

IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated Part 12. C₅–C₂₆ Hydrocarbons with Seawater

Volume Editors

David G. Shaw^{a)}

University of Alaska, Fairbanks, Alaska, USA

Andrzej Maczynski^{b)}

Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Compilers

G. T. Hefter

Murdoch University, Perth, Australia

M. Kleinschmidt

University of Alaska, Fairbanks, Alaska, USA

D. Mackay

University of Toronto, Toronto, Canada

P. A Meyers

University of Michigan, Ann Arbor, Michigan, USA

H. Miyamoto

Niigata University, Niigata, Japan

W. Y. Shiu

University of Toronto, Toronto, Canada

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The mutual solubility of C₅–C₂₆ hydrocarbons with seawater is exhaustively and critically reviewed. Reports of experimental determination of solubility in 46 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For 15 of these 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. © 2006 American Institute of Physics. [DOI: 10.1063/1.2132316]

Key words: critical evaluation; hydrocarbons; seawater; solubility; water.

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^{a)}Electronic mail: davidshaw@post.harvard.edu

^{b)}Electronic mail: macz@ichf.edu.pl

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1. Preface

1.1. Scope of this Volume

This paper is Part 12 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). An exhaustive search of the primary chemical literature through the end of 2002 showed that no new measurements of solubility of hydrocarbons in seawater had been reported since the original review was completed. All new evaluations were prepared for this revision comparing experimental results for a given hydrocarbon seawater system to one another and to the related hydrocarbon water system. In these evaluations reported solubility values are characterized as "Recommended, Tentative, Doubtful, or Rejected," based on consistency between independently determined experimental values. Recommended values are supported by two (or more) independent experimental values that agree within experimental precision and appear to be free of serious experimental problems. Tentative values are supported by two (or more) independent values in agreement with each other at a level slightly below that needed for a Recommended value or by a single value that is consistent with a Recommended value at nearby conditions of temperature or salinity. Experimental values that differ from other experimental values are Doubtful or Rejected.

A variety of units for the expression of solubility has appeared in the primary literature. 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. Where such conversions have been made, they are clearly attributed to the compiler and the source of any data not provided by the original investigators (e.g., hydrocarbon or seawater density) is specified. Defini-

tions of mass percent and mole fraction as well as their relationship to other common measures of solubility are given in the Introduction to this Volume.

The expression of the solubility of a hydrocarbon in natural seawater on a mole fraction basis presents special difficulties since the composition of seawater is not fully known and somewhat variable. However, the uncertainty introduced by this factor is generally less than 3%, smaller than the measurement uncertainty associated with many of the data. Some data for hydrocarbon solubility in seawater have been given in terms of the Setschenow (also transliterated from the Russian as Sechenov and Setchenoff) equation. A detailed discussion, "The Sechenov Salt Effect Parameter" has appeared in press.³

Most measurements of hydrocarbon solubility in seawater have been made in the temperature range considered "room temperature" (275–300 K). In most reports system pressure

is unspecified but can be assumed to be approximately 100 kPa (1 atm). For most purposes this lack of specification of system pressure is not important since hydrocarbon/water solubilities do not vary strongly with pressure.

The editors wish to acknowledge the efforts compilers, reviewers, and others whose careful work has contributed to this paper.

1.2. References for the Preface

- ¹D. Shaw, Editor, *IUPAC Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C₅ to C₇ (Pergamon, New York, 1989).
- ²D. Shaw, Editor, *IUPAC Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C₈ to C₃₆ (Pergamon, New York, 1989).
- ³R. Battino, Editor, *IUPAC Solubility Data Series*, Vol. 10, Nitrogen and Air (Pergamon, New York, 1982), pp. xxix–xlili.

2. C₅ Hydrocarbons with Seawater

2.1. Pentane+Seawater

Components:		Original Measurements:	
(1) Pentane; C ₅ H ₁₂ ; [109-66-0] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]		L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
Variables:		Prepared By:	
One temperature: 25 °C Salinity: 1–360 g (2)/kg sln		M. Kleinschmidt and D. G. Shaw	
Experimental Values			
Solubility of pentane in aqueous NaCl			
<i>t</i> /°C	10 ⁶ · <i>x</i> ₁ (compiler)	10 ³ · g (1)/100 g sln	Salinity g (2)/kg sln
25	9.19	3.68	1.002
	8.67	3.45	10.000
	7.05	2.76	34.472 ^a
	5.84	2.26	50.030
	2.95	1.09	125.100
	1.67	0.591	199.900
	0.777	0.264	279.800
	0.614	0.201	358.700

^aArtificial seawater, composition not specified but probably similar to Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
Details given in the source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) Commercial, 99+ % pure.
Estimated Error:	References:
Temperature: ±1 °C. Solubility: ±10 relative %.	¹ J. Lyman and R. H. Fleming, J. Mar. Res. 3 , 135 (1940).

2.2. Benzene+Seawater

Components:	Evaluators:
(1) Benzene; C ₆ H ₆ ; [71-43-2] (2) Seawater	D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Benzene (1) in Seawater (2)

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

Author (s)	<i>T</i> /K	Salinity g salts/kg sln
Brown and Wasik ¹	273–293	34.42
Mackay and Shiu ²	298	0–200
May <i>et al.</i> ³	298	0–40
Price ⁴	298	1–360

Reference solubility data for benzene in pure water at 298 K were reported in Part 2 (Maczynski and Shaw⁶) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 1. At 298 K and a salinity of 34.47 and 35 g salts/kg sln, the values of Mackay and Shiu,² May *et al.*,³ and Price⁴ are in very good agreement. Each group of workers has also determined the solubility of toluene in pure water and obtained results within experimental error the reference value. Therefore, the mean of the reported values, 0.135 g (1)/100 g sln, is accepted as Recommended at the indicated temperature and salinity. These studies measured solubility over range of salinities. Mackay and Shiu² reported their data in terms of the Setschenov equation. Their values may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

Brown and Wasik¹ determined the solubility of benzene in seawater at a salinity of 34.42 g salts/kg sln over the temperature range 273–293 K. Linear extrapolation by the Evaluators of these results to 298 K gives a value 0.127 g (1)/100 g. This suggests that the results of Brown and Wasik¹ may be slightly low and are Doubtful.

Rejected and Inaccessible Data

The data reported by Umamo and Hayano⁵ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

- ¹R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).
- ²D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).
- ³W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
- ⁴L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
- ⁵S. Umamo and I. Hayano, Kogyo Kagaku Zasshi **60**, 1436 (1957).
- ⁶A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater-Revised and Updated, Part 2. Benzene with Water and Heavy Water*, J. Phys. Chem. Ref. Data **34**(2), 477 (2005).

TABLE 1. Experimental values for solubility of benzene (1) in seawater (2)

<i>T</i> /K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful, R=recommended)	Reference value for pure water g (1)/100 g sln ±30%
298	35	0.136 (R; mean from Refs. 2, 3, 4)	0.18
	34.42 (Ref. 1)	0.128 (D; Ref. 1)	
	35 (Ref. 2)	0.134 (R; Ref. 2)	
	35 (Ref. 3)	0.1365 (R; Ref. 3)	
	35 (Ref. 4)	0.1391 (R; Ref. 4)	

Components:

(1) Benzene; C₆H₆; [71-43-2]
 (2) Artificial seawater

Original Measurements:

R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A
78, 453 (1974).

Variables:

Temperature: 0–20 °C
 Salinity: 34.42 g salts/kg sln

Prepared By:

G. T. Hefter and D. G. Shaw

Experimental Values

Solubility of benzene in water in artificial seawater

<i>t</i> /°C	10 ⁴ · <i>x</i> ₁ (compiler)	g (1)/100 g sln ^a
0.19	3.129	0.1323 (0.0017)
5.32	3.255	0.1376 (0.0022)
10.05	3.186	0.1347 (0.0023)
14.96	3.117	0.1318 (0.0025)
20.04	3.065	0.1296 (0.0022)

^aNumbers in parentheses are standard deviations from 4 observations.

Auxiliary Information**Method/Apparatus/Procedure:**

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibrium cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:

(1) 99.99 mole % purity; source and methods of purification not specified.
 (2) Prepared according to Sverdrup *et al.*¹ Purity not specified.

Estimated Error:

Temperature: ±0.01 °C.
 Solubility: see table above.

References:

¹H. U. Sverdrup, M. W. Johnson, and R. H. Fleming, *The Oceans* (Prentice-Hall, Englewood Cliffs, New Jersey, 1942), p. 186.

Components:

(1) Benzene; C₆H₆; [71-43-2]
 (2) Sodium Chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).

Variables:

One temperature: 25 °C
 Salinity: 0–200 g (2)/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

*S*₀ is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

*K*_{*S*} is the Setschenow constant (L/mol); and

*C*_{*S*} is the concentration of sodium chloride (L/mol);

evaluating the equation for *S* over the range of *C*_{*S*} 0–4 mol/L, *K*_{*S*} = 0.1836 ± 0.0072 (standard error) with *S*₀ = 1779.5 ± 16.4.

