IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 11. $C_{13}-C_{36}$ Hydrocarbons with Water

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The mutual solubilities and related liquid–liquid equilibria of C_{13}–C_{36} hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 56 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 17 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 homologous series of aliphatic and aromatic hydrocarbons was used. © *2006 American Institute of Physics.* [DOI: 10.1063/1.2132315]

Key words: C_{13}–C_{36} 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 11 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities 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 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.[3–6] 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 differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Calculation of reference data for some systems of polycyclic aromatic hydrocarbons was not possible because of insufficient data on solubility trends for the aromatic ring system. In evaluations of such systems, solubility values are categorized as Recommended, Tentative, Doubtful, or Rejected based on the criteria generally used in the Solubility Data Series. Recommended values are supported by two or more independent experimental values in agreement with one another and that the evaluators believe them to be reliable. Tentative values are supported by two or more independent values that lack good agreement or for some other reason are considered less reliable by the evaluators or are single values that are consistent with values at other temperatures. Doubtful values are those in disagreement with Recommended or Tentative values or are considered likely to be unreliable by the evaluators. Data that are in gross disagreement with more reliable values or that were reported without clarity are Rejected.

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.[7] The derivation of the smoothing equations used for calculate reference values for systems containing *n*-alkanes can be found in Part 10.[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 C5 to C7 (Pergamon, New York, 1989).
[2] D. Shaw, Editor, *IUPAC Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C8 to C36 (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: Alkylbenzene—Water Systems, J. Phys. Chem. Ref. Data **33**, 1159 (2004).
[7] A. Maczynski and D. G. Shaw, IUPC-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**, 5441 (2005).
[8] D. G. Shaw and A. Maczynski, IUPC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 10. C_{11} and C_{12} Hydrocarbons with Water and Heavy Water, J. Phys. Chem. Ref. Data **35**, 153 (2006).

2. C_{13}–C_{36} Hydrocarbons with Water

2.1. Fluorene+Water

Components:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Fluorene (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
Mackay and Shiu[1]	298	Walters and Luthy[4]	298
May *et al.*[2]	298	Wauchope and Getzen[5]	273–348
May *et al.*[3]	280–304		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 1 and shown in Fig. 1. At 298 K the data of Mackay and Shiu,[1] May *et al.*,[2] Walters and Luthy,[4] and Wauchope and Getzen[5] are in good agreement and are Recommended. From these data the mean value was calculated, as shown in Fig. 1 all the remaining data of May *et al.*[3] and Wauchope and Getzen[5] over the temperature range 273–348 K are consistent with the mean value at 298 K and are Tentative.

References:

[1]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
[3]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).
[4]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[5]R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

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

T/K	Experimental values x_1 (R=Recommended; T=tentative)	Mean value
273.2	$7.20\cdot10^{-8}$ (T; Ref. 5)	
279.8	$7.786\cdot10^{-8}$ (T; Ref. 3)	
286.4	$1.048\cdot10^{-7}$ (T; Ref. 3)	
291.2	$1.304\cdot10^{-7}$ (T; Ref. 3)	
297.2	$1.751\cdot10^{-7}$ (T; Ref. 3)	
297.8	$2.02\cdot10^{-7}$ (T; Ref. 5)	
298.2	$2.14\cdot10^{-7}$ (R; Ref. 1), $1.826\cdot10^{-7}$ (R; Ref. 2), $2.06\cdot10^{-7}$ (R; Ref. 4), $2.06\cdot10^{-7}$ (R; Ref. 5)	$2.0\cdot10^{-7}$
300.2	$2.000\cdot10^{-7}$ (T; Ref. 3)	
303.1	$2.57\cdot10^{-7}$ (T; Ref. 5)	
303.5	$2.61\cdot10^{-7}$ (T; Ref. 5)	
304.3	$2.436\cdot10^{-7}$ (T; Ref. 3)	
311.6	$3.82\cdot10^{-7}$ (T; Ref. 5)	
313.3	$4.16\cdot10^{-7}$ (T; Ref. 5)	
320.7	$6.00\cdot10^{-7}$ (T; Ref. 5)	
323.2	$6.82\cdot10^{-7}$ (T; Ref. 5)	
323.3	$6.85\cdot10^{-7}$ (T; Ref. 5)	
323.4	$6.88\cdot10^{-7}$ (T; Ref. 5)	
327.9	$8.69\cdot10^{-7}$ (T; Ref. 5)	
332.4	$1.10\cdot10^{-6}$ (T; Ref. 5)	
333.7	$1.18\cdot10^{-6}$ (T; Ref. 5)	
338.3	$1.53\cdot10^{-6}$ (T; Ref. 5)	
343.9	$2.09\cdot10^{-6}$ (T; Ref. 5)	
345.1	$2.23\cdot10^{-6}$ (T; Ref. 5)	
346.6	$2.44\cdot10^{-6}$ (T; Ref. 5)	
348.2	$2.68\cdot10^{-6}$ (T; Ref. 5)	

Components:	Original Measurements:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (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 fluorene in water at 25 °C was reported to be 1.98 mg (1)/L sln and $x_1 = 2.14 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $1.98 \cdot 10^{-4}$ 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 allowed to settle 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).

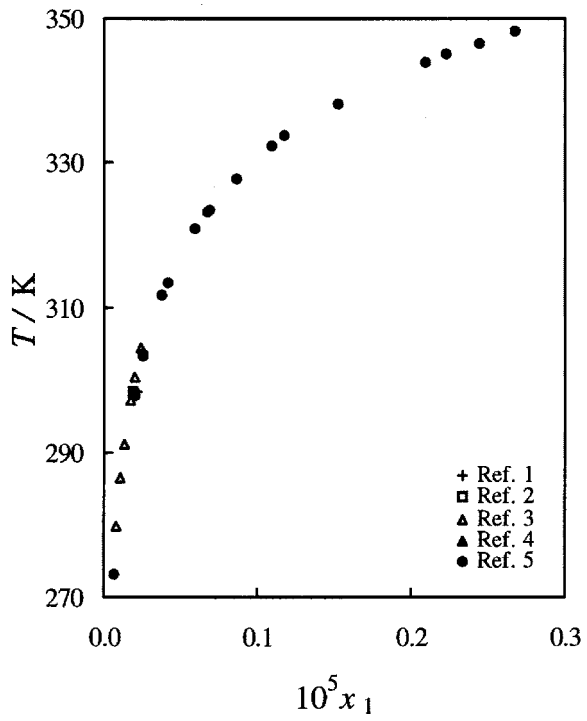

FIG. 1. All the solubility data for fluorene (1) in water (2).

Components:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of fluorene in water at 25 °C was reported to be 1.685 mg (1)/kg (2).

The corresponding mass percent and mole fraction (x_1) values, calculated by compiler, are $1.685 \cdot 10^{-4}$ g (1)/100 g sln and $1.826 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.005 mg (1)/100 kg (2) (standard deviation).

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7]
(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: 270.75–304.25 K

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

Experimental Values

Solubility of fluorene in water

T/K	$10^4 \cdot$ g (1)/100 g sln (compilers)	$10^7 \cdot x_1$
279.75	0.718	0.7786
286.35	0.967	1.048
291.15	1.203	1.304
297.15	1.616	1.751
300.15	1.845	2.000
304.25	2.248	2.436

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 (2) through a column containing the solute (1) coated on Chromosorb W. The high performance liquid chromatograph (hplc) method and ultraviolet (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) Fluorene; $C_{13}H_{10}$; [86-73-7]
(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 fluorene in water

t/°C	$10^6 \cdot x_1$ (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	7.2	0.66	—	0.66(0.01)
24.6	20.2	1.86	1.93, 1.87, 1.88	1.86
25.0	20.6	1.90	—	1.90(0.03)
29.9	25.7	2.37	2.41, 2.33, 2.34	2.37
30.3	26.1	2.41	2.10, 2.25, 2.23	2.41
38.4	38.2	3.53	3.72, 3.73	3.53
40.1	41.6	3.84	3.88, 3.84, 3.85	3.84
47.5	60.0	5.54	5.59, 5.62, 5.68	5.54
50.0	68.2	6.29	—	6.29(0.05)
50.1	68.5	6.32	6.31, 6.42, 6.54	6.32
50.2	68.8	6.35	6.27	6.35
54.7	86.9	8.02	8.31, 8.41, 8.56	8.02
59.2	110	10.2	10.5, 10.5	10.2
60.5	118	10.9	10.7, 11.0, 11.6	10.9
65.1	153	14.1	14.2, 14.1, 14.2	14.1
70.7	209	19.3	18.5, 18.5, 18.9	19.3
71.9	223	20.6	18.8	20.6
73.4	244	22.5	21.5	22.5
75.0	268	24.7		24.7(0.4)

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.

Components:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7]
(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 fluorene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	1.90±0.057	$1.91 \cdot 10^{-4}$	$2.06 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as auxiliary property to 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

2.2. Diphenylmethane (1,1′-Methylenebisbenzene)+Water

Components:	**Original Measurements:**
(1) Diphenylmethane; $C_{13}H_{12}$; [101-81-5] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Values

The solubility of diphenylmethane in water at 25 °C was reported to be $1.41 \cdot 10^{-4}$ g (1)/100 g sln.

The corresponding mole fraction (x_1) value calculated by compiler is $1.51 \cdot 10^{-7}$.

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; purified by fractional freezing; melting point 25 °C.
(2) Not specified.

Estimated Error:

Not specified.

2.3. 4-Phenyltoluene (4-Methyl-1,1′-biphenyl)+Water

Components:	**Original Measurements:**
(1) 4-Phenyltoluene; $C_{13}H_{12}$; [644-08-6] (2) Water; H_2O; [7732-18-5]	W. J. Doucette and A. W. Andren, Chemosphere **17**, 243 (1988).
Variables:	**Prepared By:**
Temperature: 4.9–40.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of 4-phenyltoluene 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)
4.9	1.09±0.07	1.83	1.96
25.0	2.41±0.08	4.06	4.35
40.0	4.18±0.17	7.09	7.59

Auxiliary Information

Method/Apparatus/Procedure:

The generator column described in Stolzenberg and Andren[1] was used. Details of the apparatus and procedures were described in the paper. Water was pumped through the generator at a flow rate 1–2 mL/min and the effluent flows through a Sep-Pak into a tarred flask. Water was removed by a stream of nitrogen. The solute was eluted in isooctane and analyzed by a Hewlett-Packard (5730A) glc equipped with a ^{63}Ni electron-capture detector. Four or five replicate determinations were made at each temperature.

Source and Purity of Materials:

(1) Ultra Scientific (Hope, RI); purity 99%; used as received.
(2) Milli Q water irradiated with UV light.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: as above (standard deviation).

References:

[1]T. Stolzenberg and A. W. Andren, Anal. Chim. Acta **151**, 271 (1983).

2.4. 1,4,5-Trimethylnaphthalene+Water

Components:
(1) 1,4,5-Trimethylnaphthalene; $C_{13}H_{14}$; [2131-41-1]
(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 1,4,5-trimethylnaphthalene in water at 25 °C was reported to be 2.1 mg (1)/L sln and $x_1 = 2.15 \cdot 10^{-7}$.
The corresponding mass percent calculated by the compiler is $2.1 \cdot 10^{-4}$ 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 allowed to settle 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).

2.5. (2-Ethylcyclopentyl)benzene+Water

Components:
(1) (2-Ethylcyclopentyl)benzene; $C_{13}H_{18}$; [4810-07-5]
(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 Z. Maczynska

Experimental Values

Solubility of water in (2-ethylcyclopentyl)benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	1.00	0.0103
20	1.62	0.0168
30	2.64	0.0273

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.

2.6. 2-Cyclopentyloctane+Water

Components:	**Original Measurements:**
(1) 2-Cyclopentyloctane; $C_{13}H_{26}$; [4810-01-9] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10–30 °C	A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in 2-cyclopentyloctane

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
10	4.86	0.0048
20	7.59	0.0075
30	12.34	0.0122

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.

2.7. Tridecane+Water

Components:	**Original Measurements:**
(1) Tridecane; $C_{13}H_{28}$; [629-50-5] (2) Water; H_2O; [7732-18-5]	P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
Variables:	**Prepared By:**
Temperature: 25 and 40 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of water in tridecane

t/°C	$10^4 \cdot x_2$	mg (2)/kg sln
25	6.1	60[a]
40	12.6	123[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 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 though 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).

2.8. Anthracene+Water

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Anthracene (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
Akiyoshi *et al.*[1]	298	May *et al.*[9]	298
Davis *et al.*[2]	300	May *et al.*[10]	278–302
Haines and Sandler[3]	298	Sawamura[11]	298
Hashimoto *et al.*[4]	293	Schwarz[12]	282–304
Kishi and Hashimoto[5]	293	Schwarz and Wasik[13]	298
Klevens[6]	298	Walters and Luthy[14]	298
Mackay and Shiu[7]	298	Wauchope and Getzen[15]	273–348
May *et al.*[8]	278–302		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 2 and shown in Fig. 2. At 298 K the data of Akiyoshi *et al.*,[1] Haines and Sandler,[3] May *et al.*,[9] and Schwarz[12] are in good agreement and are Recommended. From these data the mean value was calculated. As shown in Fig. 2, the data of Klevens,[6] Mackay and Shiu,[7] Sawamura,[11] Walters and Luthy,[14] and Wauchope and Getzen[15] seem to be high and Doubtful. The data of Davis *et al.*[2] at 300 K seem to be low and Doubtful. All the remaining data over the temperature range 273–348 K are consistent with the mean value at 298 K and are Tentative.

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

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[11] at 298 K and 0.1–200 MPa have not been critically evaluated because only a single data set are available.

References:

[1]M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn. **60**, 3935 (1987).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[3]R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).
[4]Y. Hashimoto, K. Tokura, K. Ozaki, and W. M. J. Strachan, Chemosphere **11**, 991 (1982).
[5]H. Kishi and Y. Hashimoto, Chemosphere **18**, 1749 (1989).
[6]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[7]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[8]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[9]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
[10]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).
[11]S. Sawamura, J. Solution Chem. **29**, 369 (2000).
[12]F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
[13]F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).
[14]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[15]R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

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

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
273.2	$2.20\cdot10^{-9}$ (T; Ref. 15)	
278.4	$1.28\cdot10^{-9}$ (T; Refs. 8 and 10)	
281.8	$2.36\cdot10^{-9}$ (T; Ref. 12)	
282.9	$1.637\cdot10^{-9}$ (T; Ref. 10)	
283.2	$1.77\cdot10^{-9}$ (T; Refs. 8 and 10)	
284.3	$2.47\cdot10^{-9}$ (T; Ref. 12)	
285.4	$2.59\cdot10^{-9}$ (T; Ref. 12)	
287.2	$2.77\cdot10^{-9}$ (T; Ref. 12)	
287.3	$2.24\cdot10^{-9}$ (T; Refs. 8 and 10)	
288.7	$3.00\cdot10^{-9}$ (T; Ref. 12)	
289.8	$2.537\cdot10^{-9}$ (T; Ref. 10)	
291.4	$3.26\cdot10^{-9}$ (T; Ref. 12)	
291.5	$2.94\cdot10^{-9}$ (T; Refs. 8 and 10)	
293.2	$3.3\cdot10^{-9}$ (T; Ref. 4), $4.2\cdot10^{-9}$ (T; Ref. 5)	
293.5	$4.00\cdot10^{-9}$ (T; Ref. 12)	
295.6	$3.76\cdot10^{-9}$ (T; Refs. 8 and 10)	
296.2	$4.21\cdot10^{-9}$ (T; Ref. 12)	
296.4	$3.821\cdot10^{-9}$ (T; Ref. 10)	
296.5	$4.14\cdot10^{-9}$ (T; Ref. 12)	
297.8	$4.39\cdot10^{-9}$ (T; Refs. 8 and 10)	
298.2	$4.5\cdot10^{-9}$ (R; Ref. 1), $4.30\cdot10^{-9}$ (R; Ref. 3), $4.40\cdot10^{-9}$ (R; Ref. 3), $4.34\cdot10^{-9}$ (R; Ref. 3), $8.07\cdot10^{-9}$ (D; Ref. 6), $7.57\cdot10^{-9}$ (D; Ref. 7), $4.51\cdot10^{-9}$ (R; Ref. 9), $6.2\cdot10^{-9}$ (D; Ref. 11), $4.14\cdot10^{-9}$ (R; Ref. 12), $3.04\cdot10^{-9}$ (R; Ref. 13), $7.60\cdot10^{-9}$ (D; Ref. 14), $7.08\cdot10^{-9}$ (D; Ref. 15)	$4.4\cdot10^{-9}$
299.4	$4.81\cdot10^{-9}$ (T; Ref. 12)	
300.2	$7.6\cdot10^{-11}$ (D; Ref. 2)	
301.7	$5.85\cdot10^{-9}$ (T; Ref. 12)	
301.9	$5.63\cdot10^{-9}$ (T; Refs. 8 and 10)	
302.2	$5.76\cdot10^{-9}$ (T; Ref. 9)	
302.4	$5.781\cdot10^{-9}$ (T; Ref. 10)	
304.5	$7.02\cdot10^{-9}$ (T; Ref. 12)	
308.6	$1.24\cdot10^{-8}$ (T; Ref. 15)	
312.5	$1.61\cdot10^{-8}$ (T; Ref. 15)	
317.9	$2.16\cdot10^{-8}$ (T; Ref. 15)	
320.7	$2.52\cdot10^{-8}$ (T; Ref. 15)	
323.2	$2.89\cdot10^{-8}$ (T; Ref. 15)	
323.3	$2.91\cdot10^{-8}$ (T; Ref. 15)	
327.9	$3.76\cdot10^{-8}$ (T; Ref. 15)	
332.4	$4.86\cdot10^{-8}$ (T; Ref. 15)	
337.7	$6.7E\cdot10^{-8}$ (T; Ref. 15)	
338.3	$6.9E\cdot10^{-8}$ (T; Ref. 15)	
343.0	$9.1E\cdot10^{-8}$ (T; Ref. 15)	
343.9	$9.6E\cdot10^{-8}$ (T; Ref. 15)	
345.1	$1.03\cdot10^{-7}$ (T; Ref. 15)	
347.9	$1.22\cdot10^{-7}$ (T; Ref. 15)	
348.2	$1.24\cdot10^{-7}$ (T; Ref. 15)	

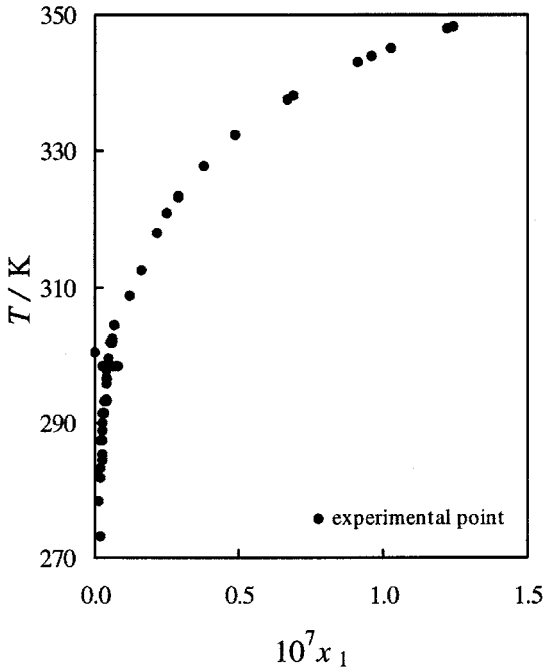

FIG. 2. All the solubility data for anthracene (1) in water (2).

