solubility: ±0.001 mole fraction.
Pressure: ±0.25 bar.

Components:	**Original Measurements:**
(1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Water; H_2O; [7732-18-5]	C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of dodecane in water at 25 °C was reported to be $3.7 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction x_1 of $4 \cdot 10^{-10}$.

Auxiliary Information

Method/Apparatus/Procedure:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 h. The flasks were then allowed to stand for 24 h. Aliquots of 100 mL were removed, filtered though a 0.45 μm Millipore filter, then extracted thee times with 10 mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

Source and Purity of Materials:

(1) Analabs Inc., 99+%.
(2) Doubly distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±16%.

3. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

4. Registry Number Index

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5. Author Index

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