The corresponding mass percent and mole fraction, *x*₁, at salinity = 35 g (2)/kg sln calculated by the compilers are 0.1340 g (1)/100 g sln and 3.227 · 10^{−4} assuming a solution density of 1.025 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

Solubility was determined by vapor phase extraction and gas chromatograph analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.

Source and Purity of Materials:

(1) Research grade, 99.9+ %, from Phillips Petroleum Co.
 (2) and (3) Not specified.

Estimated Error:

Temperature: ±0.1 °C.
 Solubility: 95% confidence limit is about 8%.

Components:

- (1) Benzene; C₆H₆; [71-43-2]
 (2) Sodium Chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [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
 Salinity: 0–40 g(2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackey

Experimental Values

The solubility of benzene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol);

evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S=0.175$ with $S_0=1791$.

The corresponding mass percent and mole fraction x_1 , at salinity=35 g (2)/kg sln calculated by the compilers are 0.1365 g (1)/100 g sln and $3.22 \cdot 10^{-4}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a generation column which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an extractor column packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
 (2) Reagent grade.
 (3) Distilled from potassium–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.006 ; $S_0 \pm 10$.

Components:

- (1) Benzene; C₆H₆; [71-43-2]
 (2) Sodium Chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:

One temperature: 25 °C
 Salinity: 1–360 g (2)/kg sln

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

Solubility of benzene in aqueous NaCl at 25 °C

10 ⁴ · x ₁ (compiler)	g (1)/100 g sln	Salinity g (2)/kg sln
3.96	0.1718	1.002
3.78	0.1628	10.000
3.28	0.1391	34.472 ^a
2.85	0.1194	50.030
1.48	0.0593	125.100
1.01	0.0388	199.900
0.581	0.0214	279.800
0.378	0.0134	358.700

^aArtificial seawater, composition not specified but probably similar to Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

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

Source and Purity of Materials:

(1) Commercial, 99+ % pure.

Estimated Error:

Temperature: ± 1 °C.
 Solubility: ± 0 relative %.

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

Auxiliary Information

Components:

(1) Benzene; C₆H₆; [71-43-2]
 (2) Sodium Chloride; NaCl; [76-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

S. Umano and I. Hayano, Kogyo Kagaku Zasshi **60**, 1436 (1957).

Variables:

Temperature: 20–284 °C
 Concentration of NaCl

Prepared By:

H. Miyamoto and G. T. Hefter

Experimental Values

Solubility of water in benzene at system pressure

<i>t</i> /°C	10 ² · <i>x</i> ₂ (compiler)	g (3)/100 g sln	Concn. NaCl ^a
281.0	63.29	28.46	0.0
271.5	59.24	25.11	0.0
250.1	47.41	17.22	0.0
223.0	29.95	8.98	
186.0	16.7	4.42	
78.0	0.103	0.240	9.939
66.0	0.814	0.189	
40.0	3.29	0.0762	
20.2	1.82	0.042	
284.0	62.11	27.44	10.0
265.0	50.27	18.91	
249.0 ^b	39.35	13.02	
223.0 ^c	26.4	7.65	
183.5	14.3	3.70	
81.0	0.67	0.155	19.200
63.0	0.34	0.079	
40.0	0.16	0.037	
21.0	0.10	0.024	
280.0	48.6	17.93	20.0
265.0	40.5	13.56	
245.0	27.3	7.96	
221.0	15.2	3.98	
178.0	6.3	1.52	
277.5	43.7	15.17	
268.5	38.2	12.47	
245.5	23.7	6.69	
219.0	14.8	3.85	
178.0	6.5	1.58	

^aStated as % in the paper; presumably g (2)/100 g sln (compilers).

^bGiven as 294.0 in the original (corrected in personal communication by the authors to H. Miyamoto).

^c*P* = 54.23 atm.

Method/Apparatus/Procedure:

At higher temperatures (1) and the aqueous brine were placed in an autoclave, described in detail in the paper, and equilibrated by stirring. After settling, the solubility of (3) in (1) was determined volumetrically by withdrawing layers from the autoclave into a burette. At lower temperatures (1) and the aqueous solution were refluxed in a flask at constant temperature. After equilibration, an aliquot of the water rich layer was withdrawn and analyzed argentometrically and the solubility of (3) in (1) calculated. The solubility of NaCl in benzene was determined to be negligible in these experiments ($8 \cdot 10^{-5}$ mol/L at 223 °C and 54.23 atm).

Source and Purity of Materials:

(1) C. P. grade; source not specified; purified by single fractional distillation.
 (2) Not specified.
 (3) C. P. grade; source not specified; recrystallized.

Estimated Error:

Not specified.

2.3. Methylcyclopentane+Seawater

Components:		Original Measurements:	
(1) Methylcyclopentane; C ₆ H ₁₂ ; [96-37-7]		L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).	
(2) Sodium Chloride; NaCl; [7647-14-5]			
(3) Water; H ₂ O; [7732-18-5]			
Variables:		Prepared By:	
One temperature: 25 °C		M. Kleinschmidt and D. G. Shaw	
Salinity: 1–360 g (2)/kg sln			
Experimental Values			
Solubility of methylcyclopentane in aqueous NaCl			
<i>t</i> /°C	10 ⁶ · <i>x</i> ₁ (compiler)	g (1)/100 g sln	g (2)/100 g sln
25	8.14	0.00380	1.002
	7.82	0.00363	10.000
	6.40	0.00292	34.472 ^a
	5.98	0.00270	50.030
	2.94	0.00127	125.100
	1.38	0.000572	199.900
	0.847	0.000336	279.800
	0.495	0.000189	358.700

^aArtificial sea water, composition not specified but probably similar to Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Commercial, 99+ % pure.

Estimated Error:

Temperature: ± 1 °C.
Solubility: ± 10 relative %.

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.4. Hexane+Seawater

Components:		Evaluators:	
(1) Hexane; C ₆ H ₁₄ ; [110-54-3]		D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.	
(2) Seawater		A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.	

Critical Evaluation of Solubility of Hexane (1) in Seawater (2)

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

Author (s)	<i>T</i> /K	Salinity g salts/kg sln
Aquan-Yuen <i>et al.</i> ¹	298	17.9–132.7
Freearde <i>et al.</i> ²	not specified	not specified
Krasnoshchekova and Gubergits ³	298	6

Reference solubility data for hexane in pure water at 298 K were reported in Part 4 (Maczynski and Shaw⁴) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 2. Two determinations of Aquan-Yuen *et al.*¹ and Krasnoshchekova and Gubergits³ were made at somewhat different salinities and thus cannot be directly compared. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergits³ are Doubtful. The data of Aquan-Yuen *et al.*¹ are Tentative.

Rejected and Inaccessible Data

The data reported by Freearde *et al.*² lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

¹M. Aquan-Yuen, D. Mackay, and W. Y. Shiu, J. Chem. Eng. Data **24**, 30 (1979).

²M. M. Freearde, C. G. Hatchard, and C. A. Parker, Lab Pract. **20**, 35 (1971).

³P. Ya. Krasnoshchekova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

⁴A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 4. C₆H₁₄ Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **34**(2), 754 (2005).

TABLE 2. Experimental values for solubility of hexane (1) in seawater (2)

<i>T</i> /K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative, D=doubtful)	Reference value for pure water g (1)/100 g sln ± 30%
298	17.9 (Ref. 1)	1.035 · 10 ⁻³ (T; Ref. 1)	1.15 · 10 ⁻³
	35.3 (Ref. 1)	7.86 · 10 ⁻⁴ (T; Ref. 1)	
	56.2 (Ref. 1)	7.25 · 10 ⁻⁴ (T; Ref. 1)	
	82.6 (Ref. 1)	4.60 · 10 ⁻⁴ (T; Ref. 1)	
	108.2 (Ref. 1)	3.47 · 10 ⁻⁴ (T; Ref. 1)	
	132.7 (Ref. 1)	2.32 · 10 ⁻⁴ (T; Ref. 1)	
	6 (Ref. 3)	7.55 · 10 ⁻³ (D; Ref. 3)	

Components:

- (1) Hexane; C₆H₁₄; [110-54-3]
 (2) Sodium Chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

M. Aquan-Yuen, D. Mackay, and W. Y. Shiu, J. Chem. Eng. Data
24, 30 (1979).

Variables:

One temperature: 25 °C
 Salinity: 18–130 g (2)/kg sln.

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

Solubility of hexane in aqueous NaCl

<i>t</i> /°C	10 ⁶ · <i>x</i> ₁ ^a	10 ⁴ · g (1)/100 g sln ^a	10 ³ · g (1)/L sln	g (2)/kg sln ^a	mol (2)/L sln
25	2.19	10.35	10.48	17.9	0.31
	1.68	7.86	8.06	35.3	0.62
	1.58	7.25	7.54	56.2	1.00
	1.08	4.60	4.88	82.6	1.50
	0.846	3.47	3.75	108.2	2.00
	0.583	2.32	2.55	132.7	2.50

^aCalculated by compilers.

Auxiliary Information**Method/Apparatus/Procedure:**

Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 h and then allowed to settle for 48 h. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.

Source and Purity of Materials:

- (1) 99% pure from Fisher Scientific.
 (2) Reagent grade.