Components: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (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 anthracene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(2.5 \pm 0.1) \cdot 10^{-7}$	$4.6 \cdot 10^{-6}$	$4.5 \cdot 10^{-9}$

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 $CHCl_3$, dehydrated, 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 average was taken as the solubility.

Source and Purity of Materials:

(1) Wako Pure and Nakarai Chemicals Co.; guaranteed sample; 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) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values
Solubility of anthracene in water

t/°C	$10^7 \cdot$ g (1)/L (2)
27	7.5±0.8
	7.2±0.5
	7.5±0.5

The best value recommended by the authors is $7.5 \cdot 10^{-7}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $7.5 \cdot 10^{-8}$ g (1)/100 g sln and $7.6 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Eastman Kodak Company; 450×; melting point range 215.6–216.5 °C; used as received; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).

Variables:
One temperature: 25.0 °C

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

Experimental Values
Solubility of anthracene in water

t/°C	g (1)/100 g sln (compilers)	x_1
25.0	$4.30 \cdot 10^{-6}$	$4.34 \cdot 10^{-9}$

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 for 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 two 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: 2.3% (reproducibility).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. Hashimoto, K. Tokura, K. Ozaki, and W. M. J. Strachan, Chemosphere **11**, 991 (1982).

Variables:
One temperature: 20.0 °C

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

Experimental Values
Solubility of anthracene in water

t/°C	mg (1)/L	g (1)/100 g sln (compilers)	x_1 (compilers)
20.0	0.033	$3.3 \cdot 10^{-6}$	$3.3 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
A microcolumn method,[1] containing glass beads coated with anthracene was used. The variation of water flow rate from 5 to 50 mL/h and recycling the solution through the column twice showed no significant differences in concentration. Samples were analyzed using a fluorophotometer (Model FP-550, Nippon Bunko Co.).

Source and Purity of Materials:
(1) Wako Janyaku Co.; melting point 216 °C; used as received.
(2) Tap water, passed through an ion-exchange column, doubly distilled.

Estimated Error:
Not stated.

References:
[1]OECD Guidelines for Testing of Chemicals, Section 1: Physicochemical-Properties 105 Water Solubility.

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Kishi and Y. Hashimoto, Chemosphere **18**, 1749 (1989).

Variables:
One temperature: 20.0 °C

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

Experimental Values
Solubility of anthracene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
20.0	0.041 ± 0.021	$4.16 \cdot 10^{-6}$	$4.20 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
The average of experimental results obtained at 17 laboratories in Japan by the procedures in the manuals collected by Environmental Agency, Japan,[1] are presented. The flask procedure was used in experiments. An excess of component (1) was coated on glass beads and added to 100 mL water, shaking for 48 h, equilibrated for 24 h, and filtered through a glass fiber filter and analyzed (domestic ring test). Details of mixtures preparation, equilibration, sampling, and analysis were described in the paper.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Solubility: as above.

References:
[1]*Measurement Method of Physical and Chemical Properties of Chemicals* (Japan Environment Association, Sangyo-tosho, 1987).

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of anthracene in water at 25 °C was reported to be $7.5 \cdot 10^{-5}$ g (1)/L sln and $4.47 \cdot 10^{-7}$ mol (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $7.5 \cdot 10^{-6}$ g (1)/100 g sln and $8.07 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (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 anthracene in water at 25 °C was reported to be 0.073 mg (1)/L sln and $x_1 = 7.57 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $7.3 \cdot 10^{-6}$ 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 allowed to settle 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) Anthracene; $C_{14}H_{10}$; [120-12-7]
(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: 278.35–302.45 K

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

Experimental Values

Solubility of anthracene in water

T/K	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$
278.35	1.270	1.284
282.85	1.619	1.637
283.15	1.750	1.769
287.25	2.221	2.245
289.75	2.510	2.537
291.45	2.910	2.941
295.55	3.720	3.760
296.35	3.780	3.821
297.75	4.340	4.387
301.85	5.570	5.630
302.45	5.719	5.781

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) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 and 997 (1978).

Variables:
Temperature: 5.2–29.0 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of anthracene in water

t/°C	$10^9 \cdot x_1$ (compiler)	$10^6 \cdot$ g (1)/100 g sln (compiler)	μg (1)/kg (2)
5.2	1.28	1.27	12.7±0.4
10.0	1.77	1.75	17.5±0.3
14.1	2.24	2.22	22.2±0.1
18.3	2.94	2.91	29.1±0.6
22.4	3.76	3.72	37.2±1.1
24.6	4.39	4.34	43.4±0.1
25.0	4.51	4.46	44.6±0.2
28.7	5.63	5.57	55.7±0.7
29.0	5.76	5.7	57.0±3.0

μg (1)/kg (2) = 8.21 + 0.8861 t + 0.0097 t^2 + 0.0013 t^3

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: standard deviation, see above.

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, J. Solution Chem. **29**, 369 (2000).

Variables:
One temperature: 25.00 °C
Pressure: 0.1–200 MPa

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

Experimental Values

Solubility of anthracene in water

t/°C	P/MPa	x_p/x_0	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$ (compilers)
25.00	0.1	1	6.1	6.2 (Ref. 2)
	50	0.72	4.5	4.5
	100	0.55	3.4	3.4
	100	0.53	3.3	3.3
	150	0.36	2.2	2.2
	150	0.38	2.4	2.4
	200	0.33	2.1	2.1
	200	0.30	1.9	1.9
	200	0.29	1.8	1.8

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from the relation of absorption of saturated solutions at high and normal pressures. A piston-and-cylinder type pressure vessel with a valve was used for a preparation of saturated solution.[1] Samples were shaken for over 50 h, kept in a water bath for 30 min, and filtered. Absorbance was measured with a Hitachi Model 340 spectrophotometer. Details of equilibration, sampling, and calculation were described in the paper. Pressure was monitored with a Bourdon-tube gauge and water bath temperature was regulated and monitored by a platinum-wire resistance thermometer. The concentration of (1) in the saturated solution was determined on the basis of spectrophotometric measurements and recommended solubility values at 25.00 °C and 0.1 MPa reported in Shaw.[2]

Source and Purity of Materials:
(1) Nakarai Tesque; recrystallized four times from methanol+water and sublimed.
(2) Distilled after de-ionization.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. Sawamura, M. Tsuchiya, T. Ishigami, Y, Taniguchi, and K. Suzuki, J. Solution Chem. **22**, 727 (1993).
[2]D. G. Shaw, ed., *IUPAC Solubility Data Series*, Vol. 38 (Pergamon, New York, 1989).

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 8.6–31.3 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of anthracene in water

t/°C	$10^9 \cdot x_1$ (compiler)	$10^6 \cdot$ g (1)/100 g sln (compiler)	$10^7 \cdot$ mol (1)/L
8.6	2.36	2.33	1.31±0.04
11.1	2.47	2.44	1.37±0.03
12.2	2.59	2.57	1.44±0.03
14.0	2.77	2.74	1.54±0.04
15.5	3.00	2.96	1.66±0.03
18.2	3.26	3.23	1.81±0.03
20.3	4.00	3.96	2.22±0.03
23.0	4.21	4.17	2.34±0.03
23.3	4.14	4.10	2.30±0.04
25.0	4.14	4.10	2.30±0.05
26.2	4.81	4.76	2.67±0.03
28.5	5.85	5.79	3.25±0.06
31.3	7.02	6.95	3.90±0.02

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 74 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 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) Anthracene; $C_{14}H_{10}$; [120-12-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).

Variables:
One temperature: 25.0 °C

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

Experimental Values

Solubility of anthracene in water

t/°C	μg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	30	$3.0 \cdot 10^{-6}$	$3.0 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was calculated from fluorescence measurements. A saturated solution was prepared by slowly stirring an excess of hydrocarbon in water for several days in a sealed flask. The sample was then diluted over 2 orders of magnitude by the addition of known volumes of water. Details of sample preparation, apparatus, and measurements were described in the paper.

Source and Purity of Materials:
(1) Source not specified; recrystallized from a solvent.
(2) Distilled and passed through a Sephadex column.

Estimated Error:
Not specified.

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(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 anthracene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	0.0698 ± 0.0075	$7.00 \cdot 10^{-6}$	$7.08 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as an auxiliary property to the adsorption measurements.
The mean value of four 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

Components:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7]
(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 anthracene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2) experiment	mg (1)/kg (2) smoothed with (standard deviation)
0.0	0.22	0.22	—	0.022 (0.001)
25.0	0.76	0.75	—	0.075 (0.002)
35.4	1.24	1.23	0.125, 0.122, 0.119	0.123
39.3	1.61	1.59	0.152, 0.151, 0.148	0.159
44.7	2.16	2.14	0.208, 0.210, 0.206	0.214
47.5	2.52	2.49	0.279	0.249
50.0	2.89	2.86	—	0.286 (0.003)
50.1	2.91	2.88	0.301, 0.297, 0.302	0.288
54.7	3.76	3.72	0.391, 0.389, 0.402	0.372
59.2	4.86	4.81	0.480, 0.488, 0.525	0.481
64.5	6.7	6.6	0.72, 0.62, 0.64	0.66
65.1	6.9	6.8	0.67, 0.64, 0.67	0.68
69.8	9.1	9.0	0.92	0.90
70.7	9.6	9.5	0.90, 0.97, 0.96	0.95
71.9	10.3	10.2	0.91	1.02
74.7	12.2	12.1	1.19, 1.13, 1.26	1.21
75.0	12.4	12.3	—	1.23 (0.02)

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.

2.9. Phenanthrene+Water

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Phenanthrene (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
Andrews and Keefer[1]	298	May *et al.*[8]	277–303
Davis *et al.*[2]	300	Sawamura[9]	298
Eganhouse and Calder[3]	298	Schwarz[10]	298
Klevens[4]	298	Vesala[11]	298
Mackay and Shiu[5]	298	Walters and Luthy[12]	298
May *et al.*[6]	282–303	Wauchope and Getzen[13]	273–348
May *et al.*[7]	298		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic system. All the experimental data are listed in Table 3 and shown in Fig. 3. At 298 K the data of Andrews and Keefer,[1] Eganhouse and Calder,[3] Mackay and Shiu,[5] Schwarz,[10] Vesala,[11] Walters and Luthy,[12] and Wauchope and Getzen[13] are in good agreement and are Recommended. From these data the mean value was calculated as shown in Fig. 3. The data of Klevens[4] seem to be high and Doubtful. The data of May *et al.*[7] at 298 and 302 K seem to be low and Doubtful. At 303 K the data of May *et al.*[6,8] and Wauchope and Getzen[13] are in good agreement and are Recommended. All the remaining data over the temperature range 273–348 K are consistent with the mean value at 298 K and are Tentative.

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

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[9] at 298 K and 0.1–200 MPa have not been critically evaluated because only a single data set is available.

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[3]R. P. Eganhouse and J. A. Calder, Geochim. Cosmochim. Acta **40**, 555 (1976).
[4]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[5]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[6]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[7]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
[8]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).
[9]S. Sawamura, J. Solution Chem. **29**, 369 (2000).
[10]F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
[11]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[12]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[13]R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

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

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
273.2	$3.90\cdot10^{-8}$ (T; Ref. 13)	
277.2	$3.649\cdot10^{-8}$ (T; Ref. 8)	
281.6	$5.060\cdot10^{-8}$ (T; Ref. 10)	
281.7	$4.270\cdot10^{-8}$ (T; Ref. 6)	
281.7	$4.275\cdot10^{-8}$ (T; Ref. 8)	
283.2	$4.730\cdot10^{-8}$ (T; Ref. 6), $4.730\cdot10^{-8}$ (T; Ref. 8)	
284.3	$5.570\cdot10^{-8}$ (T; Ref. 10)	
285.7	$5.170\cdot10^{-8}$ (T; Ref. 6), $5.175\cdot10^{-8}$ (T; Ref. 8)	
287.2	$6.470\cdot10^{-8}$ (T; Ref. 10)	
288.2	$6.070\cdot10^{-8}$ (T; Ref. 6), $6.075\cdot10^{-8}$ (T; Ref. 8)	
290.7	$7.920\cdot10^{-8}$ (T; Ref. 10)	
293.2	$7.955\cdot10^{-8}$ (T; Ref. 8)	
293.4	$8.900\cdot10^{-8}$ (T; Ref. 10)	
294.2	$8.250\cdot10^{-8}$ (T; Ref. 6), $8.248\cdot10^{-8}$ (T; Ref. 8)	
296.5	$1.097\cdot10^{-7}$ (T; Ref. 10)	
297.5	$1.006\cdot10^{-7}$ (T; Ref. 6), $9.653\cdot10^{-8}$ (T; Ref. 8)	
297.8	$1.17\cdot10^{-7}$ (T; Ref. 13)	
298.2	$1.004\cdot10^{-7}$ (R; Ref. 1), $1.08\cdot10^{-7}$ (R; Ref. 3), $1.6\cdot10^{-7}$ (D; Ref. 4), $1.3\cdot10^{-7}$ (R; Ref. 5), $1.013\cdot10^{-8}$ (D; Ref. 7), $1.163\cdot10^{-7}$ (R; Ref. 10), $1.22\cdot10^{-7}$ (R; Ref. 11), $1.31\cdot10^{-7}$ (R; Ref. 12), $1.19\cdot10^{-7}$ (R; Ref. 13)	$1.2\cdot10^{-7}$
300.2	$1.62\cdot10^{-7}$ (D; Ref. 2)	
302.2	$1.233\cdot10^{-8}$ (D; Ref. 7)	
302.5	$1.387\cdot10^{-7}$ (T; Ref. 10)	
303.1	$1.291\cdot10^{-7}$ (R; Ref. 6), $1.240\cdot10^{-7}$ (R; Ref. 8), $1.51\cdot10^{-7}$ (R; Ref. 13)	
303.5	$1.54\cdot10^{-7}$ (T; Ref. 13)	
305.0	$1.644\cdot10^{-7}$ (T; Ref. 10)	
311.6	$2.29\cdot10^{-7}$ (T; Ref. 13)	
313.3	$2.50\cdot10^{-7}$ (T; Ref. 13)	
320.7	$3.67\cdot10^{-7}$ (T; Ref. 13)	
323.2	$4.18\cdot10^{-7}$ (T; Ref. 13)	
323.3	$4.20\cdot10^{-7}$ (T; Ref. 13)	
323.4	$4.23\cdot10^{-7}$ (T; Ref. 13)	
327.9	$5.40\cdot10^{-7}$ (T; Ref. 13)	
332.4	$6.92\cdot10^{-7}$ (T; Ref. 13)	
333.7	$7.50\cdot10^{-7}$ (T; Ref. 13)	
338.3	$9.70\cdot10^{-7}$ (T; Ref. 13)	
343.9	$1.34\cdot10^{-6}$ (T; Ref. 13)	
345.1	$1.44\cdot10^{-6}$ (T; Ref. 13)	
346.6	$1.58\cdot10^{-6}$ (T; Ref. 13)	
348.2	$1.74\cdot10^{-6}$ (T; Ref. 13)	

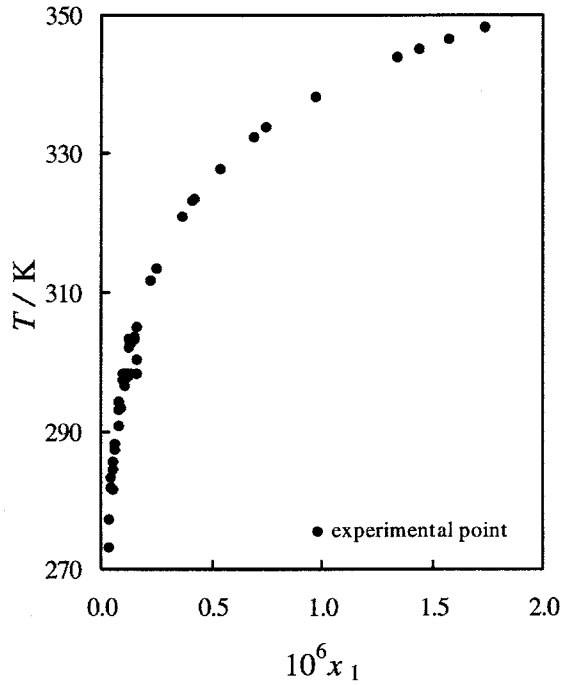

FIG. 3. All the solubility data for phenanthrene (1) in water (2).