Estimated Error:

Solubility: ± 1 relative %.

Components:

- (1) Hexane; C₆H₁₄; [110-54-3]
 (2) Seawater

Original Measurements:

P. Ya. Krasnoshechekova and M. Ya. Gubergrits, Neftekhimiya
13, 885 (1973).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of hexane in seawater was reported to be $7.55 \cdot 10^{-3}$ g (1)/100 g sln and the corresponding mole fraction, $x_1 = 1.3 \cdot 10^{-5}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

Source and Purity of Materials:

- (1) "Chemically pure."
 (2) Distilled water plus salt mixture.

Estimated Error:

Not specified.

2.5. Toluene+Seawater

Components:

(1) Toluene; C₇H₈; [108-88-3]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Toluene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Brown and Wasik ¹	273–293	34.42
Mackay and Shiu ²	298	0–200
Price ³	298	1–360
Rossi and Thomas ⁴	288–298	35
Sada <i>et al.</i> ⁵	298	29–108
Sutton and Calder ⁶	298	34.5

Reference solubility data for toluene in pure water at 298 K were reported in Part 5 (Maczynski and Shaw⁷) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 3. At 298 K and a salinity of 35 g salts/kg sln, the values of Mackay and Shiu,² Price,³ and Sutton and Calder,⁶ and are in very good agreement. Each group of workers has also determined the solubility of toluene in pure water and obtained results within experimental error the reference value. Therefore, the mean of the reported values, $3.87 \cdot 10^{-2}$ g(1)/100 g sln, is accepted as the Recommended value at the indicated temperature and salinity. Mackay and Shiu² measured solubility over a range of salinities and reported their data in terms of the Setschenov equation. Their values may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

Brown and Wasik¹ determined the solubility of toluene in seawater at a salinity of 34.42 salts/kg sln over the temperature range 273–293 K. Linear extrapolation by the Evaluators of these results to 298 K gives a value $3.80 \cdot 10^{-2}$ g(1)/100 g. This suggests that the results of Brown and Wasik¹ may be consistent with the Recommended value. The values reported by Sada *et al.*,⁵ and Rossi and Thomas⁴ are in poorer agreement with the remaining data and are Doubtful.

References:

- ¹R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).
²D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).
³L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
⁴S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
⁵E. Sada, S. Kito, and Y. Ito, J. Chem. Eng. Data **20**, 373 (1975).
⁶C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
⁷A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series, 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 5. C₇ Hydrocarbons with Water and Heavy Water*, J. Phys. Chem. Ref. Data **34**(3), (2005).

TABLE 3. Experimental values for solubility of toluene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful, R=recommended)	Reference value for pure water g (1)/100 g sln ± 30%
298	35	$3.87 \cdot 10^{-2}$ (R; mean from Refs. 2, 3, and 6)	$5.6 \cdot 10^{-2}$
	34.42 (Ref. 1)	$3.80 \cdot 10^{-2}$ (R; Ref. 1)	
	35 (Ref. 2)	$3.79 \cdot 10^{-2}$ (R; Ref. 2)	
	34.47 (Ref. 3)	$4.02 \cdot 10^{-2}$ (R; Ref. 3)	
	35 (Ref. 4)	$4.2 \cdot 10^{-2}$ (D; Ref. 4)	
	28.72 (Ref. 5)	$3.48 \cdot 10^{-2}$ (D; Ref. 5)	
	34.5 (Ref. 6)	$3.793 \cdot 10^{-2}$ (R; Ref. 6)	

Components: (1) Toluene; C ₇ H ₈ ; [108-88-3] (2) Artificial seawater	Original Measurements: R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A 78, 453 (1974).
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Variables: Temperature: 0–20 °C Salinity: 34.42 g salts/kg sln	Prepared By: G. T. Hefter and D. G. Shaw
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Experimental Values
Solubility of toluene in artificial seawater

<i>t</i> /°C	10 ⁵ · <i>x</i> ₁ (compiler)	g (1)/100 g sln ^a
0.19	9.0	0.0449 (0.0006)
5.32	8.60	0.0429 (0.0007)
10.05	8.34	0.0416 (0.0008)
14.96	8.12	0.0405 (0.0008)
20.04	7.96	0.0397 (0.0008)

^aNumbers in parentheses are standard deviations from 4 observations.

Auxiliary Information

Method/Apparatus/Procedure: Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.	Source and Purity of Materials: (1) 99.99 mole % purity; source and methods of purification not specified. (2) Prepared according to Sverdrup <i>et al.</i> ¹ Purity not specified. Estimated Error: Temperature: ±0.01 °C. Solubility: see table above. References: ¹ H. U. Sverdrup, M. W. Johnson, and R. H. Fleming, <i>The Oceans</i> (Prentice-Hall, Englewood Cliffs, New Jersey, 1942), p. 186.
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Components: (1) Toluene; C ₇ H ₈ ; [108-88-3] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. 53, 239 (1975).
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Variables: One temperature: 25 °C Salinity: 0–200 g (2)/kg sln	Prepared By: M. Kleinschmidt and D. G. Shaw
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Experimental Values

The solubility of benzene in solutions of sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S*₀ is the solubility of (1) in water (mg/L);
- S* is the solubility of (1) in solution (mg/L);
- K*_{*S*} is the Setschenow constant (L/mol); and
- C*_{*S*} is the concentration of sodium chloride (L/mol)

evaluating the equation for *S* over the range of *C*_{*S*} 0–4 mol/L, *K*_{*S*} = 0.2052 ± 0.0056 (standard error) with *S*₀ = 519.5 ± 9.6.

The corresponding mass percent and mole fraction, *x*₁, at salinity = 35 g (2)/kg sln calculated by the compilers are 3.79 · 10⁻² g (1)/100 g sln and 7.743 · 10⁻⁵ assuming a solution density of 1.025 kg/L.

Auxiliary Information

Method/Apparatus/Procedure: Solubility was determined by vapor phase extraction and gas chromatograph analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.	Source and Purity of Materials: (1) Research grade, 99.9+%, from Phillips Petroleum Co. (2) and (3) Not specified. Estimated Error: Temperature: ±0.1 °C. Solubility: 95% confidence limit is about 8%.
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Components: (1) Toluene; C ₇ H ₈ ; [108-88-3] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: L. C. Price, Am. Assoc. Pet. Geol. Bull. 60 , 213 (1976).
Variables: One temperature: 25 °C Salinity: 1–360 g (2)/kg sln	Prepared By: M. Kleinschmidt and D. Shaw

Experimental Values
Solubility of toluene in aqueous NaCl

<i>t</i> /°C	10 ⁵ · <i>x</i> ₁ (compiler)	g (1)/100 g sln	g (2)/kg sln
25	10.3	0.0526	1.002
25	9.65	0.0490	10.000
25	8.04	0.0402	34.472 ^a
25	7.26	0.0359	50.030
25	3.85	0.0182	125.100
25	2.34	0.0106	199.900
25	1.24	0.00538	279.800
25	0.890	0.00372	358.700

^aArtificial seawater, composition not specified but probably similar to Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Commercial, 99+ % pure.

Estimated Error:

Temperature: ± 1 °C.
Solubility: ± 10 relative %.

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

Components: (1) Toluene; C ₇ H ₈ ; [108-88-3] (2) Seawater; natural; H ₂ O	Original Measurements: S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. 15 , 715 (1981).
Variables: Temperature: 15–25 °C Salinity: 35 g/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values
Solubility of toluene in seawater

<i>t</i> /°C	10 ⁵ · <i>x</i> ₁	g (1)/100 g sln	μg (1)/g sln
15	8.2	0.041	410
20	8.2	0.041	410
25	8.4	0.042	418.5

Auxiliary Information

Method/Apparatus/Procedure:

Saturate solution was prepared by equilibrating seawater with an excess of hydrocarbon for 24 h in a constant temperature gyrotary shaker followed by 12 h stationary period. A 100 mL aliquot was extracted three times with hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the hydrocarbon concentration.

Source and Purity of Materials:

(1) From Burdick and Jackson, triple distilled in glass
(2) Collected off Scripps Pier and filtered twice through 0.22 μm membrane and twice extracted with hexane then its salinity adjusted to 35%.
(3) Hexane doubly distilled in glass.

Estimated Error:

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

Components:

- (1) Toluene; C₇H₈; [108-88-3]
 (2) Sodium Chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

E. Sada, S. Kito, and Y. Ito, *J. Chem. Eng. Data* **20**, 373 (1975).

Variables:

One temperature: 25 °C
 Salinity: 29–108 g (3)/kg sln

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

Solubility of toluene in aqueous sodium chloride solutions

<i>t</i> /°C	10 ⁵ · <i>x</i> ₁ ^a	g (1)/100 g sln ^a	L (1)/10 ³ L sln	g (2)/kg sln ^a	mol (2)/L sln
25	6.95	0.0348	0.410	28.72	0.5011
	5.06	0.0248	0.298	56.14	0.9991
	3.76	0.0182	0.223	82.66	1.4933
	2.87	0.0136	0.169	107.9	1.9933

^aCalculated by compilers using density and other physical data for NaCl solutions from Weast¹ and the assumption that the density of (1) is 0.8669 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

Experimental apparatus and procedure used similar to those in Sobotka and Kahn.² Toluene stained with 0.1% by weight. Sudan IV was added dropwise from a microburet into aqueous salt solution retained in a 1 L dissolution flask which was kept at 25.00 ± 0.01 °C in a thermostatically controlled water bath. The aqueous by a magnetic stirring device. Before saturation was reached, the Sudan IV was precipitated and floated on the surface as a solid. At saturation, the excess toluene appeared as immiscible red liquid droplets suspended in the aqueous solution. To ensure complete saturation, 24 h was allowed for equilibration.

Source and Purity of Materials:

- (1) Reagent grade, source not specified.
 (2) Reagent grade, source not specified.
 (3) Not specified.

Estimated Error:

Solubility: 10⁻⁶ L (1)/L sln.

References:

- ¹R. C. Weast, *CRC Handbook of Chemistry and Physics*, 59th Ed. (CRC, Boca Raton, FL, 1972), pp. D299–D300.
²H. Sobotka and J. Kahn, *J. Am. Chem. Soc.* **53**, 2935 (1948).

Components:

- (1) Toluene; C₇H₈; [108-88-3]
 (2) Artificial seawater (Ref. 1)

Original Measurements:

C. Sutton and J. A. Calder, *J. Chem. Eng. Data* **20**, 320 (1975).

Variables:

One temperature: 25 °C
 Salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of toluene in artificial seawater is reported to be 379.3 mg (1)/kg sln.

The corresponding mass percent and mole fraction, *x*₁ calculated by the compiler are 0.03793 g (1)/100 g sln and 7.61 · 10⁻⁵ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 2.8 (standard deviation).

References:

- ¹J. Lyman and R. H. Fleming, *J. Mar. Res.* **3**, 135 (1940).

2.6. Heptane+Seawater

Components:

(1) Heptane; C₇H₁₆; [142-82-5]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Heptane (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Freegarde <i>et al.</i> ¹	not specified	not specified
Krasnoshchekova and Gubergrits ²	298	6

Reference solubility data for heptane in pure water at 298 K were reported in Part 5 (Maczynski and Shaw³) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 4. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergrits² are considered Doubtful.

Rejected and Inaccessible Data

The data reported by Freegarde *et al.*¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

¹M. M. Freegarde, C. G. Hatchard, and C. A. Parker, Lab Pract. **20**, 35 (1971).

²P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

³A. Maczynski and D. Shaw, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 5. C₇ Hydrocarbons with Water and Heavy Water*, J. Phys. Chem. Ref. Data **34**(3), (2005).

Components:

(1) Heptane; C₇H₁₆; [142-82-5]
 (2) Seawater

Original Measurements:

P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of heptane in seawater was reported to be $1.03 \cdot 10^{-3}$ g (1)/100 g sln and the corresponding mole fraction, $x_1 = 1.9 \cdot 10^{-6}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution

Source and Purity of Materials:

(1) "Chemically pure."
 (2) Distilled water plus salt mixture.

Estimated Error:

Not specified.

TABLE 4. Experimental values for solubility of heptane (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful)	Reference value for pure water g (1)/100 g sln $\pm 30\%$
298	6 (Ref. 2)	$1.03 \cdot 10^{-3}$ (D; Ref. 2)	$2.95 \cdot 10^{-4}$

2.7. *o*-Xylene+Seawater

Components:

- (1) *o*-Xylene; C₈H₁₀; [95-47-6]
(2) Artificial seawater (Ref. 1)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of *o*-xylene in artificial seawater is reported to be 129.6 mg (1)/kg sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.01296 g (1)/100 g sln and $2.26 \cdot 10^{-5}$ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: 1.8 (standard deviation)

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.8. *m*-Xylene+Seawater

Components:

- (1) *m*-Xylene; C₈H₁₀; [108-38-3]
(2) Artificial seawater (Ref. 1)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility *m*-xylene in artificial seawater is reported to be 106.0 mg (1)/kg sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.01060 g (1)/100 g sln and $1.85 \cdot 10^{-5}$ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: 0.6 (standard deviation)

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.9. *p*-Xylene+Seawater**Components:**

(1) *p*-Xylene; C₈H₁₀; [106-42-3]
 (2) Artificial seawater

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
 One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of *p*-xylene in artificial seawater is reported to be 110.9 mg (1)/kg sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.01109 g (1)/100 g sln and $1.93 \cdot 10^{-5}$ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

(1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 0.9 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.10. Ethylbenzene+Seawater

Components:

(1) Ethylbenzene; C₈H₁₀; [100-41-4]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Ethylbenzene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Brown and Wasik ¹	273–293	34.4
Sutton and Calder ²	298	34.5

Reference solubility data for ethylbenzene in pure water at 273–298 K were reported in Part 6 (Shaw and A. Maczynski³) and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 5. The reported data are all from different temperatures, thus precluding direct comparison. Since the data are in only fair agreement with each other and with the reference values for the solubility of ethylbenzene in pure water, all the values are Tentative.

References:

¹R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).

²C. Sutton and J. A. Calder, Environ. Sci. Technol. **8**, 654 (1974).

³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 6. C₆H₆–C₈H₁₀ Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **34**(3), (2005).

TABLE 5. Experimental values for solubility of ethylbenzene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative)	Reference value for pure water g (1)/100 g sln $\pm 30\%$
273	34.42	$1.40 \cdot 10^{-2}$ (T; Ref. 1)	$2.00 \cdot 10^{-2}$
278	34.42	$1.33 \cdot 10^{-2}$ (T; Ref. 1)	$1.94 \cdot 10^{-2}$
283	34.42	$1.29 \cdot 10^{-2}$ (T; Ref. 1)	$1.88 \cdot 10^{-2}$
288	34.42	$1.25 \cdot 10^{-2}$ (T; Ref. 1)	$1.82 \cdot 10^{-2}$
293	34.42	$1.22 \cdot 10^{-2}$ (T; Ref. 1)	$1.88 \cdot 10^{-2}$
298	34.5	$1.11 \cdot 10^{-2}$ (T; Ref. 2)	$1.88 \cdot 10^{-2}$

Components: (1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Artificial seawater	Original Measurements: R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A 78 , 453 (1974).
Variables: Temperature: 0–20 °C Salinity: 34.42 g salts/kg sln	Prepared By: G. T. Hefter and D. G. Shaw

Experimental Values

Solubility of ethylbenzene in artificial seawater

<i>t</i> /°C	10 ³ · <i>x</i> ₁ (compiler)	g (1)/100 g sln
0.19	2.44	0.0140 (0.0002)
5.32	2.31	0.0133 (0.0003)
10.05	2.25	0.0129 (0.0003)
14.96	2.18	0.0125 (0.0003)
20.04	2.12	0.0122 (0.0003)

Auxiliary Information**Method/Apparatus/Procedure:**

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 L of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities is not given.

Source and Purity of Materials:

(1) 99.99 mole % purity; source and methods of purification not specified.
(2) Prepared according to Sverdrup *et al.*¹ Purity not specified.

Estimated Error:

Temperature: ±0.01 °C.
Solubility: see table above.

References:

¹H. U. Sverdrup, M. W. Johnson, and R. H. Fleming, *The Oceans* (Prentice-Hall, Englewood Cliffs, New Jersey, 1942), p. 186.

Components: (1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Artificial seawater (Lyman and Fleming ¹)	Original Measurements: C. Sutton and J. A. Calder, J. Chem. Eng. Data 20 , 320 (1975).
Variables: One temperature: 25.0 °C One salinity: 34.5 g salts/kg sln	Prepared By: M. Kleinschmidt

Experimental Values

The solubility of ethylbenzene in artificial seawater is reported to be 111.0 mg (1)/kg sln.

The corresponding mass percent and mole fraction, *x*₁, calculated by the compiler are 0.01110 g (1)/100 g sln and 1.9 · 10⁻⁵ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

(1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1.3 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.11. Octane+Seawater

Components:

(1) Octane; C₈H₁₈; [111-65-9]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Octane (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Freegarde <i>et al.</i> ¹	not specified	not specified
Krasnoshchekova and Gubergits ²	298	6

Reference solubility data for octane in pure water at 298 K were reported in Part 7, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 6. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergits² are considered Doubtful.

Rejected and Inaccessible Data

The data reported by Freegarde *et al.*¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

¹M. M. Freegarde, C. G. Hatchard, and C. A. Parker, Lab Pract. **20**, 35 (1971).

²P. Ya. Krasnoshchekova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 7. C₈H₁₂–C₈H₁₈ Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **34**(4), (2005).

Components:

(1) Octane; C₈H₁₈; [111-65-9]
 (2) Seawater (composition not specified)

Original Measurements:

M. Freegarde, C. G. Hatchard, and C. A. Parker, Lab Pract. **20**, 35 (1971).

Variables:

Temperature, pressure, and salinity not given

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of octane was reported to be 1.0 mg/L. The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $1.0 \cdot 10^{-4}$ g (1)/100 g sln and $1.6 \cdot 10^{-7}$, respectively, assuming a solution density of 1.02 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

None given except that analysis was done using gas chromatography.