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Values

The solubility of phenanthrene in water at 25 °C was reported to be $9.94 \cdot 10^{-5}$ g (1)/100 g sln.

The corresponding mole fraction (x_1), calculated by compiler, is $1.004 \cdot 10^{-7}$.

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; recrystallized twice from ethanol; melting point 101.0 °C.
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of phenanthrene in water

t/°C	$10^3 \cdot$ g (1)/L (2)
27	1.55
	1.62
	1.65

The best value recommended by the authors is $1.60 \cdot 10^{-3}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.60 \cdot 10^{-4}$ g (1)/100 g sln and $1.62 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Eastman Kodak Company; 599; melting point range 100.0– 100.9 °C; used as received; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: $\pm 5 \cdot 10^{-5}$ g (1)/L (2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	Original Measurements:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (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 phenanthrene in water at 25 °C was reported to be 1.07 mg (1)/kg (2) and $6 \cdot 10^{-6}$ mol (1)/L (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.07 \cdot 10^{-4}$ g (1)/100 g sln and $1.08 \cdot 10^{-7}$, 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 Hewlett-Packard instrument (model 5700 A) 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) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of phenanthene in water at 25 °C was reported to be $1.6 \cdot 10^{-8}$ g (1)/L sln and $9.0 \cdot 10^{-6}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.6 \cdot 10^{-4}$ g (1)/100 g sln and $1.62 \cdot 10^{-7}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(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 phenanthrene in water at 25 °C was reported to be 1.29 mg (1)/L sln and $x_1 = 1.3 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $1.29 \cdot 10^{-4}$ 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 allowed to settle 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: ±0.07 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 and 997 (1978).

Variables:
Temperature: 8.5–29.9 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of phenanthrene in water

t/°C	$10^7 \cdot x_1$ (compiler)	$10^4 \cdot$ g (1)/100 g sln (compiler)	μg (1)/kg (2)
8.5	0.427	0.423	423±4
10.0	0.473	0.468	468±2
12.5	0.517	0.512	512±1
15.0	0.607	0.601	601±7
21.0	0.825	0.816	816±8
24.3	1.006	0.995	995±1
25.0	1.013	1.002	1002±11
29.0	1.233	1.220	1220±13
29.9	1.291	1.277	1277±11

μg (1)/kg (2) = $324.0 + 5.413\,t + 0.8059\,t^2 + 0.0025\,t^3$

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: standard deviation see above.

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(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 phenanthrene in water at 25 °C was reported to be 1.29 mg (1)/L sln and $x_1 = 1.3 \cdot 10^{-7}$.

The corresponding mass percent calculated by the compiler is $1.29 \cdot 10^{-4}$ 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 allowed to settle 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: ±0.07 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, J. Solution Chem. **29**, 369 (2000).

Variables:
One temperature: 25.00 °C
Pressure: 0.1–200 MPa

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

Experimental Values

Solubility of phenanthrene in water

t/°C	P/MPa	x_p/x_0	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$ (compilers)
25.00	0.1	1	1.1	1.1 (Ref. 2)
	50	0.800	0.87	0.88
	100	0.618	0.67	0.68
	150	0.468	0.51	0.51
	200	0.367	0.40	0.40

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from the relation of absorption of saturated solutions at high and normal pressures. A piston-and-cylinder type pressure vessel with a valve was used for a preparation of saturated solution.[1] Samples were shaken for over 50 h, kept in a water bath for 30 min, and filtered. Absorbance was measured with a Hitachi Model 340 spectrophotometer. Details of equilibration, sampling, and calculation were described in the paper. Pressure was monitored with a Bourdon-tube gauge and water bath temperature was regulated and monitored by a platinum-wire resistance thermometer. The concentration of (1) in the saturated solution was determined on the basis of spectrophotometric measurements and recommended solubility values at 25.00 °C and 0.1 MPa reported in Shaw.[2]

Source and Purity of Materials:
(1) Nakarai Tesque; recrystallized four times from methanol+water and sublimed.
(2) Distilled after de-ionization.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. Sawamura, M. Tsuchiya, T. Ishigami, Y, Taniguchi, and K. Suzuki, J. Solution Chem. **22**, 727 (1993).
[2]D. G. Shaw, ed., *IUPAC Solubility Data Series*, Vol. 38 (Pergamon, New York, 1989).

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 8.4–31.8 °C

Prepared By:
A. Maczynski

Experimental Values
Solubility of phenanthrene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	$10^6 \cdot$ mol (1)/L
8.4	5.06	5.01	2.81±0.07
11.1	5.57	5.51	3.09±0.07
14.0	6.47	6.40	3.59±0.06
17.5	7.92	7.84	4.40±0.04
20.2	8.90	8.80	4.94±0.09
23.3	10.97	10.85	6.09±0.07
25.0	11.63	11.51	6.46±0.02
29.3	13.87	13.72	7.7±0.2
31.8	16.44	16.27	9.13±0.08

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 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) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(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 phenanthrene in water

T/K	mol (1)/g (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(6.77\pm0.08)\cdot10^{-9}$	$1.21\cdot10^{-6}$	$1.22\cdot10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibration was carried out in a modified vessel,[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) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(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 phenanthrene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	1.29±0.14	$1.29 \cdot 10^{-4}$	$1.31 \cdot 10^{-7}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as an auxiliary property to the adsorption measurements.
The mean value of four 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

Components:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]
(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 phenanthrene 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	0.39	0.39	—	0.39 (0.01)
24.6	1.17	1.16	1.12, 1.11	1.16
25.0	1.19	1.18	—	1.18 (0.02)
29.9	1.51	1.49	1.49, 1.49	1.49
30.3	1.54	1.52	1.47, 1.48	1.52
38.4	2.29	2.27	2.44, 2.45	2.27
48.1	2.50	2.47	2.27, 2.28, 2.25	2.47
47.5	3.67	3.63	3.81, 3.88, 3.87	3.63
50.0	4.18	4.14	—	4.14 (0.04)
50.1	4.20	4.16	4.30, 4.38, 4.32	4.16
50.2	4.23	4.19	4.08, 4.04, 411	4.19
54.7	5.40	5.34	5.66, 5.64, 5.63	5.34
59.2	6.92	6.85	7.17, 7.19, 7.21	6.85
60.5	7.5	7.4	7.2, 7.2, 7.6	7.4
65.1	9.7	9.6	9.8, 9.7, 9.8	9.6
70.7	13.4	13.3	12.4, 12.6, 12.4	13.3
71.9	14.4	14.2	12.9	14.2
73.4	15.8	15.6	18.2	15.6
75.0	17.4	17.2	—	17.2 (0.3)

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.

2.10. *trans*-Stilbene+Water

Components:
(1) *trans*-Stilbene; $C_{14}H_{12}$; [103-30-0]
(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 of *trans*-stilbene in water at 25 °C was reported to be $2.9 \cdot 10^{-5}$ g (1)/100 g sln.
The corresponding mole fraction (x_1), calculated by the compilers, is $2 \cdot 10^{-8}$.

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) From the State University of Iowa; melting point 120–121 °C.
(2) Not specified.

Estimated Error:
Not specified.

2.11. 4,4′-Dimethyl-1,1′-biphenyl+Water

Components:
(1) 4,4′-Dimethyl-1,1′-biphenyl; $C_{14}H_{14}$; [613-33-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. J. Doucette and A. W. Andren, Chemosphere **17**, 243 (1988).

Variables:
Temperature: 4.0–40.0 °C

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

Experimental Values

Solubility of 4,4′-dimethyl-1,1′-biphenyl in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
4.0	$(3.77 \pm 0.23) \cdot 10^{-7}$	$6.87 \cdot 10^{-6}$	$6.79 \cdot 10^{-9}$
25.0	$(9.59 \pm 0.42) \cdot 10^{-7}$	$1.75 \cdot 10^{-5}$	$1.73 \cdot 10^{-8}$
40.0	$(2.42 \pm 0.12) \cdot 10^{-6}$	$4.45 \cdot 10^{-5}$	$4.39 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:
The generator column described in Stolzenberg and Andren[1] was used. Details of the apparatus and procedures were described in the paper. Water was pumped through the generator at a flow rate 1–2 mL/min and the effluent flowed through a Sep-Pak into a tarred flask. Water was removed by a stream of nitrogen, the solute was eluted in isooctane, and analyzed by a Hewlett-Packard (5730A) glc equipped with a ^{63}Ni electron-capture detector. Five or six replicate determinations were made at each temperature.

Source and Purity of Materials:
(1) Ultra Scientific (Hope, RI); purity 99%; used as received.
(2) Milli Q water irradiated with UV light.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: as above (standard deviation).

References:
[1]T. Stolzenberg and A. W. Andren, Anal. Chim. Acta **151**, 271 (1983).

2.12. 1,4-Dicyclopentylbutane+Water

Components:	**Original Measurements:**
(1) 1,4-Dicyclopentylbutane; $C_{14}H_{26}$; [2980-70-3] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10–30 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 1,4-dicyclopentylbutane

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	0.94	0.0088
20	1.50	0.0139
30	2.59	0.0241

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.

2.13. Tetradecane+Water

Components:	**Evaluators:**
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, March, 2004.

Critical Evaluation of the Solubility of Tetradecane (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
Franks[1]	298	Sutton and Calder[4]	298
Mackay and Shiu[2]	not specified		

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 4. The data of Franks[1] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful. The data of Sutton and Calder[4] 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 Tetradecane (1)

The experimental solubility data for (2) in (1) have been investigated by Schatzberg[3] at 313 K only. Therefore the data were not critically evaluated.

Rejected and Inaccessible Data

The data of Mackay and Shiu[2] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

[1]F. Franks, Nature (London) **210**, 87 (1966).
[2]D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).
[3]P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
[4]C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

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

T/K	Experimental values x_1 (T=tentative; D=doubtful)	Reference values $x_1 \pm 30\%$
298	$6.3 \cdot 10^{-10}$ (D; Ref. 1), $2.1 \cdot 10^{-10}$ (T; Ref. 4)	$2.4 \cdot 10^{-10}$

Components:	Original Measurements:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	F. Franks, Nature (London) **210**, 87 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Values

The solubility of tetradecane in water at 25 °C was reported to be in mole fraction $x_1 = 6.3 \cdot 10^{-10}$.

The corresponding mass percent calculated by the compiler is $6.94 \cdot 10^{-7}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
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.	(1) Fluka; purum grade; purity >97% (chromatographic analysis). (2) Not specified. **Estimated Error:** Solubility: ±12%.

Components:	Original Measurements:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).
Variables:	**Prepared By:**
Not specified	M. C. Haulait-Pirson

Experimental Values

The authors reported a value of 0.0259 mg (1)/L sln for the solubility of tetradecane in water.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent, calculated by the compiler, is $2.59 \cdot 10^{-6}$ g (1)/100 g sln and the corresponding mole fraction (x_1) is $2.4 \cdot 10^{-9}$.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.	(1) Not specified. (2) Not specified. **Estimated Error:** Not estimated.

Components:	Original Measurements:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
Variables:	**Prepared By:**
One temperature: 40 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of water in tetradecane at 40 °C was reported to be 114 mg (2)/kg sln corresponding to a mole fraction (x_2) of $1.26 \cdot 10^{-5}$.

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.; pure grade; 99+ mole %; passed repeatedly though 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: 0%–2% (deviations from the mean).

Components:	Original Measurements:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (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 tetradecane in water at 25 °C was reported to be $2.2 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction (x_1) of $2 \cdot 10^{-10}$.

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 through 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%.

2.14. 2-Methylanthracene+Water

Components:
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of 2-Methylanthracene (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
Mackay and Shiu[1]	298	May *et al.*[3]	279–304
May *et al.*[2]	279–304		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the data are listed in Table 5 and shown in Fig. 4. The data of Mackay and Shiu[1] at 298 K are in poor agreement with the data of May *et al.*[2,3] at 279–304 K. All data are considered Doubtful.

References:

[1]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 and 997 (1978).
[3]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).

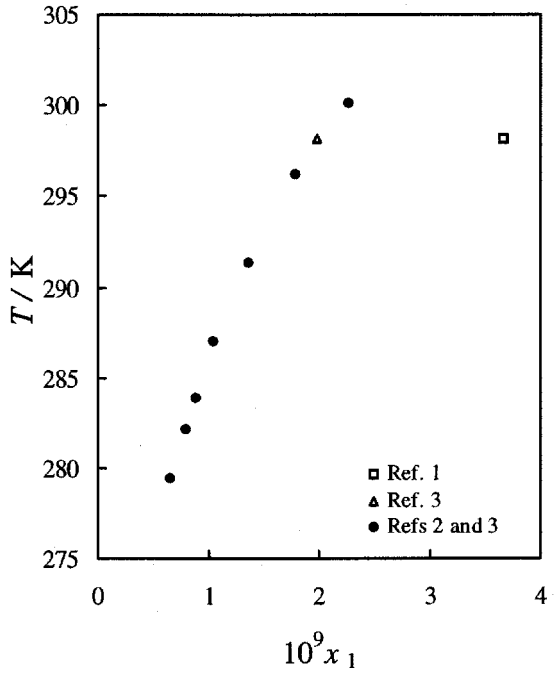

FIG. 4. All the solubility data for 2-methylanthracene (1) in water (2).

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

T/K	Experimental values x_1
279.4	$6.61 \cdot 10^{-10}$ (Refs. 2 and 3)
282.2	$7.95 \cdot 10^{-10}$ (Refs. 2 and 3)
283.9	$8.84 \cdot 10^{-10}$ (Refs. 2 and 3)
287.0	$1.04 \cdot 10^{-9}$ (Refs. 2 and 3)
291.4	$1.36 \cdot 10^{-9}$ (Refs. 2 and 3)
296.2	$1.79 \cdot 10^{-9}$ (Refs. 2 and 3)
298.2	$3.67 \cdot 10^{-9}$ (Ref. 1), $1.99 \cdot 10^{-9}$ (Refs. 2 and 3)
300.1	$2.27 \cdot 10^{-9}$ (Refs. 2 and 3)
304.2	$3.01 \cdot 10^{-9}$ (Refs. 2 and 3)

Components:	**Original Measurements:**
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7] (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 2-methylanthracene in water at 25 °C was reported to be 0.039 mg (1)/L sln and $x_1 = 3.67 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $3.9 \cdot 10^{-6}$ 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 allowed to settle 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: ±0.004 mg (1)/L sln (maximum deviation from several determinations).

Components:	**Original Measurements:**
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7] (2) Water; H_2O; [7732-18-5]	W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 and 997 (1978).
Variables:	**Prepared By:**
Temperature: 6.3–31.1 °C	A. Maczynski

Experimental Values

Solubility of 2-methylanthracene in water

t/°C	$10^9 \cdot x_1$ (compiler)	$10^6 \cdot$ g (1)/100 g sln (compiler)	μg (1)/kg (2)
6.3	0.661	0.706	7.06±0.18
9.1	0.794	0.848	8.48±0.09
10.8	0.883	0.943	9.43±0.37
13.9	1.04	1.11	11.1±0.3
18.3	1.36	1.45	14.5±0.1
23.1	1.79	1.91	19.1±0.6
25.0	1.99	2.13	21.3±0.3
27.0	2.27	2.42	24.2±0.1
31.1	3.01	3.21	32.1±0.3

μg (1)/kg (2) = $2.78 + 0.8180\,t + 0.0306\,t^2 + 0.0011\,t^3$

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:

Temperature: ±0.05 °C.
Solubility: standard deviation, see above.

References:

[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]
(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: 279.45–304.25 K

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

Experimental Values

Solubility of 2-methylanthracene in water

T/K	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$
279.45	0.7059	0.6615
282.25	0.8480	0.7946
283.95	0.9429	0.8836
287.05	1.110	1.040
291.45	1.450	1.359
296.25	1.910	1.790
300.15	2.420	2.268
304.25	3.210	3.008

The same data were reported in May *et al.*[1]

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).

2.15. 9-Methylanthracene+Water

Components:
(1) 9-Methylanthracene; $C_{15}H_{12}$; [779-02-2]
(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 9-methylanthracene in water at 25 °C was reported to be 0.261 mg (1)/L sln and $x_1 = 2.44 \cdot 10^{-8}$.
The corresponding mass percent calculated by the compiler is $2.61 \cdot 10^{-5}$ 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 allowed to settle 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: ±0.002 mg (1)/L sln (maximum deviation from several determinations).

2.16. 1-Methylphenanthrene+Water

Components:
(1) 1-Methylphenanthrene; $C_{15}H_{12}$; [832-69-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 and 997 (1978).

Variables:
Temperature: 6.6–29.9 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of 1-methylphenanthrene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	μg (1)/kg (2)
6.6	0.892	0.952	95.2±0.2
8.9	1.07	1.14	114.0±4.0
14.0	1.38	1.47	147.0±1.0
19.2	1.81	1.93	193.0±1.0
24.1	2.39	2.55	255.0±5.0
25.0	2.69	2.69	269.0±3.0
26.9	2.85	3.04	304.0±1.0
29.9	3.32	3.55	355.0±2.0

$\mu g\ (1)/kg\ (2) = 55.42 + 6.8016\ t + 0.1301\ t^2 + 0.0080\ t^3$

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generarting saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chomatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: standard deviation, see above.

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) 1-Methylphenanthrene; $C_{15}H_{12}$; [832-69-9]
(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: 279.75–303.05 K

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

Experimental Values

Solubility of 1-methylphenanthrene in water

T/K	$10^5 \cdot$ g (1)/100 g sln (compilers)	$10^8 \cdot x_1$
279.75	0.9520	0.8921
282.05	1.140	1.068
287.15	1.469	1.377
292.35	1.929	1.808
297.25	2.549	2.389
300.05	3.040	2.849
303.05	3.549	3.326

The same data were reported in May *et al.*[1]

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).

2.17. Fluoranthene+Water

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Fluoranthene (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
Akiyoshi *et al.*[1]	298	Mackay and Shiu[6]	298
Davis *et al.*[2]	300	May *et al.*[7]	298 and 302
Hashimoto *et al.*[3]	293	May *et al.*[8]	281–303
Kishi and Hashimoto[4]	288–298	Schwarz and Wasik[9]	298
Klevens[5]	298	Walters and Luthy[10]	298

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 6 and shown in Fig. 5. At 293 K the data of Hashimoto *et al.*,[3] Kishi and Hashimoto,[4] and May *et al.*[8] are in good agreement and are Recommended. From these data the mean value was calculated. As shown in Fig. 5, the data of Akiyoshi *et al.*[1] at 298 K, the higher values of Kishi and Hashimoto[4] at 288 and 298 K, Klevens,[5] and Mackay and Shiu[6] at 298 K seem to be high and Doubtful. At 298 K the data of Kishi and Hashimoto,[4] May *et al.*,[7,8] Schwartz and Wasik,[9] and Walters and Luthy[10] are in good agreement and are Recommended. From these data, the mean value was calculated. All the remaining data over the temperature range 281–303 K are consistent with the mean values at 293 and 298 K and are Tentative.

Refernces:

[1]M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn. **60**, 3935 (1987).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[3]Y. Hashimoto, K. Tokura, K. Ozaki, and W. M. J. Strachan, Chemosphere **11**, 991 (1982).
[4]H. Kishi and Y. Hashimoto, Chemosphere **18**, 1749 (1989).
[5]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[6]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[7]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
[8]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).
[9]F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).
[10]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

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

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
281	$7.3\cdot10^{-7}$ (T; Ref. 8)	
286	$9.5\cdot10^{-7}$ (T; Ref. 8)	
288	$1.2\cdot10^{-8}$ (T; Ref. 4), $2.5\cdot10^{-8}$ (D; Ref. 4)	
293	$1.7\cdot10^{-8}$ (R; Ref. 3), $1.5\cdot10^{-8}$ (R; Ref. 4), $1.3\cdot10^{-8}$ (R; Ref. 8)	$1.5\cdot10^{-8}$
298	$2.5\cdot10^{-8}$ (D; Ref. 1), $2.0\cdot10^{-8}$ (R; Ref. 4), $3.3\cdot10^{-8}$ (D; Ref. 4), $2.4\cdot10^{-8}$ (D; Ref. 5), $2.3\cdot10^{-8}$ (D; Ref. 6), $1.8\cdot10^{-8}$ (R; Ref. 7), $1.8\cdot10^{-8}$ (R; Ref. 8), $2.1\cdot10^{-8}$ (R; Ref. 9), $1.78\cdot10^{-8}$ (R; Ref. 10)	$1.9\cdot10^{-8}$
300	$2.15\cdot10^{-8}$ (T; Ref. 2)	
302	$2.4\cdot10^{-8}$ (T; Ref. 7)	
303	$2.5\cdot10^{-8}$ (T; Ref. 8)	

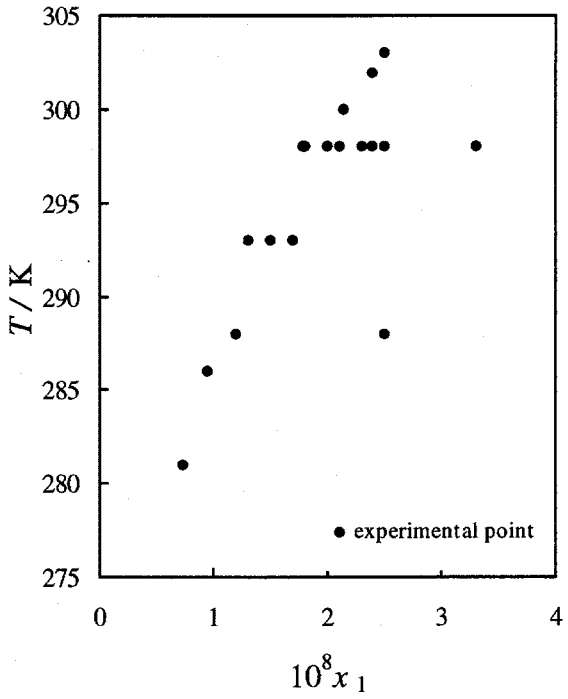

FIG. 5. All the solubility data for fluoranthene (1) in water (2).

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(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 fluoranthene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(1.4 \pm 0.1) \cdot 10^{-6}$	$2.8 \cdot 10^{-5}$	$2.5 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Aqueous solutions saturated with vapor of (1) were prepared in the apparatus described in Sanmasa *et al.*[1] Samples were extracted with $CHCl_3$, dehydrated, 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 an 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) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of fluoranthene in water

t/°C	$10^4 \cdot$ g (1)/L (2)
27	2.40±0.20
	2.25±0.20
	2.40±0.20

The best value recommended by the authors is $2.40 \cdot 10^{-4}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.40 \cdot 10^{-5}$ g (1)/100 g sln and $2.15 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 110.0–110.7 °C; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Kishi and Y. Hashimoto, Chemosphere **18**, 1749 (1989).

Variables:
Temperature: 15.0–25.0 °C

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

Experimental Values

Solubility of fluoranthene in water

t/°C	mg (1)/L sln	$10^5 \cdot$ g (1)/100 g sln (compilers)	$10^8 \cdot x_1$ (compilers)
15.0[b]	0.133 ± 0.027	1.34	1.19
15.0[c]	0.275	2.75	2.45
20.0[a]	0.166 ± 0.034	1.66	1.48
25.0[b]	0.222 ± 0.031	2.22	1.98
25.0[c]	0.373	3.74	3.33

Auxiliary Information

Method/Apparatus/Procedure:
The average of experimental results obtained at laboratories in Japan (up to 17 laboratories) by the procedures in the manuals collected by Environmental Agency, Japan. Three procedures were used:
(a) Flask method; an excess of component (1) was coated on glass beads and added to 100 mL water, shaken for 48 h, equilibrated for 24 h, and filtrated through a glass fiber filter and analyzed; domestic ring test;
(b) Column elution method; glass beads coated with component (1) were added to the glass column, then water at a flow rate 20–30 mL/h was passed; the effluent was collected and analyzed (Japanese values of OECD ring test);
(c) Column elution method; as above; (values of OECD ring test[1]).
Details of mixtures preparation, equilibration, sampling, and analysis were described in the paper.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Temperature: ± 0.5 K (column elution method).
Solubility: as above.

References:
[1] *OECD Guidelines for Testing of Chemicals*, Section 1, Physical-Chemical Properties, 105, Water Solubillity (OECD, 1981).

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. Hashimoto, K. Tokura, K. Ozaki, and W. M. J. Strachan, Chemosphere **11**, 991 (1982).

Variables:
One temperature: 20.0 °C

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

Experimental Values

Solubility of fluoranthene in water

t/°C	mg (1)/L	g (1)/100 g sln (compilers)	x_1 (compilers)
20.0	0.19	$1.9 \cdot 10^{-5}$	$1.7 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:
A microcolumn,[1] containing glass beads coated with fluoranthene was used. Variation of water flow rate from 5 to 50 mL/h and recycling the solution through the column twice showed no significant differences in concentration. Samples were analyzed using a fluorophotometer (Model FP-550, Nippon Bunko Co.).

Source and Purity of Materials:
(1) Wako Janyaku Co.; melting point 110.3 °C; used as received.
(2) Tap water, passed through an ion-exchange column, doubly distilled.

Estimated Error:
Not stated.

References:
[1] *OECD Guidelines for Testing of Chemicals*, Section 1: Physicochemical-Properties, 105, Water Solubility (OECD, 1981).

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of fluoranthene in water at 25 °C was reported to be $2.65 \cdot 10^{-4}$ g (1)/L sln and $1.32 \cdot 10^{-6}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.65 \cdot 10^{-5}$ g (1)/100 g sln and $2.37 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.	(1) Not specified. (2) Not specified. **Estimated Error:** Not specified.

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (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 fluoranthene in water at 25 °C was reported to be 0.26 mg (1)/L sln and $x_1 = 2.28 \cdot 10^{-8}$.

The corresponding mass percent calculated by the compiler is $2.6 \cdot 10^{-5}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently allowed to settle 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.	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) Doubly distilled. **Estimated Error:** Solubility: ±0.002 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
Temperature: 25 and 29 °C

Prepared By:
A. Maczynski

Experimental Values
Solubility of fluoranthene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2)
25	1.83	2.06	0.206
29	2.35	2.64	0.264

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled-column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.002 mg (1)/100 kg (2) (standard deviation).

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(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: 281.25–303.05 K

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

Experimental Values
Solubility of fluoranthene in water

T/K	10^5 g (1)/100 g sln (compilers)	$10^8 \cdot x_1$
281.25	0.8200	0.7304
286.35	1.0700	0.9531
292.85	1.483	1.321
297.75	2.026	1.805
303.05	2.793	2.488

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:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of fluoranthene in water

t/°C	μg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	236	$2.37 \cdot 10^{-5}$	$2.11 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was calculated from fluorescence measurements. A saturated solution was prepared by slowly stirring an excess of hydrocarbon in water for several days in a sealed flask. The sample was then diluted over 2 orders of magnitude by the addition of known volumes of water. Details of sample preparation, apparatus, and measurements were described in the paper.

Source and Purity of Materials:

(1) Source not specified; recrystallized from a solvent.
(2) Distilled and passed through a Sephadex column.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Water; H_2O; [7732-18-5]	R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of fluoranthene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	0.199 ± 0.011	$2.00 \cdot 10^{-5}$	$1.78 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:

The method and procedure were not described. Solubility was treated as an auxiliary property in the adsorption measurements.
The mean value of four 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:

See above.

2.18. Pyrene+Water

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Pyrene (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
Davis *et al.*[1]	300	Rossi and Thomas[6]	298
Klevens[2]	298	Schwarz[7]	285–304
Mackay and Shiu[3]	298	Schwarz and Wasik[8]	298
May *et al.*[4]	293 and 302	Walters and Luthy[9]	298
May *et al.*[5]	278–303	Wauchope and Getzen[10]	273–348

Calculation of reference data for this sytem was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 7 and shown in Fig. 6. At 298 K the data of Klevens,[2] Mackay and Shiu,[3] May *et al.*,[4] Schwarz,[7] Walters and Luthy,[9] and Wauchope and Getzen[10] are in good agreement and are Recommended. All these data were used for calculation of the mean value. At 298 K the data of Rossi and Thomas[6] seem to be low and are Doubtful and the data of Schwarz and Wasik[8] seem to be high and are Doubtful. As shown in Fig. 6, all the remaining data over the temperature range 273–348 K are consistent with the mean value and are Tentative.

References:

[1]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[3]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[4]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[5]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).
[6]S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
[7]F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
[8]F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).
[9]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).
[10]R. D. Wauchope and F. W. Getzen, J. Chem. Eng. Data **17**, 38 (1972).

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

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
273.2	$4.40\cdot10^{-9}$ (T; Ref. 10)	
277.9	$4.382\cdot10^{-9}$ (T; Ref. 5)	
282.7	$5.211\cdot10^{-9}$ (T; Ref. 5)	
285.4	$4.86\cdot10^{-9}$ (T; Ref. 7)	
287.5	$6.413\cdot10^{-9}$ (T; Ref. 5)	
288.2	$6.11\cdot10^{-9}$ (T; Ref. 7)	
290.6	$7.04\cdot10^{-9}$ (T; Ref. 7)	
291.9	$8.31\cdot10^{-9}$ (T; Ref. 5)	
293.5	$8.23\cdot10^{-9}$ (T; Ref. 7)	
294.4	$9.709\cdot10^{-9}$ (T; Ref. 5)	
295.4	$1.15\cdot10^{-8}$ (T; Ref. 10)	
296.2	$1.04\cdot10^{-8}$ (T; Ref. 7)	
296.5	$1.05\cdot10^{-8}$ (T; Ref. 7)	
298.2	$1.39\cdot10^{-8}$ (R; Ref. 2), $1.2\cdot10^{-8}$ (R; Ref. 3), $1.18\cdot10^{-8}$ (R; Ref. 4), $6.4\cdot10^{-10}$ (D; Ref. 6), $1.15\cdot10^{-8}$ (R; Ref. 7), $1.53\cdot10^{-8}$ (D; Ref. 8), $1.19\cdot10^{-8}$ (R; Ref. 9), $1.32\cdot10^{-8}$ (R; Ref. 10)	$1.24\cdot10^{-8}$
298.7	$1.211\cdot10^{-8}$ (T; Ref. 5)	
299.4	$1.28\cdot10^{-8}$ (T; Ref. 7)	
299.9	$1.29\cdot10^{-8}$ (T; Ref. 7)	
300.2	$1.45\cdot10^{-8}$ (T; Ref. 1)	
301.7	$1.49\cdot10^{-8}$ (T; Ref. 7)	
302.2	$1.44\cdot10^{-8}$ (T; Ref. 4)	
303.1	$1.514\cdot10^{-8}$ (T; Ref. 5)	
304.5	$1.67\cdot10^{-8}$ (T; Ref. 7)	
307.7	$2.09\cdot10^{-8}$ (T; Ref. 10)	
317.9	$3.55\cdot10^{-8}$ (T; Ref. 10)	
323.2	$4.74\cdot10^{-8}$ (T; Ref. 10)	
323.3	$4.75\cdot10^{-8}$ (T; Ref. 10)	
328.8	$6.50\cdot10^{-8}$ (T; Ref. 10)	
329.2	$6.60\cdot10^{-8}$ (T; Ref. 10)	
333.9	$8.60\cdot10^{-8}$ (T; Ref. 10)	
338.4	$1.13\cdot10^{-7}$ (T; Ref. 10)	
345.1	$1.69\cdot10^{-7}$ (T; Ref. 10)	
347.9	$2.01\cdot10^{-7}$ (T; Ref. 10)	
348.2	$2.06\cdot10^{-7}$ (T; Ref. 10)	

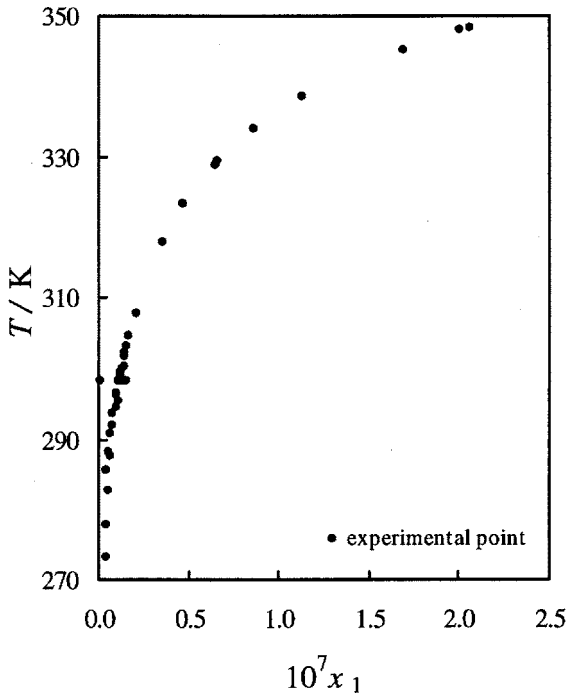

FIG. 6. All the solubility data for pyrene (1) in water (2).

Components:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of pyrene in water

t/°C	$10^4 \cdot$ g (1)/L (2)
27	1.60 ± 0.10
	1.65 ± 0.05

The best value recommended by the authors is $1.65 \cdot 10^{-4}$ g (1)/L (2).

Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.65 \cdot 10^{-5}$ g (1)/100 g sln and $1.45 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 149.6–150.5 °C; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ± 3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of pyrene in water at 25 °C was reported to be $1.75 \cdot 10^{-4}$ g (1)/L sln and $7.7 \cdot 10^{-7}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.75 \cdot 10^{-5}$ g (1)/100 g sln and $1.39 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (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 pyrene in water at 25 °C was reported to be 0.135 mg (1)/L sln and $x_1 = 1.2 \cdot 10^{-8}$.

The corresponding mass percent calculated by the compiler is $1.35 \cdot 10^{-5}$ 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 allowed to settle 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: ±0.005 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
Temperature: 25 and 29 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of pyrene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2)
25	1.18	1.32	0.132
29	1.44	1.62	0.162

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled-column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.01 mg (1)/kg (2) (standard deviation).