Source and Purity of Materials:

Not given.

Estimated Error:

Not specified.

TABLE 6. Experimental values for solubility of octane (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful)	Reference value for pure water g (1)/100 g sln $\pm 30\%$
298	6 (Ref. 2)	$2.5 \cdot 10^{-4}$ (D; Ref. 2)	$6.3 \cdot 10^{-5}$

2.12. 1,2,3-Trimethylbenzene+Seawater

Components: (1) Octane; C ₈ H ₁₈ ; [111-65-9] (2) Seawater	Original Measurements: P. Ya. Krasnoshechekova and M. Ya. Gubergrits, Neflekimiya 13, 885 (1973).
Variables: One temperature: 25 °C Salinity: 6 g/kg sln	Prepared By: M. Kleinschmidt

Experimental Values

The solubility of octane in seawater was reported to be $2.5 \cdot 10^{-4}$ g (1)/100 g sln, and the corresponding mole fraction, $x_1 = 4.0 \cdot 10^{-7}$.

Auxiliary Information

Method/Apparatus/Procedure: A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.	Source and Purity of Materials: (1) "Chemically pure." (2) Distilled water plus salt mixture.
	Estimated Error: Not specified.

Components: (1) 1,2,3-Trimethylbenzene; C ₉ H ₁₂ ; [526-73-8] (2) Artificial seawater (Lyman and Fleming ¹)	Original Measurements: C. Sutton and J. A. Calder, J. Chem. Eng. Data 20 , 320 (1975).
Variables: One temperature: 25.0 °C One salinity: 34.5 g salts/kg sln	Prepared By: M. Kleinschmidt

Experimental Values

The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg (1)/kg sln. The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $4.86 \cdot 10^{-3}$ g (1)/100 g sln and $7.47 \cdot 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure: A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.	Source and Purity of Materials: (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure. (2) Made from doubly distilled water and salts 99+ % pure.
	Estimated Error: Temperature: ± 0.1 °C. Solubility: 0.5 (standard deviation).
	References: ¹ J. Lyman and R. H. Fleming, J. Mar. Res. 3 , 135 (1940).

2.13. 1,2,4-Trimethylbenzene+Seawater

Components:

- (1) 1,2,4-Trimethylbenzene; C₉H₁₂; [95-63-6]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
 One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of 1,2,4-trimethylbenzene in artificial seawater is reported to be 39.6 mg (1)/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $3.96 \cdot 10^{-3}$ g (1)/100 g sln and $6.09 \cdot 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 0.5 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.14. Mesitylene+Seawater

Components:

- (1) Mesitylene (1,3,5-trimethylbenzene); C₉H₁₂; [108-67-8]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
 One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of mesitylene in artificial seawater is reported to be 31.3 mg (1)/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $3.13 \cdot 10^{-3}$ g (1)/100 g sln and $4.81 \cdot 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 0.2 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.15. Cumene+Seawater

Components:

- (1) Cumene (isopropylbenzene); C₉H₁₂; [98-82-8]
(2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of cumene in artificial seawater is reported to be 42.5 mg (1)/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $4.25 \cdot 10^{-3}$ g (1)/100 g sln and $6.54 \cdot 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
(2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: 0.5 (standard deviation).

References:

- ¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.16. Nonane+Seawater

Components:

- (1) Nonane; C₉H₂₀; [111-84-2]
(2) Seawater

Original Measurements:

P. Ya. Krasnoshechkova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

Variables:

One temperature: 25 °C
Salinity: 6 g/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of nonane in seawater was reported to be $4.3 \cdot 10^{-5}$ g (1)/100 g sln and the corresponding mole fraction, $x_1 = 6.0 \cdot 10^{-8}$.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

Source and Purity of Materials:

- (1) "Chemically pure."
(2) Distilled water plus salt mixture.

Estimated Error:

Not specified.

2.17. Naphthalene+Seawater

Components:	Evaluators:
(1)Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Seawater	D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Naphthalene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Eganhouse and Calder ¹	298	35
Gordon and Thorne ²	298	31.7
Gordon and Thorne ³	298	35
May <i>et al.</i> ⁴	298	35
Paul ⁵	298	30.59
Schwarz ⁶	281–303	30

Reference solubility data for naphthalene in pure water at 298 K were reported in Part 9, Shaw and Maczynski,⁷ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 7. At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder,¹ Gordon and Thorne,³ and May *et al.*,⁴ are in good agreement. Therefore all these data and the mean value, $2.28 \cdot 10^{-3}$ are adopted as the Recommended value at this temperature and salinity. Since the value of Schwarz⁶ is lower than would be expected with decreasing salinity, it is considered Doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul⁵ and of Gordon and Thorne² are in fair agreement. Therefore their data are adopted as Tentative values. Gordon and Thorne² and May *et al.*⁴ report data for a range of salinities using the Setschenow equation. Schwarz⁶ reports data over the temperature range 281–303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

References:

- ¹R. P. Eganhouse and J. A. Calder, *Geochim. Cosmochim. Acta* **40**, 555 (1976).
- ²J. E. Gordon and R. L. Thorne, *Geochim. Cosmochim. Acta* **31**, 2433 (1967).
- ³J. E. Gordon and R. L. Thorne, *J. Phys. Chem.* **71**, 4390 (1967).
- ⁴W. E. May, S. P. Wasik, and D. H. Freeman, *Anal. Chem.* **50**, 997 (1978).
- ⁵M. A. Paul, *J. Am. Chem. Soc.* **74**, 5274 (1952).
- ⁶F. P. Schwarz, *J. Chem. Eng. Data* **22**, 273 (1977).
- ⁷D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 9. C₁₀ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **35**(1), (2005).

TABLE 7. Experimental values for solubility of naphthalene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful, R=recommended, T=tentative)	Reference value for pure water g (1)/100 g sln ± 30%
298	35	$2.28 \cdot 10^{-3}$ (R; mean from Refs. 1, 3, and 4)	$3.06 \cdot 10^{-3}$
	35 (Ref. 1)	$2.20 \cdot 10^{-3}$ (R; Ref. 1)	
	31.7 (Ref. 2)	$2.47 \cdot 10^{-3}$ (T; Ref. 2)	
	35 (Ref. 3)	$2.36 \cdot 10^{-3}$ (R; Ref. 3)	
	35 (Ref. 4)	$2.29 \cdot 10^{-3}$ (R; Ref. 4)	
	30.59 (Ref. 5)	$2.53 \cdot 10^{-3}$ (T; Ref. 5)	
	30 (Ref. 6)	$4.76 \cdot 10^{-3}$ (D; Ref. 6)	

Components:

(1) Naphthalene; C₁₀H₈; [91-20-3]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

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

Variables:

One temperature: 25.0 °C
 Salinity: 35 g/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of naphthalene in seawater is reported to be 22.0 mg/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $2.20 \cdot 10^{-3}$ g (1)/100 g sln and $3.18 \cdot 10^{-6}$, respectively.

Graphical results for other salinities are also reported.

Auxiliary Information**Method/Apparatus/Procedure:**

Equilibrium was obtained in a 1 L Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. Mixtures were agitated 12+h at 215 rpm on a New Brunswick gyrotary shaker; a 24 h stationary equilibrium period followed. Hydrocarbons were extracted with doubly distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard. Analysis was by gas chromatography.

Source and Purity of Materials:

(1) Analytical grade salts for artificial seawater solution reagent grade.
 Water: doubly distilled.

Estimated Error:

Temperature: ± 0.5 °C.
 Solubility: ± 0.293 (95% confidence interval).

References:

¹J. Lyman and R. H. Fleming, *J. Mar. Res.* **3**, 135 (1940).

Components:

(1) Naphthalene; C₁₀H₈; [91-20-3]
 (2) Natural seawater

Original Measurements:

J. E. Gordon and R. L. Thorne, *Geochim. Cosmochim. Acta* **31**, 2433 (1967).

Variables:

One temperature: 25 °C
 Salinity: 10–32 g/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

Solubility of naphthalene in natural seawater at 25 °C

$10^6 \cdot x_1^b$	10^3 (1)/100 g sln ^b	Chlorosity (%)	Salinity ^b g/kg sln	Treatment ^a
3.47	2.47	17.96	31.8	MF
3.45	2.46		31.8	
3.49	2.48	17.96	31.8	GFF
3.49	2.49		31.8	
3.56	2.53	18.00	31.9	CENT
3.53	2.51		31.9	
3.42	2.44	17.81	31.5	MF
3.41	2.45		31.5	
3.44	2.43	17.95	31.8	GFF
3.41	2.45		31.8	
3.45	2.47	17.72	31.7	MF
3.46	2.465		31.7	
3.41	2.45	17.80	31.5	GFF
3.43	2.44		31.5	
4.22	3.005	5.45	9.8	MF
4.22	3.005		9.8	
4.23	3.01	5.45	9.8	GFF
4.20	2.99		9.8	

^aMF, membrane (0.45 μ m) filtered; GFF, glass fiber filtered; CENT, centrifuged.