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(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: 277.85–303.05 K

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

Experimental Values

Solubility of pyrene in water

T/K	10^5 g(1)/100 g sln (compilers)	$10^8 \cdot x_1$
277.85	0.4919	0.4382
282.65	0.5850	0.5211
287.45	0.7200	0.6413
291.85	0.9329	0.8310
294.35	1.0900	0.9709
298.65	1.3595	1.211
303.05	1.6997	1.514

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:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
Variables:	**Prepared By:**
Temperature: 12.2–31.3 °C	A. Maczynski

Experimental Values

Solubility of pyrene in water

t/°C	$10^9 \cdot x_1$ (compiler)	$10^6 \cdot$ g (1)/100 g sln (compiler)	$10^7 \cdot$ mol (1)/L
12.2	4.86	5.46	2.70±0.03
15.5	6.11	6.86	3.39±0.03
17.4	7.04	7.91	3.91±0.05
20.3	8.23	9.25	4.57±0.04
23.0	10.41	11.69	5.78±0.06
23.3	10.48	11.77	5.82±0.03
25.0	11.53	12.95	6.40±0.05
26.2	12.84	14.42	7.13±0.07
26.7	12.93	14.53	7.18±0.04
28.5	16.90	16.37	8.09±0.08
31.3	16.75	18.81	9.3±0.1

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. Sealed fluorescence cells containing 5 mL of the aqueous solution and an excess of (1) were rotated at least 74 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 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:	**Original Measurements:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Values

The solubility of pyrene in distilled water at 25 °C was reported to be 0.13 μg/g, corresponding to a mole fraction (x_1) of $6.4 \cdot 10^{-10}$. The corresponding mass percent calculated by the compiler is $1.3 \cdot 10^{-5}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

500 mL of water and an excess of (1) were equilibrated for at least 24 h in a 1 L Erlenmeyer flask placed in a constant temperature (±0.1 °C) gyrotary shaker (200 rpm). After a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass–wool plug into a calibrated separatory funnel. Pyrene was isolated from solution by triplicate extraction with 10 mL of hexane (recovery >99%) and determined on a Hewlett-Packard Model 5840A gas chromatograph (GC) using a WCOTSP-2100 glass column (30 m/mL 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally determined by UV spectrophotometry (Beckman ACTA MVI). Agreement between GC and UV analyses was typically within 2%. Further details are given in the paper.

Source and Purity of Materials:

(1) Aldrich; purified by derivatization with 2,4,6-trinitrophenol.
(2) Doubly distilled in all-glass apparatus; free of trace organics.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±0.01 μg/g (standard deviation for six determinations).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).

Variables:
One temperature: 25.0 °C

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

Experimental Values
Solubility of pyrene in water

t/°C	μg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	171	$1.72 \cdot 10^{-5}$	$1.53 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was calculated from fluorescence measurements. A saturated solution was prepared by slow stirring an excess of hydrocarbon in water for several days in a sealed flask. The sample was then diluted over 2 orders of magnitude by the addition of known volumes of water. Details of sample preparation, apparatus, and measurements were described in the paper.

Source and Purity of Materials:
(1) Source not specified; recrystallized from a solvent.
(2) Distilled and passed through a Sephadex column.

Estimated Error:
Not specified.

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(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 pyrene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	0.133 ± 0.033	$1.33 \cdot 10^{-5}$	$1.19 \cdot 10^{-8}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated as an auxiliary property to the adsorption measurements.
The mean value of four 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 Continental Water Co; pH in the range 6.8–7.2.

Estimated Error:
See above.

2.19. 9,10-Dimethylanthracene+Water

Components:
(1) 9,10-Dimethylanthracene; $C_{16}H_{14}$; [781-43-1]
(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 9,10-dimethylanthracene in water at 25 °C was reported to be 0.056 mg (1)/L sln and $x_1 = 4.90 \cdot 10^{-9}$.
The corresponding mass percent calculated by the compiler is $5.6 \cdot 10^{-6}$ 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 allowed to settle 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: ±0.0005 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(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 pyrene in water

t/°C	$10^8 \cdot x_1$ (compiler)	$10^5 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2) experiment	mg (1)/kg (2) smoothed with (standard deviation)
0.0	0.44	0.49	—	0.049(0.001)
22.2	1.15	1.30	0.129, 0.128, 0.124	0.130
25.0	1.32	1.48	—	0.148(0.002)
34.5	2.09	2.35	0.228, 0.235	0.235
44.7	3.55	3.99	0.397, 0.395, 0.405	0.399
50.0	4.74	5.32	—	0.532(0.004)
50.1	4.75	5.34	0.558, 0.576, 0.556	0.534
55.6	6.5	7.3	0.75, 0.75, 0.77	0.73
56.0	6.6	7.4	0.74	0.74
60.7	8.6	9.7	0.96, 0.95, 0.90	0.97
65.2	11.3	12.7	1.27, 1.29	1.27
71.9	16.9	19.0	1.83, 1.86, 1.89	1.90
74.7	20.1	22.6	2.21	2.26
75.0	20.6	23.1	—	2.31(0.03)

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.

2.20. 2,4,6-Trimethyl-2-phenylheptane+Water

Components:	**Original Measurements:**
(1) 2,4,6-Trimethyl-2-phenylheptane; $C_{16}H_{26}$; [4810-06-4] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10–30 °C	A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in 2,4,6-trimethyl-2-phenylheptene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	1.16	0.0096
20	1.87	0.0154
30	3.05	0.0252

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.

2.21. 7,8-Dimethyltetradecane+Water

Components:	**Original Measurements:**
(1) 7,8-Dimethyltetradecane; $C_{16}H_{34}$; [2801-86-7] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 20–50 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in 7,8-dimethyltetradecane

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
20	9.67	0.0077
30	16.83	0.0134
40	27.48	0.0219
50	43.09	0.0344

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.

2.22. Hexadecane+Water

Components:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Hexadecane (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
Franks[2]	298	Sutton and Calder[8]	298
Hellinger and Sandler[3]	298	Yoshida and Yamane[9]	not specified

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.

The experimental and reference data of Franks,[2] Hellinger and Sandler,[3] and Sutton and Calder[8] at 298 K are listed in Table 8.

All the data at 298 K are in poor agreement with the reference data (greater than 30% relative standard deviation) and are Doubtful.

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

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

Author (s)	T/K	Author (s)	T/K
Englin *et al.*[1]	293–323	Schatzberg[4]	298 and 313
Hellinger and Sandler[3]	298		

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 hexadecane in water calculated with Eq. (1). The input solubility data at other temperatures were 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 data of Englin *et al.*[1] at 293–323 K, Hellinger and Sandler[3] at 298 K, and Schatzberg[4] at 298 and 313 K are listed in Table 9. The data of Englin *et al.*[1] at 293–323 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Hellinger and Sandler[3] at 298 K, and Schatzberg[4] at 298 and 313 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Rejected and Inaccessible Data

The data reported by Yoshida and Yamane[9] lack sufficient information to justify evaluation. Therefore these data are Rejected.

High Pressure Solubility Data

The experimental high pressure solubility of (1) in (2) investigated by Skripka[5] and Sultanov and Skripka[7] at 523–598 K, and 3.9 and 78.5 MPa, and solubility of (2) in (1) investigated by Skripka and Namiot[6] at 598 K and 1.7 and 13.18 MPa have not been critically evaluated because only a single data set is available.

References:

[1]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[2]F. Franks, Nature (London) **210**, 87 (1966).
[3]S. Hellinger and S. I. Sandler, J. Chem. Eng. Data B, 321 (1995).
[4]P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).
[5]V. G. Skripka, Tr. Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).
[6]V. G. Skripka and A. Yu. Namiot, Zh. Fiz. Khim. **48**, 782 (1974).
[7]R. G. Sultanov and V. G. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).
[8]C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).
[9]F. Yoshida and T. Yamane, Biotechnol. Bioeng. **13**, 691 (1971).

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

T/K	Experimental values x_1 (D=doubtful)	Reference values $x_1 \pm 30\%$
298	$5\cdot10^{-10}$ (D; Ref. 2), $2.94\cdot10^{-10}$ (D; Ref. 3), $2.98\cdot10^{-10}$ (D; Ref. 3), $7\cdot10^{-11}$ (D; Ref. 7)	$1.8\cdot10^{-10}$

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

T/K	Experimental values x_2 (T=tentative; D=doubtful)	Reference values $x_2 \pm 30\%$
293	$8.67\cdot10^{-4}$ (T; Ref. 1)	$1.1\cdot10^{-3}$
298	$7.50\cdot10^{-4}$ (D; Ref. 3), $7.4\cdot10^{-4}$ (D; Ref. 3), $6.8\cdot10^{-4}$ (D; Ref. 4)	$1.3\cdot10^{-3}$
303	$1.55\cdot10^{-3}$ (T; Ref. 1)	$1.6\cdot10^{-3}$
313	$2.62\cdot10^{-3}$ (T; Ref. 1), $1.13\cdot10^{-3}$ (D; Ref. 4)	$2.4\cdot10^{-3}$
323	$4.16\cdot10^{-3}$ (T; Ref. 1)	$3.6\cdot10^{-3}$

Components:	Original Measurements:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 20–50 °C	A. Maczynski and M. C. Haulait-Pirson

Experimental Values

Solubility of water in hexadecane

t/°C	$10^4 \cdot x_2$ (compiler)	g (2)/100 g sln
20	8.67	0.0069
30	15.45	0.0123
40	26.22	0.0209
50	41.59	0.0332

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:	Original Measurements:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O; [7732-18-5]	F. Franks, Nature (London) **210**, 87 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Values

The solubility of hexadecane in water at 25 °C was reported to be in mole fraction $x_1 = 5 \cdot 10^{-10}$.

The corresponding mass percent calculated by the compiler is $6.3 \cdot 10^{-7}$ 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) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Hellinger and S. I. Sandler, J. Chem. Eng. Data **40**, 321 (1995).

Variables:
One temperature: 25.0 °C

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

Experimental Values

Solubility of hexadecane in water

t/°C	$10^6 \cdot$ g (1)/100 g sln (compilers)	$10^9 \cdot x_1$
25.0	3.70	2.94
	3.75	2.98

Solubility of water in hexadecane

t/°C	$10^3 \cdot$ g (2)/100 g sln (compilers)	$10^4 \cdot x_2$
25.0	5.97	7.5
	5.89	7.4

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. An equilibrium cell thermostatically jacketed to maintain temperature to within ±0.1 °C was described in Magnussen *et al.*[1] Samples of both phases were withdrawn using a Perfectum Model MicroMate hypodermic syringe. Analysis of (1) in (2) was done using a Hewlett-Packard Model 5730 gas chromatograph with thermal conductivity detector and a Poropak Q column. For determination of (2) in (1) Karl Fischer titration[2] was used. Every sample was analyzed three times.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity 99%; used as received.
(2) De-ionized with Barnstead NANO pure equipment.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±2%.

References:
[1]T. Magnussen, P. Rasmussen, and Aa. Fredenslund, Ind. Eng. Chem. Process Des. Dev. **20**, 331 (1981).
[2]C. McAuliffe, Nature (London) **200**, 1002 (1963).

Components:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(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 hexadecane

t/°C	$10^4 \cdot x_2$	mg (2)/kg sln
25	6.8	54[a]
40	13.1	104[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 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) Humphrey-Wilkinson, Inc.; ASIM normal cetane; 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) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. G. Skripka, Tr. Vses. Neftegazov. Nauch. Issled. Inst. **61**, 139 (1976).
R. G. Sultanov and V. G. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).

Variables:

Temperature: 250–325 °C
Pressure: 3.9–78.5 MPa

Prepared By:

A. Maczynski

Experimental Values

Solubility of water in hexadecane

t/°C	x_2	g (2)/100 g sln (compiler)	P/kg·cm^{-2}	P/MPa (compiler)
250	0.230	2.32	40	3.9
	0.227	2.28	53	5.2
	0.217	2.16	93	9.1
	0.216	2.14	100	9.8
	0.212	2.10	134	13.1
	0.211	2.08	150	14.7
	0.208	2.05	200	19.6
	0.197	1.91	300	29.4
	0.193	1.87	400	39.2
	0.190	1.83	500	49.0
	0.186	1.78	600	58.8
	0.182	1.74	700	68.6
	0.178	1.69	800	78.5
275	0.355	4.19	53	5.2
	0.345	4.02	93	9.1
	0.343	3.99	100	9.8
	0.336	3.87	134	13.1
	0.333	3.82	150	14.7
	0.325	3.69	200	19.6
	0.308	3.42	300	29.4
	0.290	3.15	400	39.2
	0.273	2.90	500	49.0
	0.260	2.72	600	58.8
	0.250	2.58	700	68.6
	0.244	2.50	800	78.5
300	0.517	7.84	93	9.1
	0.505	7.51	100	9.8
	0.480	6.84	134	13.1
	0.469	6.56	150	14.7
	0.441	5.90	200	19.6
	0.404	5.11	300	29.4
	0.384	4.72	400	39.2
	0.366	4.39	500	49.0
	0.348	4.07	600	58.8
	0.329	3.75	700	68.6
	0.310	3.45	800	78.5
325	0.712	16.43	134	13.1
	0.643	12.53	150	14.7
	0.571	9.57	200	19.6
	0.509	7.62	300	29.4
	0.480	6.84	400	39.2
	0.466	6.49	500	49.0
	0.450	6.11	600	58.8
	0.435	5.77	700	68.6
	0.414	5.32	800	78.5

Auxiliary Information

Method/Apparatus/Procedure:

The experimental technique was described in Sultanov *et al.*[1]
No details reported in the paper.

Source and Purity of Materials:

(1) Source not specified, chemical reagent grade; purity not specified; used as received.
(2) Distilled.

Estimated Error:

Not specified.

References:

[1]R. G. Sultanov, V. E. Skripka, and V. G. Namiot, Gazov. Prom. **4**, 6 (1971).

Components:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skripka and A. Yu. Namiot, Zh. Fiz. Khim. **48**, 782 (1974).

Variables:
One temperature: 325 °C
Pressure: 1.7–13.18 MPa

Prepared By:
A. Maczynski

Experimental Values

Solubility of water in hexadecane

t/°C	x_2	g (2)/100 g sln (compiler)	P/kg·cm^{-2}	P/MPa (compiler)
325	0.083	0.71	17.3	1.7
	0.232	2.34	41.5	4.07
	0.352	4.14	62.5	6.13
	0.517	7.85	94.2	9.24
	0.712	16.43	134.4	13.18

Auxiliary Information

Method/Apparatus/Procedure:
Method was described in Sultanov *et al.*[1,2] Nothing more was reported in the paper.

Source and Purity of Materials:
(1) Source not specified; CP reagent; used as received.
(2) Distilled.

Estimated Error:
Not specified.

References:
[1]R. G. Sultanov, V. G. Skripka, and V. G. Namiot, Neft. Khoz. **2**, 57 (1972).
[2]R. G. Sultanov, V. G. Skripka, and V. G. Namiot, Gazov. Delo **10**, 43 (1972).

Components:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of hexadecane in water at 25 °C was reported to be $0.9 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction (x_1) of $0.7 \cdot 10^{-10}$.

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 through a 0.45 μm Millipore filter, then extracted three 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%.

Components:	Original Measurements:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O; [7732-18-5]	F. Yoshida and T. Yamane, Biotechnol. Bioeng. **13**, 691 (1971).
Variables:	**Prepared By:**
One temperature: not specified	M. C. Haulait-Pirson

Experimental Values

The solubility of hexadecane in water was reported to be $5.57 \cdot 10^{-9}$ g (1)/mL sln.

With the assumption that a solution density of 1.00 g/mL, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $5.57 \cdot 10^{-7}$ g (1)/100 g sln and $4.45 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
The analytical method was used, 10 mL of (1) and 1200 mL of (2) were placed in a stoppered flask and agitated with a magnetic stirrer at a speed of 200 rpm for 9–24 hours (1) was extracted from 1000 mL of (2) with 2 mL of heptane and its concentration determined by gas chromatography using a Shimadzu instrument equipped with hydrogen flame detectors.	Not specified. **Estimated Error:** Not specified.

2.23. Benzo[*a*]fluorene+Water

Components:	Original Measurements:
(1) Benzo[*a*]fluorene; $C_{17}H_{12}$; [238-84-6] (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 benzo[*a*]fluorene in water at 25 °C was reported to be 0.045 mg (1)/L sln and $x_1 = 3.75 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $4.5 \cdot 10^{-6}$ g (1)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 h and subsequently allowed to settle 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.	(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) Doubly distilled. **Estimated Error:** Solubility: ±0.0012 mg (1)/L sln (maximum deviation from several determinations).

2.24. Benzo[*b*]fluorine+Water

Components:
(1) Benzo[*b*]fluorene; $C_{17}H_{12}$; [243-17-4]
(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 benzo[*b*]fluorene in water at 25 °C was reported to be 0.0020 mg (1)/L sln and $x_1 = 9.56 \cdot 10^{-10}$.
The corresponding mass percent calculated by the compiler is $2.0 \cdot 10^{-7}$ 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 allowed to settle 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: $\pm 3 \cdot 10^{-5}$ mg (1)/L sln (maximum deviation from several determinations).

2.25. Benz[*a*]anthracene+Water

Components:
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Benz[*a*]anthracene (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
Davis *et al.*[1]	300	May *et al.*[5]	298 and 302
Haines and Sandler[2]	298	May *et al.*[6]	280–303
Klevens[3]	298	Walters and Luthy[7]	298
Mackay and Shiu[4]	298		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 10 and shown in Fig. 7. The data of Klevens,[3] May *et al.*,[5] and May *et al.*[6] at 298 K are in very good agreement and are Recommended. From these data the mean value was calculated. As shown in Fig. 7, the data of Haines and Sandler[2] and Klevens[4] at 298 K seem to be high and Doubtful. Similarly the data of Walters and Luthy[7] at 298 K seem to be below and are also Doubtful. The data of Davis *et al.*[1] at 300 K, the data of May *et al.*[5] at 303 K, and the data of May *et al.*[6] at 281–303 K are in good agreement with the mean value at 298 K and are Tentative.

References:
[1]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).
[3]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[4]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[5]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
[6]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).
[7]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

TABLE 10. Experimental values for solubility of benz[*a*]anthracene (1) in water (2)

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
280.1	$2.36 \cdot 10^{-10}$ (T; Ref. 6)	
283.9	$2.98 \cdot 10^{-10}$ (T; Ref. 6)	
284.3	$2.85 \cdot 10^{-10}$ (T; Ref. 6)	
287.5	$3.78 \cdot 10^{-10}$ (T; Ref. 6)	
291.3	$4.40 \cdot 10^{-10}$ (T; Ref. 6)	
292.5	$4.99 \cdot 10^{-10}$ (T; Ref. 6)	
296.3	$6.60 \cdot 10^{-10}$ (T; Ref. 6)	
296.8	$6.31 \cdot 10^{-10}$ (T; Ref. 6)	
298.2	$1.15 \cdot 10^{-9}$ (D; Ref. 2), $7.78 \cdot 10^{-10}$ (R; Ref. 3), $1.10 \cdot 10^{-9}$ (D; Ref. 4), $7.40 \cdot 10^{-10}$ (R; Ref. 5), $6.79 \cdot 10^{-10}$ (R; Ref. 6), $1.33 \cdot 10^{-10}$ (D; Ref. 7)	$7.3 \cdot 10^{-10}$
300.2	$8.7 \cdot 10^{-10}$ (T; Ref. 1)	
302.2	$9.6 \cdot 10^{-10}$ (T; Ref. 5)	
302.7	$9.76 \cdot 10^{-10}$ (T; Ref. 6)	
302.9	$1.00 \cdot 10^{-9}$ (T; Ref. 6)	

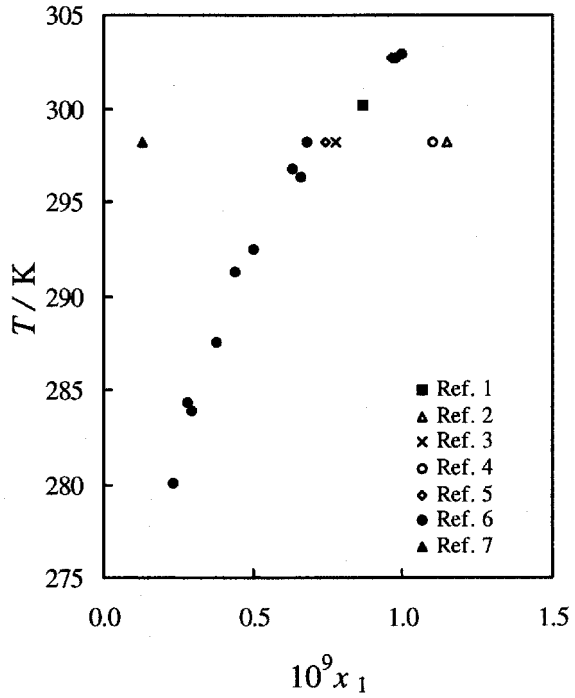

FIG. 7. All the solubility data for benz[*a*]anthracene (1) in water (2).

Components:	**Original Measurements:**
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of benz[*a*]anthracene in water

t/°C	$10^5 \cdot$ g (1)/L(2)
27	1.1
	1.1
	1.2

The best value recommended by the authors is $1.1 \cdot 10^{-5}$ g (1)/L(2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.1 \cdot 10^{-6}$ g (1)/100 g sln and $8.7 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 161.4–161.8 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: $\pm 10^{-6}$ g (1)/L(2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. I. S. Haines and S. I. Sandler, J. Chem. Eng. Data **40**, 833 (1995).

Variables:
One temperature: 25.0 °C

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

Experimental Values

Solubility of benz[*a*]anthracene in water

t/°C	g (1)/100 g sln (compilers)	x_1
25.0	$1.46 \cdot 10^{-6}$	$1.15 \cdot 10^{-9}$

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 for 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 two 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: 2.7% (reproducibility).

Components:
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of benz[*a*]anthracene in water at 25 °C was reported to be 10^{-5} g (1)/L sln and $4.31 \cdot 10^{-8}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $9.83 \cdot 10^{-7}$ g (1)/100 g sln and $7.78 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:	**Original Measurements:**
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3] (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 benz[*a*]anthracene in water at 25 °C was reported to be 0.014 mg (1)/L sln and $x_1 = 1.1 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $1.4 \cdot 10^{-6}$ 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 allowed to settle 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: ±0.0002 mg (1)/L sln (maximum deviation from several determinations).

Components:	**Original Measurements:**
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3] (2) Water; H_2O; [7732-18-5]	W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
Variables:	**Prepared By:**
Temperature: 25 and 29 °C	A. Maczynski

Experimental Values

Solubility of benz[*a*]anthracene in water

t/°C	$10^{10} \cdot x_1$ (compiler)	$10^6 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2)
25	7.4	0.94	0.0094
29	9.6	1.22	0.0122

Auxiliary Information

Method/Apparatus/Procedure:

The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled-column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:

(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Haas, Philadelphia, Pa.).

Estimated Error:

Temperature: ±0.05 °C.
Solubility: ±0.001 mg (1)/kg (2) (standard deviation).

References:

[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3]
(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: 277.85–303.05 K

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

Experimental Values
Solubility of benz[*a*]anthracene in water

T/K	10^6 g (1)/100 g sln (compilers)	$10^9 \cdot x_1$
280.05	0.2989	0.2359
283.85	0.3780	0.2983
284.25	0.3610	0.2849
287.45	0.4790	0.3780
291.25	0.5579	0.4403
292.45	0.6330	0.4995
296.25	0.8370	0.6605
296.75	0.8000	0.6313
298.15	0.8609	0.6794
302.65	1.2399	0.9785
302.85	1.2697	1.002

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) Benz[*a*]anthracene; $C_{18}H_{12}$; [56-55-3]
(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 benz[*a*]anthracene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	0.0168±0.0011	$1.68 \cdot 10^{-6}$	$1.33 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated an an auxiliary property to the 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

2.26. Chrysene+Water

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Chrysene (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
Davis *et al.*[1]	300	May *et al.*[4]	298 and 302
Klevens[2]	298	May *et al.*[5]	280–302
Mackay and Shiu[3]	298	Walters and Luthy[6]	298

Calcualtion of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 11 and shown in Fig. 8. The data of Mackay and Shiu,[3] May *et al.*,[4] and May *et al.*[5] at 298 K are in very good agreement and are Recommended. From these data the mean value was calculated. As shown in Fig. 8, the data of Davis *et al.*[1] at 300 K seem to be low and are Doubtful. Similarly, the data of Klevens[2] and Walters and Luthy[6] at 298 K seem to be high and are Doubtful. All remaining data over the temperature range 280–302 K are consistent with the mean value for 298 K and are Tentative.

References:

[1]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[3]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[4]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[5]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).
[6]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

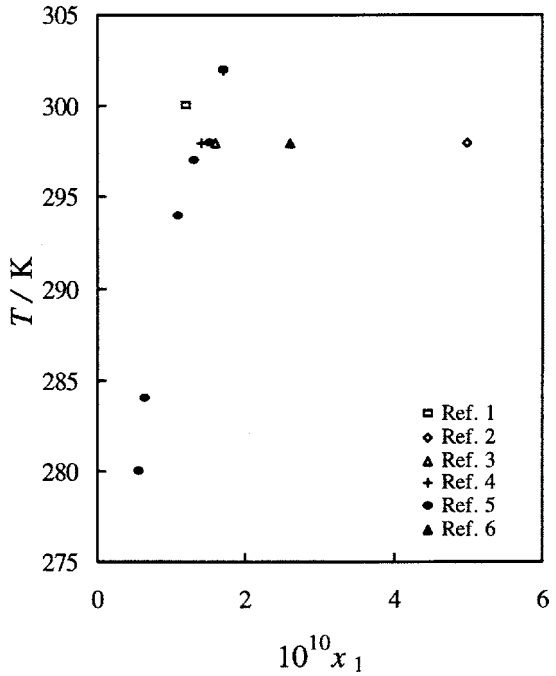

FIG. 8. All the solubility data for chrysene (1) in water (2).

TABLE 11. Experimental values for solubility of chrysene (1) in water (2)

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
280	$5.6\cdot10^{-11}$ (T; Ref. 5)	
284	$6.3\cdot10^{-11}$ (T; Ref. 5)	
294	$1.1\cdot10^{-10}$ (T; Ref. 5)	
297	$1.3\cdot10^{-10}$ (T; Ref. 5)	
298	$5.0\cdot10^{-10}$ (D; Ref. 2), $1.6\cdot10^{-10}$ (R; Ref. 3), $1.4\cdot10^{-10}$ (R; Ref. 4), $1.5\cdot10^{-10}$ (R; Ref. 5), $2.59\cdot10^{-10}$ (D; Ref. 6)	$1.5\cdot10^{-10}$
300	$1.2\cdot10^{-10}$ (D; Ref. 1)	
302	$1.7\cdot10^{-10}$ (T; Ref. 4), $1.7\cdot10^{-10}$ (T; Ref. 5)	

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of chrysene in water

t/°C	$10^6 \cdot$ g (1)/L (2)
27	1.5±0.5
	1.5±0.2

The best value recommended by the authors is $1.5 \cdot 10^{-6}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.5 \cdot 10^{-7}$ g (1)/100 g sln and $1.2 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis *et al.*[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 253.2–253.8 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of chrysene in water at 25 °C was reported to be $6 \cdot 10^{-6}$ g (1)/L sln and $2.76 \cdot 10^{-8}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $6.29 \cdot 10^{-7}$ g (1)/100 g sln and $4.98 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(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 chrysene in water at 25 °C was reported to be 0.0020 mg (1)/L sln and $x_1 = 1.58 \cdot 10^{-10}$.
The corresponding mass percent calculated by the compiler is $2 \cdot 10^{-7}$ 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 allowed to settle 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: ±0.00017 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
Temperature: 25 and 29 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of chrysene in water

t/°C	$10^{10} \cdot x_1$ (compiler)	$10^7 \cdot$ g (1)/100 g sln (compiler)	mg (1)/kg (2)
25	1.4	1.8	0.0018
29	1.7	2.2	0.0022

Auxiliary Information

Method/Apparatus/Procedure:
The DCCLC method was based on generating saturated solutions by pumping water through a column packed with glass beads that had been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled-column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Haas, Philadelphia, Pa.).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.001 mg (1)/kg (2) (standard deviation).

References:
[1]W. May, S. Chesler, S. Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9]
(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: 279.65–301.85 K

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

Experimental Values
Solubility of chrysene in water

T/K	10^7 g (1)/100 g sln (compilers)	$10^{10} \cdot x_1$
279.65	0.7100	0.5603
284.15	0.8000	0.6313
293.55	1.400	1.105
297.15	1.680	1.326
298.45	1.889	1.491
301.85	2.210	1.744

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) Chrysene; $C_{18}H_{12}$; [218-01-9]
(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 chrysene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25	0.00327±0.00043	$3.28 \cdot 10^{-7}$	$2.59 \cdot 10^{-10}$

Auxiliary Information

Method/Apparatus/Procedure:
The method and procedure were not described. Solubility was treated an an auxiliary property to the adsorption measurements.
The mean value of four 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

2.27. Naphthacene+Water

Components:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Naphthacene (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
Davis *et al.*[1]	300	Mackay and Shiu[3]	298
Klevens[2]	298		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 12. The data of Davis *et al.*[1] and Mackay and Shiu[3] reported at 300 and 298 K, respectively, are in good agreement and are Tentative. From these data the mean value was calculated. The remaining value of Klevens[2] seems to be high and is Doubtful.

References:

[1]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[3]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 12. Experimental values for solubility of naphthacene (1) in water (2)

T/K	Experimental values x_1 (T=tentative; D=doubtful)	Mean values
298	$3.7\cdot10^{-11}$ (T; Ref. 3), $1.2\cdot10^{-10}$ (D; Ref. 2)	$5.8\cdot10^{-11}$
300	$7.9\cdot10^{-11}$ (T; Ref. 1)	$5.8\cdot10^{-11}$

Components:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of naphthacene in water

t/°C	$10^6\cdot$g(1)/L(2)
27	1.0±0.5
	1.0±0.2

The best value recommended by the authors is $1.0\cdot10^{-6}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.0\cdot10^{-7}$ g (1)/100 g sln and $7.9\cdot10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 341.5–343.0 °C; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ± 3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	Original Measurements:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of naphthacene in water at 25 °C was reported to be $6.6 \cdot 10^{-9}$ mol (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler are $1.5 \cdot 10^{-7}$ g (1)/100 g sln and $1.2 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0] (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 naphthacene in water at 25 °C was reported to be 0.00057 mg (1)/L sln and $x_1 = 3.7 \cdot 10^{-11}$.

The corresponding mass percent calculated by the compiler is $5.7 \cdot 10^{-8}$ 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 allowed to settle 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: ±0.00003 mg (1)/L sln (maximum deviation from several determinations).

2.28. Triphenylene+Water

Components:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Triphenylene (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
Akiyoshi *et al.*[1]	298	Mackay and Shiu[4]	298
Davis *et al.*[2]	300	May *et al.*[5]	281–301
Klevens[3]	298	Walters and Luthy[6]	298

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 13 and shown in Fig. 9. The data of Akiyoshi *et al.*,[1] Klevens,[3] and Mackay and Shiu[4] at 298 K, are in very good agreement and Recommended. From these data the mean value was calculated. The data of Davis *et al.*[2] at 300 K are in very good agreement with the mean value calculated at 298 K and are Tentative. All the data of May *et al.*[5] and the data of Walters and Luthy[6] seem to be low and are Doubtful.

References:

[1]M. Akiyoshi, T. Deguchi, and I. Sanemasa, Bull. Chem. Soc. Jpn. **60**, 3935 (1987).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[3]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
[4]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).
[5]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).
[6]R. W. Walters and R. G. Luthy, Environ. Sci. Technol. **18**, 395 (1984).

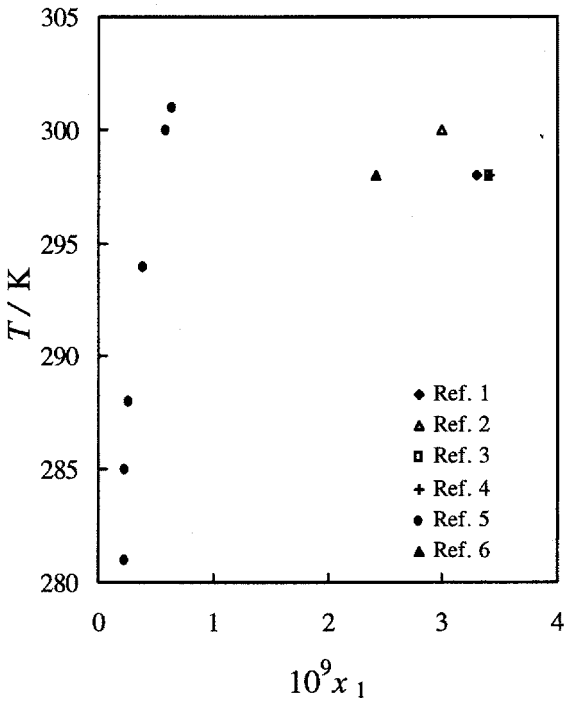

FIG. 9. All the solubility data for triphenylene (1) in water (2).

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

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
281	$2.4\cdot10^{-10}$ (D; Ref. 5)	
285	$2.4\cdot10^{-10}$ (D; Ref. 5)	
288	$2.7\cdot10^{-10}$ (D; Ref. 5)	
294	$3.9\cdot10^{-10}$ (D; Ref. 5)	
298	$3.3\cdot10^{-9}$ (R; Ref. 1), $3.4\cdot10^{-9}$ (R; Ref. 3), $3.4\cdot10^{-9}$ (R; Ref. 4), $2.43\cdot10^{-9}$ (D; Ref. 6)	$3.4\cdot10^{-9}$
300	$3.0\cdot10^{-9}$ (T; Ref. 2), $6.0\cdot10^{-10}$ (D; Ref. 5)	
301	$6.4\cdot10^{-10}$ (D; Ref. 5)	

Components:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]
(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 triphenylene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(1.8\pm0.2)\cdot10^{-7}$	$4.2\cdot10^{-6}$	$3.3\cdot10^{-9}$

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 $CHCl_3$, dehydrated, 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 97%; 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) Triphenylene; $C_{18}H_{12}$; [217-59-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of triphenylene in water

t/°C	$10^5\cdot$g (1)/L (2)
27	3.8±0.8
	3.6±0.4
	4.0±0.4

The best value recommended by the authors is $3.8\cdot10^{-5}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler are $3.8\cdot10^{-6}$ g (1)/100 g sln and $3.0\cdot10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 197.5–197.9 °C; used as received; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	Original Measurements:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of triphenylene in water at 25 °C was reported to be $4.3 \cdot 10^{-5}$ g (1)/L sln and $1.88 \cdot 10^{-7}$ mole (1)/L sln.

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction, (x_1), calculated by the compiler, are $4.28 \cdot 10^{-6}$ g (1)/100 g sln and $3.39 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (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 triphenylene in water at 25 °C was reported to be 0.043 mg (1)/L sln and $x_1 = 3.39 \cdot 10^{-9}$.