^bValues calculated by compiler.

Auxiliary Information**Method/Apparatus/Procedure:**

Details given in Gordon and Thorne.¹ Saturated solutions were prepared by equilibrating excess naphthalene and salt solution in an ampoule with shaking for 24 h. The filtered saturated solution was analyzed by a UV spectrophotometer.

Source and Purity of Materials:

(1) Naphthalene: 99.99+ % from James Hinton, Valparaiso, Florida.
 Salts: Analytical reagent grade from Mallinckrodt.
 Natural seawater: Collected at West Falmouth, Buzzards Bay, Quicks Hole, and Mashapaquitt Creek, Massachusetts.

Estimated Error:

Temperature: ± 0.03 °C (authors).
 Solubility: $\pm 3\%$ (authors).

References:

¹J. E. Gordon and R. L. Thorne, *J. Phys. Chem.* **71**, 4390 (1967).

Components: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: J. E. Gordon and R. L. Thorne, J. Phys. Chem. 71 , 4390 (1967).
Variables: One temperature: 24.91 °C Salinity: 0–108 g (2)/kg sln	Prepared By: M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S_0 is the solubility of (1) in water (mg/L);
- S is the solubility of (1) in solution (mg/L);
- K_S is the Setschenow constant (L/mol); and
- C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–2 mol/L, $K_S = 0.220 \pm 0.0041$ (95% confidence limit).

$\log S_0 = -3.590 \pm 0.004$ (95% confidence limit).

The corresponding mass percent and mole fraction, x_1 at salinity=35 g (2)/kg sln calculated by the compilers are $2.36 \cdot 10^{-3}$ g (1)/100 g sln and $3.48 \cdot 10^{-6}$ assuming a solution density of 1.025 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

Saturated solutions were prepared by equilibrating excess (1) in salt water in sealed ampoules for 24 h. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.

Source and Purity of Materials:

- (1) Recrystallized four times and sublimed or zone refined, 99.99+ % pure.
- (2) Analytical reagent grade.
- (3) Distilled from potassium permanganate and redistilled from all glass still.

Estimated Error:

Temperature: ± 0.03 °C.
Solubility: See above.

Components: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [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 Salinity: 0–40 g (2)/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S_0 is the solubility of (1) in water (mg/L);
- S is the solubility of (1) in solution (mg/L);
- K_S is the Setschenow constant (L/mol); and
- C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–7 mol/L, $K_S = 0.213$ with $S_0 = 31.69$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g(2)/kg sln, calculated by the compilers, are $2.29 \cdot 10^{-3}$ g (1)/100 g sln and $3.29 \cdot 10^{-6}$, respectively.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a generator column which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an extractor column packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.001 .
 S_0 : ± 0.23 .

Components: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: M. A. Paul, J. Am. Chem. Soc. 74 , 5274 (1952).
Variables: One temperature: 25 °C Salinity: 13–64 g (3)/kg sln	Prepared By: M. Kleinschmidt and W. Shiu

Experimental Values

Solubility of naphthalene in aqueous sodium chloride at 25 °C

g mol (3)/L	10 ⁶ · x ₁ ^a (compiler)	10 ³ · g (1)/100 g sln	g (2)/kg sln ^a (compiler)	g mol (3)/L
0.214	4.27	3.01	12.40	2.37
0.440	3.61	2.52	25.31	2.00
0.535	3.64	2.53	30.59	2.02
0.771	3.02	2.09	43.70	1.68
1.101	2.48	1.69	61.63	1.38

^aCalculated by compilers using density and other physical data for NaCl solutions from Weast.¹**Auxiliary Information****Method/Apparatus/Procedure:**

Equilibration was obtained in a 50 mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon and recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05 °C for at least 48 h and shaken occasionally during that time. Samples were withdrawn with a 10 mL transfer pipette, diluted appropriately, and analyzed using a spectrophotometer in the ultraviolet region of the spectrum.

Source and Purity of Materials:

- (1) Recrystallized from methanol.
- (2) Reagent grade, dried at 120 °C before weighing.
- (3) Redistilled.

Estimated Error:

Temperature: ± 0.05 °C.
Solubility: ± 1%.

References:

¹R. C. Weast, *CRC Handbook of Chemistry and Physics*, 59th Ed. (CRC, Boca Raton, FL, 1978), pp. D299–D300.

Components: (1) Naphthalene; C ₁₀ H ₈ ; [91-20-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: F. P. Schwarz and S. P. Wasik, J. Chem. Eng. Data 22 , 270 (1977).
Variables: Temperature: 8.6–31.8 °C Salinity: 30 g (2)/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values

Solubility of naphthalene in 0.5 g mol (2)/L

t/°C	10 ⁴ · mol (1)/L sln
8.6	0.84
11.1	0.92
14.0	1.09
17.1	1.23
20.0	1.37
23.0	1.58
25.0	1.73
31.8	2.22

The corresponding mass percent and mole fraction x₁, at 25.0 °C calculated by the compilers are 2.17 · 10⁻³ g(1)/100 g sln and 3.13 · 10⁻⁶.

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility of naphthalene in NaCl solution was determined by fluorescence and ultraviolet (UV) absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The spectrofluorimeter employed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

Naphthalene: purity >99 mole %.
Sodium chloride: reagent grade.
Ethanol: reagent grade.
Water: distilled over a KMnO₄-NaOH solution and passed through a Sephadex column.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: ± 3.3%.

2.18. Butylbenzene+Seawater

Components:

- (1) Butylbenzene; C₁₀H₁₄; [104-51-8]
 (2) Artificial seawater

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
 One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of butylbenzene in artificial seawater is reported to be 7.09 mg (1)/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $7.09 \cdot 10^{-4}$ g (1)/kg sln and $9.76 \cdot 10^{-7}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 0.07 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.19. *sec*-Butylbenzene+Seawater**Components:**

- (1) *sec*-Butylbenzene; C₁₀H₁₄; [135-98-8]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:

One temperature: 25.0 °C
 One salinity: 34.5 g salts/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of *sec*-butylbenzene in artificial seawater is reported to be 11.9 mg (1)/kg sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $1.19 \cdot 10^{-3}$ g(1)/100 g sln and $1.64 \cdot 10^{-6}$ assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information**Method/Apparatus/Procedure:**

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
 (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
 Solubility: 0.2 (standard deviation).

References:

¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.20. *tert*-Butylbenzene+Seawater

Components: (1) <i>tert</i> -Butylbenzene; C ₁₀ H ₁₄ ; [98-06-6] (2) Artificial seawater (Ref. 1)	Original Measurements: C. Sutton and J. A. Calder, J. Chem. Eng. Data 20 , 320 (1975).
Variables: One temperature: 25.0 °C One salinity: 34.5 g salts/kg sln	Prepared By: M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of *tert*-butylbenzene in artificial seawater is reported to be 21.2 mg (1)/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compiler, are $2.12 \cdot 10^{-3}$ g (1)/100 g sln and $2.92 \cdot 10^{-6}$, respectively, assuming the artificial seawater composition of Lyman and Fleming.¹

Auxiliary Information

Method/Apparatus/Procedure:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

- (1) From either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+ % pure.
- (2) Made from doubly distilled water and salts 99+ % pure.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: 0.3 (standard deviation).

References:

- ¹J. Lyman and R. H. Fleming, J. Mar. Res. **3**, 135 (1940).

2.21. Decane+Seawater

Components: (1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater	Evaluators: D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.
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Critical Evaluation of Solubility of Decane (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Freearde <i>et al.</i> ¹	not specified	not specified
Krasnoshchekova and Gubergrits ²	298	6

Reference solubility data for decane in pure water at 298 K were reported in Part 9, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 8. Because the presence of sea salts is expected to depress the solubility value below the value for pure water the data of Krasnoshchekova and Gubergrits² are considered Doubtful.

Rejected and Inaccessible Data

The data reported by Freearde *et al.*¹ lack sufficient information to justify evaluation. Therefore these data are Rejected.

References:

- ¹M. M. Freearde, C. G. Hatchard, and C. A. Parker, Lab Pract. **20**, 35 (1971).
- ²P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).
- ³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 9. C₁₀ Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **35**(1), (2006).

TABLE 8. Experimental values for solubility of decane (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful)	Reference value for pure water g (1)/100 g sln $\pm 30\%$
298	6 (Ref. 2)	$8.7 \cdot 10^{-6}$ (D; Ref. 2)	$2.6 \cdot 10^{-6}$

Components: (1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater (composition not specified)	Original Measurements: M. Freegarde, C. G. Hatchard, and C. A. Parker, Lab Pract. 20 , 35 (1971).
Variables: Temperature, pressure, salinity not given	Prepared By: M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of decane was reported to be 0.15 mg/L.

The corresponding mass percent and mole fractions (x_1), calculated by the compilers, are $1.5 \cdot 10^{-5}$ g (1)/100 g sln and $1.9 \cdot 10^{-8}$, respectively, assuming a solution density of 1.02 kg/L.

Auxiliary Information

Method/Apparatus/Procedure: None given except that analysis was done using gas chromatography.	Source and Purity of Materials: Not given.
	Estimated Error: Not specified.