The corresponding mass percent calculated by the compiler is $4.3 \cdot 10^{-6}$ 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 allowed to settle 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: ±0.00017 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]
(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: 281.15–301.35 K

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

Experimental Values

Solubility of triphenylene in water

T/K	10^7 g (1)/100 g sln (compilers)	$10^{10} \cdot x_1$
281.15	2.989	2.359
285.15	3.030	2.391
287.95	3.390	2.675
293.65	4.890	3.859
300.45	7.650	6.037
301.35	8.110	6.400

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) Triphenylene; $C_{18}H_{12}$; [217-59-4]
(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 triphenylene in water

t/°C	mg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
5	0.0307±0.0043	$3.08 \cdot 10^{-6}$	$2.43 \cdot 10^{-9}$

Auxiliary Information

Method/Apparatus/Procedure:
The method was not described. Solubility was treated as an auxiliary property to the measuring of an adsorption isotherm on activated carbon.
The mean value of four 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 Continental Water Co.; pH in the range 6.8–7.2.

Estimated Error:
See above.

2.29. 1,2-Diphenylbenzene+Water

Components:
(1) 1,2-Diphenylbenzene; $C_{18}H_{14}$; [84-15-1]
(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 1,2-diphenylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(5.38 \pm 0.02) \cdot 10^{-6}$	$1.242 \cdot 10^{-4}$	$9.72 \cdot 10^{-8}$

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 $CHCl_3$, dehydrated, 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 97%; 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).

2.30. 1,3-Diphenylbenzene+Water

Components:
(1) 1,3-Diphenylbenzene; $C_{18}H_{14}$; [92-06-8]
(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 1,3-diphenylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(6.56 \pm 0.02) \cdot 10^{-6}$	$1.515 \cdot 10^{-4}$	$1.185 \cdot 10^{-7}$

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 $CHCl_3$, dehydrated, 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 97%; 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).

2.31. 1,4-Diphenylbenzene+Water

Components:
(1) 1,4-Diphenylbenzene; $C_{18}H_{14}$; [92-94-4]
(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 1,4-diphenylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$(7.8 \pm 0.6) \cdot 10^{-8}$	$1.80 \cdot 10^{-6}$	$1.41 \cdot 10^{-9}$

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 $CHCl_3$, dehydrated, 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 97%; 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).

2.32. Octadecane+Water

Components:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3]
(2) Water; H_2O; [7732-18-5]

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

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

The experimental solubility data for (1) in (2) have been investigated by Baker,[1–3] 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 14. 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 Baker[1] are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

Rejected and Inaccessible Data

The data reported by Baker[1,3] lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:
[1]E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **1**, 5 (1956).
[2]E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **3**, C-61 (1958).
[3]E. G. Baker, Science **129**, 871 (1959).
[4]C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

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

T/K	Experimental values x_1 (T=tentative; D=doubtful)	Reference value $x_1 \pm 30\%$
298	$4 \cdot 10^{-10}$ (D; Ref. 2), $1.5 \cdot 10^{-10}$ (T; Ref. 4)	$1.4 \cdot 10^{-10}$

Components:	Original Measurements:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **1**, 5 (1956).
Variables:	**Prepared By:**
One temperature: 25–80 °C	M. C. Haulait-Pirson

Experimental Values

The authors reported that the solubility of octadecane in water increases from about 55 ppb by weight at room temperature to twice this amount at 80 °C. A graph reporting the mole fraction x_1 , a function of the reciprocal absolute temperature, is given.

Auxiliary Information

Method/Apparatus/Procedure:

Tritio-octadecane was used as a radioactive tracer. (1) was shaken with (2); the mixture was filtered through a 0.05 μm filter; 0.01 mL of filtrate was vaporized in hot oxygen and passed over CuO at 600 °C; the H_2O–T_2O derived from the vaporized solvent as well as from the combusted (1) was trapped at −78 °C; the melted ice was reduced by Zn and the gas was counted. Many details are given in the paper.

Source and Purity of Materials:

(1) Tritio-octadecane prepared by hydrogenating octadecene-1 with tritium; 100 Ci of tritium were introduced per mole of (1).
(2) Distilled.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	E. G. Baker, Am. Chem. Soc., Div. Petrol. Chem., Prepr. **3**, C-61 (1958).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of octadecane-1,2-H^3 in water at 25 °C was reported to be $6 \cdot 10^{-9}$ g (1)/g (2) and that of octadecane-1-C^{14} $5.7 \cdot 10^{-9}$ g (1)/g (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $6 \cdot 10^{-7}$ g (1)/100 g sln and $4 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Tritiated or carbon-14 labeled (1) was used as a 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) Octadecane-1,2-H^3 from Tracer Lab.; percolated through silica gel. Octadecane-1-C^{14} from 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**, 5 (1956).

Components:	Original Measurements:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (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 octadecane in water at 25 °C was reported to be $2.1 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction (x_1) of $1.5 \cdot 10^{-10}$.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
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 through a 0.45 μm Millipore filter, then extracted three 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.	(1) Analabs Inc., 99+%. (2) Doubly distilled. **Estimated Error:** Temperature: ±0.1 °C. Solubility: ±16%.

Components:	Original Measurements:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	E. G. Baker, Science **129**, 871 (1959).
Variables:	**Prepared By:**
One temperature: 25 °C	F. Kapuku

Experimental Values

The solubility of octadecane in water at 25 °C was reported to be $7.75 \cdot 10^{-7}$ mL (1)/100 mL (2).

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
Not specified.	Not specified. **Estimated Error:** Not specified.

2.33. 1-Methylbenz[*a*]anthracene+Water

Components:	**Original Measurements:**
(1) 1-Methylbenz[*a*]anthracene; $C_{19}H_{14}$; [2498-77-3] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of 1-methylbenz[*a*]anthracene in water

t/°C	$10^5 \cdot$ g (1)/L (2)
27	5.5 ± 0.2
	5.4 ± 0.4
	5.5 ± 0.2

The best value recommended by the authors is $5.5 \cdot 10^{-5}$ g (1)/L (2).

Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $5.5 \cdot 10^{-6}$ g (1)/100 g sln and $4.1 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 138.5–139.0 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ± 3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.34. 9-Methylbenz[*a*]anthracene+Water

Components:	**Original Measurements:**
(1) 9-Methylbenz[*a*]anthracene; $C_{19}H_{14}$; [2381-16-0] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of 9-methylbenz[*a*]anthracene in water at 27 °C was reported to be $6.6 \cdot 10^{-5}$ g (1)/L (2). (Two identical results have been obtained.)

With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $6.6 \cdot 10^{-6}$ g (1)/100 g sln and $4.5 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 138.0–138.8 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ± 3 °C.
Solubility: $\pm 10^{-6}$ g (1)/L (2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.35. 10-Methylbenz[*a*]anthracene+Water

Components:
(1) 10-Methylbenz[*a*]anthracene; $C_{19}H_{14}$; [2381-15-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of 10-methylbenz[*a*]anthracene in water at 27 °C was reported to be $5.5 \cdot 10^{-5}$ g (1)/L (2). (Four identical results have been obtained.)

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $5.5 \cdot 10^{-6}$ g (1)/100 g sln and $4.1 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 140.0–140.5 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: $\pm 5 \cdot 10^{-6}$ g (1)/L (2).

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.36. 5-Methylchrysene+Water

Components:
(1) 5-Methylchrysene; $C_{19}H_{14}$; [3697-24-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of 5-methylchrysene in water

t/°C	$10^5 \cdot$ g (1)/L (2)
27	6.5±0.5
	6.5±0.5
	5.8±0.5
	5.5±0.5
	6.1±0.3
	6.2±0.3

The best value recommended by the authors is $6.2 \cdot 10^{-5}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $6.2 \cdot 10^{-6}$ g (1)/100 g sln and $4.6 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at the Ohio State University; melting point range 117.3–117.7 °C; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.37. Benzo[*a*]pyrene+Water

Components:
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Benzo[*a*]pyrene (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
Barone *et al.*[1]	298	Mackay and Shiu[4]	298
Davis *et al.*[2]	300	May *et al.*[5]	283–303
Haines and Sandler[3]	298		

Calcualtion of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 15 and shown in Fig. 10. The data of Haines and Sandler,[3] and Mackay and Shiu[4] at 298 K are in good agreement and are Recommended. From these data, the mean was calculated. As shown in Fig. 10, the data of Davis *et al.*[2] at 300 K are in agreement with the mean and are Tentative. All the data of May *et al.*[5] seem to be low and Doubtful. The data of Barone *et al.*[1] seem to be high and Doubtful.

References:

[1]G. Barone, V. Crescenzi, A. M. Liquori, and F. Quadrifoglio, J. Phys. Chem. **71**, 2341 (1967).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[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]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).

TABLE 15. Experimental values for solubility of benzo[*a*]pyrene (1) in water (2)

T/K	Experimental values x_1 (R=Recommended; T=Tentative; D=Doubtful)	Mean value
283	$4.0\cdot10^{-11}$ (D; Ref. 5)	
288	$5.7\cdot10^{-11}$ (D; Ref. 5)	
293	$8.1\cdot10^{-11}$ (D; Ref. 5)	
298	$5.2\cdot10^{-10}$ (D; Ref. 1), $3.4\cdot10^{-10}$ (R; Ref. 3), $2.7\cdot10^{-10}$ (R; Ref. 4), $1.2\cdot10^{-10}$ (D; Ref. 5)	$3.1\cdot10^{-10}$
300	$2.9\cdot10^{-10}$ (T; Ref. 2)	
303	$1.6\cdot10^{-10}$ (D; Ref. 5)	

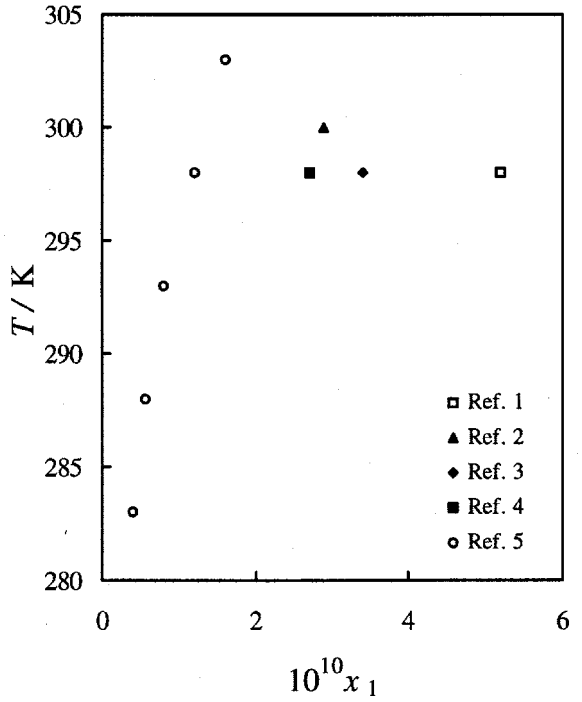

FIG. 10. All the solubility data for benzo[*a*]pyrene (1) in water (2).

Components:	**Original Measurements:**
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8] (2) Water; H_2O; [7732-18-5]	G. Barone, V. Crescenzi, A. M. Liquori, and F. Quadrifoglio, J. Phys. Chem. **71**, 2341 (1967).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzo[*a*]pyrene in water

t/°C	mol (1)/L (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.9 \cdot 10^{-8}$	$7.3 \cdot 10^{-7}$	$5.2 \cdot 10^{-10}$

Auxiliary Information

Method/Apparatus/Procedure:

A flask containing powdered crystals of component (1) suspended in the polyelectrolyte and in potassium laurate solution was shaken in a thermostat for over 10 days. Once the equilibrium was reached the solution was filtered through sintered-glass (G-4) filters and examined for the presence of microcrystals by fluoroscence spectroscopy. The concentration of component (1) was determined by carrying out ultraviolet spectral measurements on cyclohexane extracts.

Source and Purity of Materials:

(1) Source and purity not specified; purified by repeated crystallization from benzene+ethanol (1:9) mixture; melting point 176 °C.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 °C.

Components:	**Original Measurements:**
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of benzo[*a*]pyrene in water

t/°C	$10^6 \cdot$ g (1)/L (2)
27	3.0±0.5
	4.5±0.5
	4.0±0.1
	4.0±0.5
	3.5±0.5

The best value recommended by the authors is $4.0 \cdot 10^{-6}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $4.0 \cdot 10^{-7}$ g (1)/100 g sln and $2.9 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Hoffman La-Roche; used as received; melting point range 176.3–177.0 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	**Original Measurements:**
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8] (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 benzo[*a*]pyrene in water

t/°C	g (1)/100 g sln (compilers)	x_1
25.0	$4.72 \cdot 10^{-7}$	$3.37 \cdot 10^{-10}$

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 for 4 days, and equilibrated at 25 °C for 2 days. Samples were extracted and analyzed by the high performance liquid chromatograph. Analysis details are reported in the paper. The mean of two separate experiments is reported. (Confirmatory analyses were made after 2 days of additional mixing.)

Source and Purity of Materials:

(1) Aldrich Chemicals Co.; purity 98 mass %; used as received.
(2) Distilled and de-ionized water.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 2.7% (reproducibility).

Components:	**Original Measurements:**
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8] (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 benzo[*a*]pyrene in water at 25 °C was reported to be 0.0038 mg (1)/L sln and $x_1 = 2.73 \cdot 10^{-10}$.

The corresponding mass percent calculated by the compiler is $3.8 \cdot 10^{-7}$ 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 allowed to settle 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: ±0.00031 mg (1)/L sln (maximum deviation from several determinations).

Components:
(1) Benzo[*a*]pyrene; $C_{20}H_{12}$; [50-32-8]
(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: 283.15–303.15 K

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

Experimental Values

Solubility of benzo[*a*]pyrene in water

T/K	$10^7 \cdot$ g (1)/100 g sln (compilers)	$10^{10} \cdot x_1$
283.15	0.5599	0.3998
288.15	0.8000	0.5712
293.15	1.1399	0.8139
298.15	1.620	1.157
303.15	2.290	1.635

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).

2.38. Benzo[*e*]pyrene+Water

Components:
(1) Benzo[*e*]pyrene; $C_{20}H_{12}$; [192-97-2]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Benzo[*e*]pyrene (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
Barone *et al.*[1]	298	Schwarz and Wasik[3]	298
Schwarz[2]	282–305		

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. All the experimental data are listed in Table 16 and shown in Fig. 11. The data of Barone *et al.*[1] and Schwartz and Wasik[3] at 298 K are in only fair agreement and are Tentative. At all other temperatures in the range 282–305 K, only one value is reported at each temperature and therefore all are considered Tentative.

References:
[1]G. Barone, V. Crescenzi, A. M. Liquori, and F. Quadrifoglio, J. Phys. Chem. **71**, 2341 (1967).
[2]F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
[3]F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).

TABLE 16. Experimental values for solubility of benzo[*e*]pyrene (1) in water (2)

T/K	Experimental values x_1 (T=tentative)
281.75	$2.32 \cdot 10^{-10}$ (T; Ref. 2)
287.15	$2.56 \cdot 10^{-10}$ (T; Ref. 2)
290.15	$3.17 \cdot 10^{-10}$ (T; Ref. 2)
290.65	$2.81 \cdot 10^{-10}$ (T; Ref. 2)
293.15	$3.28 \cdot 10^{-10}$ (T; Ref. 2)
293.35	$3.42 \cdot 10^{-10}$ (T; Ref. 2)
296.15	$3.62 \cdot 10^{-10}$ (T; Ref. 2)
296.35	$3.82 \cdot 10^{-10}$ (T; Ref. 2)
298.15	$3.4 \cdot 10^{-10}$ (T; Ref. 1), $2.9 \cdot 10^{-10}$ (T; Ref. 3)
302.35	$4.59 \cdot 10^{-10}$ (T; Ref. 2)
304.85	$4.86 \cdot 10^{-10}$ (T; Ref. 2)

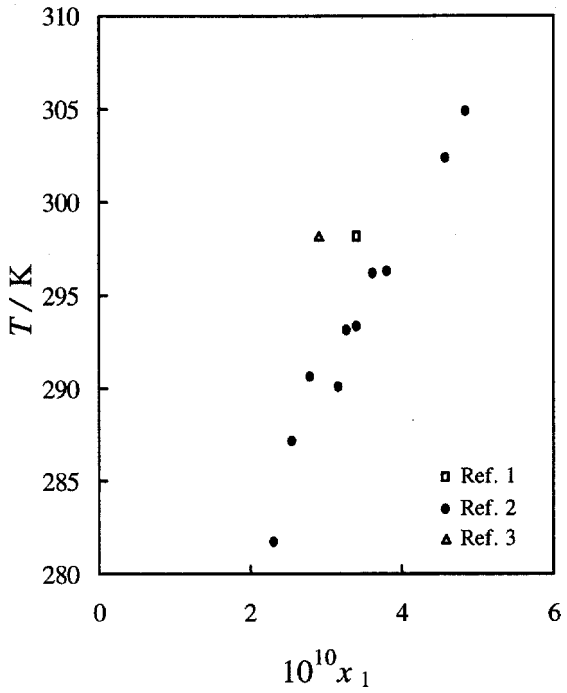

FIG. 11. All the solubility data for benzo[*e*]pyrene (1) in water (2).

Components:
(1) Benzo[*e*]pyrene; $C_{20}H_{12}$; [192-97-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. Barone, V. Crescenzi, A. M. Liquori, and F. Quadrifoglio, J. Phys. Chem. **71**, 2341 (1967).