Components: (1) Decane; C ₁₀ H ₂₂ ; [124-18-5] (2) Seawater	Original Measurements: P. Ya. Krasnoschekova and M. Ya. Gubergrits, Neftekhimiya 13 , 885 (1973).
Variables: One temperature: 25 °C Salinity: 6 g/kg sln	Prepared By: M. Kleinschmidt

Experimental Values

The solubility of decane in seawater was reported to be $8.7 \cdot 10^{-6}$ g (1)/100 g sln and the corresponding mole fraction, $x_1 = 1.1 \cdot 10^{-8}$.

Auxiliary Information

Method/Apparatus/Procedure: A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.	Source and Purity of Materials: (1) "Chemically pure." (2) Distilled water plus salt mixture.
	Estimated Error: Not specified.

2.22. 1-Methylnaphthalene+Seawater

Components:

- (1) 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 8.1–28.5 °C
 Salinity: 30 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

Solubility of 1-methylnaphthalene in 0.5 g mol (2)/L

<i>t</i> /°C	10 ⁴ ·mol(1)/L sln
8.1	1.23
11.1	1.35
15.5	1.49
17.4	1.53
18.2	1.54
20.7	1.54
23.3	1.63
25.0	1.69
28.5	1.81

The corresponding mass percent and mole fraction (*x*₁) at 25.0 °C, calculated by the compiler, are 2.34·10⁻³ g (1)/100 g sln and 3.06·10⁻⁶.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1-methylnaphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of 1-methylnaphthalene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least cell 72 h in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 320 nm. The spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of 1-methylnaphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

(1) 1-Methylnaphthalene: purity >99%.
 Sodium chloride: reagent grade.
 Ethanol: reagent grade.
 Water: distilled over a KMnO₄-NaOH solution and passed through a Sephadex column.

Estimated Error:

Temperature: ±0.1 °C (author).
 Solubility: ±3.6% (author).

2.23. Undecane+Seawater

Components:

- (1) Undecane; C₁₁H₂₄; [1120-21-4]
 (2) Seawater

Original Measurements:

P. Ya. Krasnoschekova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln

Prepared By:

M. Kleinschmidt

Experimental Values

The solubility of undecane in seawater was reported to be 1.0·10⁻⁶ g(1)/100 g sln and the corresponding mole fraction, *x*₁ = 1.2·10⁻⁹.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

Source and Purity of Materials:

- (1) "Chemically pure."
 (2) Distilled water plus salt mixture.

Estimated Error:

Not specified.

2.24. Acenaphthene+Seawater

Components: (1) Acenaphthene; C ₁₂ H ₁₀ ; [83-32-9] (2) Seawater; natural	Original Measurements: S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. 15 , 715 (1981).
Variables: Temperature: 15–25 °C Salinity: 35 g/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values
Solubility of acenaphthene in seawater

<i>t</i> /°C	10 ⁸ · <i>x</i> ₁ ^a	10 ⁵ · g (1)/100 g sln ^a	μg (1)/g (2)
15	2.56	2.14	0.214
20	6.6	5.5	0.55
25	22.0	18.4	1.84

^aCalculated by compilers.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared by equilibrating seawater with an excess of hydrocarbon for 24 h in a constant temperature gyrotary shaker followed by 12 h stationary period. A 100 mL aliquot was extracted three times with hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the hydrocarbon concentration.

Source and Purity of Materials:

Acenaphthene: from Aldrich Chemical Co. of 99% purity and doubly distilled from distilled methanol.
Hexane: doubly distilled in glass.
Seawater: collected off Scripps Pier and was filtered twice through 0.22 μm membrane and twice extracted with hexane then its salinity adjusted to 35 parts per thousand.

Estimated Error:

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

2.25. Biphenyl+Seawater

Components: (1) Biphenyl; C ₁₂ H ₁₀ ; [92-52-4] (2) Seawater	Evaluators: D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.
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Critical Evaluation of Solubility of Biphenyl (1) in Seawater (2)

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

Author (s)	<i>T</i> /K	Salinity g salts/kg sln
Eganhouse and Calder ¹	298	35
Paul ²	298	13–64

Reference solubility data for biphenyl in pure water at 298 K were reported in Part 10, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 9. The reported data are all from different salinities, which precludes direct comparison. Since the data appear consistent with each other and with the reference value for the solubility of biphenyl in pure water, the data of Eganhouse and Calder¹ and Paul² are adopted as Tentative.

References:

- ¹R. P. Eganhouse and J. A. Calder, *Geochim. Cosmochim. Acta* **40**, 555 (1976).
²M. A. Paul, *J. Am. Chem. Soc.* **74**, 5274 (1952).
³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 10. C₁₁ and C₁₂ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **35**(1), (2006).

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

<i>T</i> /K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (<i>T</i> =tentative)	Reference value for pure water g (1)/100 g sln ±30%
298	35 (Ref. 1)	4.76 · 10 ⁻⁴ (<i>T</i> ; Ref. 1)	7 · 10 ⁻⁴
	13.25 (Ref. 2)	6.08 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	26.24 (Ref. 2)	5.46 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	39.05 (Ref. 2)	4.62 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	46.28 (Ref. 2)	4.16 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	51.62 (Ref. 2)	4.13 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	63.97 (Ref. 2)	3.54 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	
	63.97 (Ref. 2)	3.45 · 10 ⁻⁴ (<i>T</i> ; Ref. 2)	

Components:

(1) Biphenyl; C₁₂H₁₀; [92-52-4]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

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

Variables:

One temperature: 25.0 °C
 Salinity: 35 g/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of biphenyl in seawater is reported to be 4.76 mg/kg.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $4.76 \cdot 10^{-4}$ g (1)/100 g sln and $5.70 \cdot 10^{-7}$, respectively. Graphical results for other salinities are also reported.

Auxiliary Information**Method/Apparatus/Procedure:**

Equilibrium was obtained in a 1 L Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ h at 215 rpm on a New Brunswick gyrotary shaker; a 24 h stationary equilibrium period followed. Hydrocarbons were extracted with doubly distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard. Analysis: Gas chromatography

Source and Purity of Materials:

(1) Analytical grade salts for artificial seawater solution reagent grade.
 Water: doubly distilled.

Estimated Error:

Temperature: ± 0.5 °C.
 Solubility: ± 0.293 (95% confidence interval).

References:

¹J. Lyman and R. H. Fleming, *J. Mar. Res.* **3**, 135 (1940).

Components:

(1) Biphenyl; C₁₂H₁₀; [92-52-4]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

M. A. Paul, *J. Am. Chem. Soc.* **74**, 5274 (1952).

Variables:

One temperature: 25 °C
 Salinity: 13–64 g (3)/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

Solubility of biphenyl and aqueous solution sodium chloride

$10^7 \cdot x_1^*$	$10^4 \cdot \text{g (1)/100 g sln}^a$	g (2)/kg sln^a	$10^5 \cdot \text{mol(1)/L}$	mol (2)/L
7.16	6.08	13.25	3.98	0.229
6.49	5.46	26.24	3.61	0.458
5.55	4.62	39.05	3.08	0.687
5.02	4.16	46.28	2.79	0.818
5.01	4.13	51.62	2.78	0.916
4.32	3.54	63.97	2.40	1.145
4.21	3.45	63.97	2.34	1.145

^aCalculated by compilers using density and other physical data for NaCl solutions from Weast.¹

Auxiliary Information**Method/Apparatus/Procedure:**

Equilibration was obtained in a 50 mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05 °C for at least 48 h, and shaken occasionally during that time. Samples were withdrawn with a 10 mL transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultraviolet region of the spectrum.

Source and Purity of Materials:

(1) Recrystallized from methanol.
 (2) Reagent grade, dried at 120 °C before weighing.
 (3) Redistilled.
 Sources not specified.

Estimated Error:

Temperature: ± 0.05 °C.
 Solubility: $\pm 2.6\%$.

References:

¹R. C. Weast, *CRC Handbook of Chemistry and Physics*, 59th ed. (CRC, Boca Raton, FL, 1978), pp. D299–D300.

2.26. Dodecane+Seawater

Components:

(1) Dodecane; C₁₂H₂₆; [112-40-3]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Dodecane (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Button ¹	298	12
Krasnoshechekova and Gubergits ²	298	6
Sutton and Calder ³	298	35

Reference solubility data for dodecane in pure water at 298 K were reported in Part 10, Shaw and Maczynski,⁴ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 10. The reported data are all from different salinities, which precludes direct comparison. The data are in only fair agreement with each other and with the reference values for the solubility of dodecane in pure water. Since hydrocarbon solubilities in saline solutions are expected to be less than in pure water, the data of Krasnoshechekova and Gubergits² are Doubtful. The remaining data are Tentative.

References:

¹D. K. Button, *Geochim. Cosmochim. Acta* **40**, 435 (1975).

²P. Ya. Krasnoshechekova and M. Ya. Gubergits, *Neftekhimiya* **13**, 885 (1973).

³C. Sutton and J. A. Calder, *Environ. Sci. Technol.* **8**, 654 (1974).