Variables:
One temperature: 25.0 °C

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

Experimental Values

Solubility of benzo[*e*]pyrene in water

t/°C	mol (1)/L (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$2.9 \cdot 10^{-8}$	$4.8 \cdot 10^{-7}$	$3.4 \cdot 10^{-10}$

Auxiliary Information

Method/Apparatus/Procedure:
A flask containing powdered crystals of component (1) suspended in the polyelectrolyte and in potassium laurate solution was shaken in a thermostat for over 10 days. Once the equilibrium was reached solution was filtered through sintered-glass (G-4) filters and examined for the presence of microcrystals by fluoroscence spectroscopy. The concentration of component (1) was determined by carrying out ultraviolet spectral measurements on cyclohexane extracts.

Source and Purity of Materials:
(1) Source and purity not specified; purified according to Sangster and Irvine;[1] melting point 179.5 °C.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.

References:
[1]R. C. Sangster and J. W. Irvine, J. Chem. Phys. **24**, 670 (1956).

Components:
(1) Benzo[*e*]pyrene; $C_{20}H_{12}$; [192-97-2]
(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 benzo[*e*]pyrene in water

t/°C	$10^{10} \cdot x_1$ (compiler)	$10^7 \cdot$ g (1)/100 g sln (compiler)	$10^8 \cdot$ mol (1)/L
8.6	2.32	3.25	1.29 ± 0.07
14.0	2.56	3.58	1.42 ± 0.05
17.0	3.17	4.44	1.76 ± 0.13
17.5	2.81	3.94	1.56 ± 0.08
20.0	3.28	4.59	1.82 ± 0.09
20.2	3.42	4.79	1.90 ± 0.14
23.0	3.62	5.07	2.01 ± 0.20
23.2	3.82	5.35	2.12 ± 0.10
29.2	4.59	6.43	2.55 ± 0.02
31.7	4.86	6.81	2.70 ± 0.15

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 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) Benzo[*e*]pyrene; $C_{20}H_{12}$; [192-97-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and S. P. Wasik, Anal. Chem. **48**, 524 (1976).

Variables:
One temperature: 25.0 °C

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

Experimental Values

Solubility of benzo[*e*]pyrene in water

t/°C	μg (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	≈4	$4.0 \cdot 10^{-7}$	$2.9 \cdot 10^{-10}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was calculated from fluorescence measurements. A saturated solution was prepared by slowly stirring an excess of hydrocarbon in water for several days in a sealed flask. The sample was then diluted over 2 orders of magnitude by the addition of known volumes of water. Details of sample preparation, apparatus, and measurements were described in the paper.

Source and Purity of Materials:
(1) Source not specified; recrystallized from a solvent.
(2) Distilled and passed through a Sephadex column.

Estimated Error:
Not specified.

2.39. Perylene+Water

Components:	Original Measurements:
(1) Perylene; $C_{20}H_{12}$; [198-55-0] (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 perylene in water at 25 °C was reported to be 0.0004 mg (1)/L sln and $x_1 = 2.83 \cdot 10^{-11}$.

The corresponding mass percent calculated by the compiler is $4 \cdot 10^{-8}$ 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 allowed to settle 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: $\pm 2 \cdot 10^{-5}$ mg (1)/L sln (maximum deviation from several determinations).

2.40. Cholanthrene+Water

Components:	Original Measurements:
(1) Cholanthrene; $C_{20}H_{14}$; [479-23-2] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of cholantrene in water at 27 °C was reported to be $3.5 \cdot 10^{-6}$ g (1)/L (2). (Two identical results were obtained.)

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $3.5 \cdot 10^{-7}$ g (1)/100 g sln and $2.5 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 170.1–170.6 °C; used as received; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: $\pm 10^{-6}$ g (1)/L (2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.41. 7,12-Dimethylbenz[*a*]anthracene+Water

Components:
(1) 7,12-Dimethylbenz[*a*]anthracene; $C_{20}H_{16}$; [57-97-6]
(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 7,12-dimethylbenz[*a*]anthacene in water at 25 °C was reported to be 0.061 mg (1)/L sln and $x_1 = 4.26 \cdot 10^{-9}$.
The corresponding mass percent calculated by the compiler is $6.1 \cdot 10^{-6}$ 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 allowed to settle 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: $\pm 6 \cdot 10^{-4}$ mg (1)/L sln (maximum deviation from several determinations).

2.42. 9,10-Dimethylbenz[*a*]anthracene+Water

Components:
(1) 9,10-Dimethylbenz[*a*]anthracene; $C_{20}H_{16}$; [56-56-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of 9,10-dimethylbenz[*a*]anthracene in water

t/°C	$10^5 \cdot$ g (1)/L (2)
27	4.3 ± 0.2
	4.5 ± 0.4
	4.5 ± 0.1
	4.3 ± 0.3
	3.9 ± 0.4

The best value recommended by the authors is $4.3 \cdot 10^{-5}$ g (1)/L (2).

With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $4.3 \cdot 10^{-6}$ g (1)/100 g sln and $3.0 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 122.6–122.9 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ± 3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.43. 10-Ethylbenz[*a*]anthracene+Water

Components:	**Original Measurements:**
(1) 10-Ethylbenz[*a*]anthracene; $C_{20}H_{16}$; [14854-08-1] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of 10-Ethylbenz[*a*]anthracene in water

t/°C	$10^5 \cdot$ g (1)/L (2)
27	4.5±0.5
	4.5±0.5
	3.5±0.5
	4.5±0.3
	4.5±0.5
	4.0±0.5
	4.0±0.8

The best value recommended by the authors is $4.5 \cdot 10^{-5}$ g (1)/L (2).

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are $4.5 \cdot 10^{-6}$ g (1)/100 g sln and $3.2 \cdot 10^{-9}$.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 112.4–112.8 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.44. Eicosane+Water

Components:	**Original Measurements:**
(1) Eicosane; $C_{20}H_{42}$; [112-95-8] (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 eicosane in water at 25 °C was reported to be $1.9 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction (x_1) of $1.1 \cdot 10^{-10}$.

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 through 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%.

2.45. 5-Methylbenzo[*a*]pyrene+Water

Components:
(1) 5-Methylbenzo[*a*]pyrene; $C_{21}H_{14}$; [31647-36-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of 5-methylbenzo[*a*]pyrene in water

t/°C	$10^7 \cdot$ g (1)/L (2)
27	8±2
	10±4
	8±2

The best value recommended by the authors is $8 \cdot 10^{-7}$ g (1)/L (2).

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $8 \cdot 10^{-8}$ g (1)/100 g sln and $6 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at Harvard University; melting point range 216.6–217.3 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.46. 3-Methylcholantrene+Water

Components:
(1) 3-Methylcholantrene; $C_{21}H_{16}$; [56-49-5]
(2) Water; H_2O; [7732-18-5]

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

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

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. The experimental solubility data for (1) in (2) have been investigated by Davis *et al.*[1] at 300 K and Mackay and Shiu[2] at 298 K. Both the experimental data are listed in Table 17. The data are in poor agreement and both are considered Doubtful.

References:
[1]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

TABLE 17. Experimental values for solubility of 3-methylcholantrene (1) in water (2)

T/K	Experimental values x_1 (D=Doubtful)
298	$1.9 \cdot 10^{-10}$ (D: Ref. 1)
300	$1.0 \cdot 10^{-10}$ (D: Ref. 2)

Components:	**Original Measurements:**
(1) 3-Methylcholantrene; $C_{21}H_{16}$; [56-49-5] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility of 3-methylcholantrene in water

t/°C	$10^6 \cdot$ g (1)/L (2)
27	1.1
	1.8
	1.8

The best value recommended by the authors is $1.5 \cdot 10^{-6}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.5 \cdot 10^{-7}$ g (1)/100 g sln and $1.0 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Hoffman La-Roche; used as received; melting point 175.3–177.1 °C; used as received; (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: $\pm 3 \cdot 10^{-7}$ g (1)/L (2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	**Original Measurements:**
(1) 3-Methylcholantrene; $C_{21}H_{16}$; [56-49-5] (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 3-methylcholantrene in water at 25 °C was reported to be 0.0029 mg (1)/L sln and $x_1 = 1.92 \cdot 10^{-10}$.
The corresponding mass percent calculated by the compiler is $2.9 \cdot 10^{-7}$ 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 allowed to settle 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: $\pm 2.1 \cdot 10^{-4}$ mg (1)/L sln (maximum deviation from several determinations).

2.47. Benzo[*ghi*]perylene+Water

Components:
(1) Benzo[*ghi*]perylene; $C_{22}H_{12}$; [191-24-2]
(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 benzo[*ghi*]perylene in water at 25 °C was reported to be 0.00026 mg (1)/L sln and $x_1 = 1.73 \cdot 10^{-11}$.
The corresponding mass percent calculated by the compiler is $2.6 \cdot 10^{-8}$ 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 allowed to settle 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: $\pm 10^{-5}$ mg (1)/L sln (maximum deviation from several determinations).

2.48. Dibenz[*a,h*]anthracene+Water

Components:
(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of Dibenz[*a,h*]anthracene (1) in Water (2)

Calculation of reference data for this system was not possible because of insufficient data on solubility trends for this aromatic ring system. The experimental solubility data for (1) in (2) have been investigated by Davis *et al.*[1] at 300 K and Klevens[2] at 298 K.

Both the experimental data are listed in Table 18. The data reported at similar temperatures are in very good agreement with each other and are Tentative.

References:
[1]W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
[2]H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

TABLE 18. Experimental values for solubility of dibenz[a,h]anthracene (1) in water (2)

T/K	Experimental values x_1 (T=tentative)	Mean values
298	$3.9 \cdot 10^{-11}$ (T; Ref. 2)	$3.45 \cdot 10^{-11}$
300	$3.0 \cdot 10^{-11}$ (T; Ref. 1)	$3.45 \cdot 10^{-11}$

Components:	Original Measurements:
(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of dibenz[a,h]anthracene in water at 27 °C was reported to be $5 \cdot 10^{-7}$ g (1)/L (2). (Two identical results have been obtained.)

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $5 \cdot 10^{-8}$ g (1)/100 g sln and $3 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Eastman Kodak Company; purified; melting point range 266.6–266.9 °C or Hoffman La Roche; melting point range 262.7–264 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ±3 °C.
Solubility: $\pm 10^{-7}$ g (1)/L (2).

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

Components:	Original Measurements:
(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3] (2) Water; H_2O; [7732-18-5]	H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Values

The solubility of dibenz[a,h]anthracene in water at 25 °C was reported to be $2.15 \cdot 10^{-9}$ mol (1)/L sln.

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $5.84 \cdot 10^{-8}$ g (1)/100 g sln and $3.88 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

2.49. Dibenz[*a,j*]anthracene+Water

Components:
(1) Dibenz[*a*,*j*]anthracene; $C_{22}H_{14}$; [224-41-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of dibenz[*a*,*j*]anthracene in water

t/°C	$10^5 \cdot$ g (1)/L (2)
27	1.1±0.1
	1.0±0.2
	1.3±0.2

The best value recommended by the authors is $1.2 \cdot 10^{-5}$ g (1)/L (2).

Assuming that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.2 \cdot 10^{-6}$ g (1)/100 g sln and $7.8 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at the Ohio State University; melting point range 198.0–198.4 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C.
Solubility: see above.

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.50. Picene+Water

Components:
(1) Picene; $C_{22}H_{14}$; [213-46-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).

Variables:
One temperature: 27 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of picene in water at 27 °C was reported to be $2.5 \cdot 10^{-6}$ g (1)/L (2).

With the assumption that 1.00 L sln=1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.5 \cdot 10^{-7}$ g (1)/100 g sln and $1.6 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:
(1) Prepared at the Ohio State University; melting point range 363.5–364.5 °C (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:
Temperature: ±3 °C
Solubility: $\pm 5 \cdot 10^{-7}$ g (1)/L (2).

References:
[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.51. 10-Butylbenz[*a*]anthracene+Water

Components:	**Original Measurements:**
(1) 10-Butylbenz[*a*]anthracene; $C_{22}H_{20}$; [31632-63-0] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility 10-butylbenz[*a*]**anthracene in water**

t/°C	$10^6 \cdot$ g (1)/L (2)
27	7 ± 0.7
	7 ± 0.7
	7 ± 0.7
	8 ± 1
	8 ± 1

The best value recommended by the authors is $8 \cdot 10^{-6}$ g (1)/L (2).

Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $8 \cdot 10^{-7}$ g (1)/100 g sln and $5.1 \cdot 10^{-10}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 96.4–96.7 °C. (cf. Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ± 3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.52. 7-Pentylbenz[*a*]anthracene+Water

Components:	**Original Measurements:**
(1) 7-Pentylbenz[*a*]anthracene; $C_{23}H_{22}$; [63019-00-1] (2) Water; H_2O; [7732-18-5]	W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **64**, 108 (1942).
Variables:	**Prepared By:**
One temperature: 27 °C	M. C. Haulait-Pirson

Experimental Values

Solubility 7-pentylbenz[*a*]**anthracene in water**

t/°C	$10^6 \cdot$ g (1)/L (2)
27	9 ± 1
	8 ± 3
	8 ± 2

The best value recommended by the authors is $8 \cdot 10^{-7}$ g (1)/L (2).

Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $8 \cdot 10^{-8}$ g (1)/100 g sln and $5 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100 mm was employed. Many details are reported in Davis and Parker.[1]

Source and Purity of Materials:

(1) Prepared at Harvard University; melting point range 82.6–83.3 °C. (Davis *et al.*[2]).
(2) Dust-free.

Estimated Error:

Temperature: ± 3 °C.
Solubility: see above.

References:

[1]W. W. Davis, Jr. and T. V. Parker, J. Am. Chem. Soc. **64**, 101 (1942).
[2]W. W. Davis, M. E. Krahl, and G. H. A. Cloves, J. Am. Chem. Soc. **62**, 3086 (1940).

2.53. Coronene+Water

Components:
(1) Coronene; $C_{24}H_{12}$; [191-07-1]
(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 coronene in water at 25 °C was reported to be 0.00014 mg (1)/L sln and $x_1 = 8.56 \cdot 10^{-12}$.
The corresponding mass percent calculated by the compiler is $1.4 \cdot 10^{-8}$ 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 allowed to settle 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: $\pm 2 \cdot 10^{-5}$ mg (1)/L sln (maximum deviation from several determinations).

2.54. Hexacosane+Water

Components:
(1) Hexacosane; $C_{26}H_{54}$; [630-01-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of hexacosane in water at 25 °C was reported to be $1.7 \cdot 10^{-7}$ g (1)/100 g (2) corresponding to a mole fraction (x_1) of $8 \cdot 10^{-11}$.

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 through a 0.45 μm Millipore filter, then extracted three 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%.

2.55. Squalene+Water

Components:
(1) Squalane; $C_{30}H_{62}$; [111-01-3]
(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: 637.2–658.9 K
Pressure: 197.9–312.1 bar

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

Experimental Values

Solubility of squalane in water

T/K	P/bar	g (1)/100 g sln (compilers)	x_1
637.2	197.9	1.4	0.0006
	201.5	3.0	0.0013
	204.9	3.2	0.0014
	208.3	2.5	0.0011
	225.6	1.4	0.0006
	268.8	0.7	0.0003
	312.0	0.5	0.0002
642.2	221.1[a]	22.2	0.0120
	221.4	10.5	0.0050
	224.3	13.1	0.0064
	226.0	7.6	0.0035
	242.9	3.2	0.0014
	243.0	2.5	0.0011
	277.5	1.4	0.0006
	312.1	0.7	0.0003
653.2	265.2[a]	38.5	0.026
	270.5	63.1	0.068
	277.4	69.6	0.089
	294.7	75.3	0.115
658.9	292.7[a]	—	—

Solubility of water in squalane

T/K	P/bar	g (2)/100 g sln (compilers)	x_2
637.2	197.9	86.51	0.9934
	201.5	75.01	0.9860
	204.9	42.27	0.945
	208.3	26.64	0.895
	225.6	19.70	0.852
	268.8	15.29	0.809
	312.0	13.33	0.783
642.2	221.1[a]	77.82	0.988
	221.4	62.82	0.9754
	224.3	62.24	0.9748
	226.0	40.03	0.940
	242.9	22.65	0.873
	243.0	22.81	0.874
	277.5	17.53	0.833
	312.1	15.29	0.809
653.2	265.2[a]	61.48	0.974
	270.5	87.23	0.9938
	277.4	92.59	0.9966
	294.7	96.16	0.9983

[a]Liquid–liquid critical point.

Auxiliary Information

Method/Apparatus/Procedure:
A flow apparatus for the high temperature experiments was used. Streams of both components were combined, mixed, preheated, and pumped into a 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. 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 Chemical 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.

2.56. Hexatriacontane+Water

Components:
(1) Hexatriacontane; $C_{36}H_{74}$; [630-06-8]
(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 hexatriacontane-18,19-C^{14} in water at 25 °C was reported to be $1.7 \cdot 10^{-9}$ g (1)/g (2).

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $1.7 \cdot 10^{-7}$ g (1)/100 g sln and $6.1 \cdot 10^{-11}$, 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) New England Nuclear 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**, 5 (1956).

Components:
(1) Hexatriacontane; $C_{36}H_{74}$; [630-06-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. G. Baker, Science **129**, 871 (1959).

Variables:
One temperature: 25 °C

Prepared By:
F. Kapuku

Experimental Values

The solubility of hexatriacontane in water at 25 °C was reported to be $2.09 \cdot 10^{-7}$ mL (1)/100 mL (2).

Auxiliary Information

Method/Apparatus/Procedure:
Not specified.

Source and Purity of Materials:
Not specified.

Estimated Error:
Not specified.

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

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

5. Author Index

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