⁴D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 10. C₁₁ and C₁₂ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **35**(1), (2006).

TABLE 10. Experimental values for solubility of dodecane (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative, D=Doubtful)	Reference value for pure water g (1)/100 g sln ± 30%
298	12 (Ref. 1)	1.74 · 10 ⁻⁷ (T; Ref. 1)	3.4 · 10 ⁻⁷
	6 (Ref. 2)	5 · 10 ⁻⁷ (D; Ref. 2)	
	35 (Ref. 3)	2.9 · 10 ⁻⁷ (T; Ref. 3)	

Components:

(1) Dodecane; C₁₂H₂₆; [112-40-3]
 (2) Salt mixture (Ref. 1)
 (2) Water; H₂O; [7732-18-5]

Original Measurements:

D. K. Button, *Geochim. Cosmochim. Acta* **40**, 435 (1975).

Variables:

One temperature: 25 °C
 Constant salinity: 12 g (2)/kg sln
 Different periods of standing

Prepared By:

P. Meyers and D. G. Shaw

Experimental Values

Dodecene concentration in saline medium after gently stirring for 1 week and then remaining quiescent for the periods shown.

Time (weeks)	Dodecene, μg (1)/L (2)
1	2.16 ± 0.03
8	1.80 ± 0.02
16	1.78 ± 0.02

The corresponding mass percent and mole fraction calculated by the compilers for the results at 16 weeks are 1.74 · 10⁻⁷ g (1)/100 g sln and 1.89 · 10⁻¹⁰ using the assumption that the solution density is 1.02 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

Dodecane solutions were prepared in a chemically defined solution resembling dilute seawater. In addition to the mineral salts and vitamins reported (Button¹), the solution contained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121 °C for 30 min), 0.8 μL of ¹⁴C-dodecane was sprayed on to the medium surface to form a thin film. Gentle subsurface agitation was induced by a 3 in. magnet rotating at 60 rpm against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples collected from a port at the bottom of the carboy. The system was stirred for 1 week and then allowed to stand. Equilibrium appeared to have been achieved within 8 weeks.

Source and Purity of Materials:

Amersham Searle Corp. (Arlington Heights, Ill.) supplied the [¹⁴C] dodecane, 27 μCi/μmol. It was accompanied by a gas chromatogram of the preparation showing a single peak at the appropriate location.

Estimated Error:

Experimental error is estimated at ± 1%.

References:

¹D. K. Button, *Limnol. Oceanogr.* **14**, 95 (1969).

Components: (1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3] (2) Seawater	Original Measurements: P. Ya. Krasnoshechekova and M. Ya. Gubergrits, Neflekimiya 13, 885 (1973).
Variables: One temperature: 25 °C Salinity: 6 g/kg sln	Prepared By: M. Kleinschmidt

Experimental Values

The solubility of dodecane in seawater was reported to be $5 \cdot 10^{-7}$ g (1)/100 g sln and the corresponding mole fraction $x_1 = 5.0 \cdot 10^{-10}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10–12 h in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

Source and Purity of Materials:

- (1) "Chemically pure."
- (2) Distilled water plus salt mixture.

Estimated Error:

Not specified.

Components: (1) Dodecane; C ₁₂ H ₂₆ ; [112-40-3] (2) Seawater	Original Measurements: C. Sutton and J. A. Calder, Environ. Sci. Technol. 8, 654 (1974).
Variables: One temperature: 25 °C One salinity: 35 g salts/kg sln	Prepared By: P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of dodecane in seawater was reported to be $2.9 \cdot 10^{-7}$ g (1)/100 g sln and $x_1 = 3.1 \cdot 10^{-10}$.

Auxiliary Information**Method/Apparatus/Procedure:**

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through $0.45 \mu\text{m}$ membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+ % pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of $\pm 16\%$, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.27. Fluorene+Seawater

Components:

- (1) Fluorene; C₁₃H₁₀; [86-73-7]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [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
 Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of fluorene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.267$ with $S_0 = 1.685$.

The corresponding mass percent and mole fraction, x_1 at salinity=35 g (2)/kg sln calculated by the compilers are $1.20 \cdot 10^{-4}$ g (1)/100 g sln and $1.30 \cdot 10^{-7}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
 (2) Reagent grade.
 (3) Distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.

2.28. Anthracene+Seawater

Components:

- (1) Anthracene; C₁₄H₁₀; [120-12-7]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Anthracene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
May <i>et al.</i> ¹	298	35.0
Schwarz ²	281–303	30

Mean of selected experimental solubility data for anthracene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 11. The reported data are from different salinities, which precludes direct comparison. Since the data appear consistent with each other and with the mean value for the solubility of anthracene in pure water, the data of May *et al.*¹ and Schwarz² are adopted as Tentative. Schwarz² also reports data over the temperature range.

References:

¹W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

²F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).

³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 11. C₁₃–C₃₆ Hydrocarbons with Water*, J. Phys. Chem. Ref. Data **35**(2), (2006).

TABLE 11. Experimental values for solubility of anthracene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative)	Mean value for pure water g (1)/100 g sln
298	35 (Ref. 1)	$3.11 \cdot 10^{-6}$ (T; Ref. 1)	$4.3 \cdot 10^{-6}$
	30 (Ref. 2)	$3.55 \cdot 10^{-6}$ (T; Ref. 2)	

Components:

- (1) Anthracene; C₁₄H₁₀; [120-12-7]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [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
 Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S_0 is the solubility of (1) in water (mg/L);
 S is the solubility of (1) in solution (mg/L);
 K_S is the Setschenow constant (L/mol); and
 C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.238$ with $S_0 = 0.0446$.

The corresponding mass percent and mole fraction (x_1) at salinity = 35 g (2)/kg sln, calculated by the compilers, are $3.11 \cdot 10^{-6}$ g (1)/100 g sln and $3.22 \cdot 10^{-9}$.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
 (2) Reagent grade.
 (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.004 .
 S_0 : ± 0.0002 .

Components:

- (1) Anthracene; C₁₄H₁₀; [120-12-7]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 8.2–30.2 °C
 Salinity: 30 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

Solubility of anthracene in 0.5 mol (2)/L sln

$t/^\circ\text{C}$	$10^{-7} \cdot \text{mol (2)/L sln}$
8.2	0.93
8.6	1.01
11.7	1.22
19.2	1.47
21.5	1.68
25.0	2.04
25.3	1.92
27.1	2.02
30.2	2.46

The corresponding mass percent and mole fraction (x_1) at 25.0 °C, calculated by the compilers, are $3.55 \cdot 10^{-6}$ g (1)/100 g sln and $3.69 \cdot 10^{-9}$.

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility of anthracene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, a saturated solution was prepared by adding excess amount of anthracene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 365 nm. The spectrofluorimeter employed a ratio-photon counting mode where anthracene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of anthracene in ethanol solution therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

(1) Anthracene: purity >99 mole %.
 Sodium chloride: reagent grade.
 Water: distilled over a KMnO₄–NaOH solution and passed through a Sephadex column.
 Ethanol: reagent grade.

Estimated Error:

Temperature: ± 0.1 °C (author).
 Solubility: $\pm 4.3\%$ (author).

2.29. Phenanthrene+Seawater

Components:	Evaluators:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Seawater	D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Phenanthrene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Aquan-Yuen <i>et al.</i> ¹	298	29–108
Eganhouse and Calder ²	298	35
May <i>et al.</i> ³	298	35
Schwarz ⁴	284–305	30

Mean of selected experimental solubility data for phenanthrene in pure water at 298 K was reported in Part 11, Shaw and Maczynski,⁵ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 12. At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder² and of May *et al.*³ are in very good agreement. Therefore their mean, $6.9 \cdot 10^{-5}$ g (1)/100 g sln is adopted as the Recommended value for the solubility of phenanthrene at the indicated temperature and salinity. The value of Aquan-Yuen *et al.*¹ appears consistent with the data discussed above and with the mean value for the solubility of phenanthrene in pure water and is Tentative. The value of Schwarz⁴ appears slightly high and is considered Doubtful. Schwarz⁴ also reports data over a temperature range.

References:

¹M. Aquan-Yuen, D. Mackay, and W. Y. Shiu, *J. Chem. Eng. Data* **24**, 30 (1979).

²R. P. Eganhouse and J. A. Calder, *Geochim. Cosmochim. Acta* **40**, 555 (1976).

³W. E. May, S. P. Wasik, and D. H. Freeman, *Anal. Chem.* **50**, 997 (1978).

⁴F. P. Schwarz, *J. Chem. Eng. Data* **22**, 273 (1977).

⁵D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated, Part 11. C₁₃–C₃₆ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **35**(2), (2005).

Components:	Original Measurements:
(1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	M. Aquan-Yuen, D. Mackay, and W. Y. Shiu, <i>J. Chem. Eng. Data</i> 24 , 30 (1979).
Variables:	Prepared By:
One temperature: 25 °C Salinity: 29–108 g (2)/kg sln	M. Kleinschmidt and W. Y. Shiu

Experimental Values
Solubility of phenanthrene in aqueous NaCl

10 ⁸ · x ₁ ^a	10 ⁵ · g (1)/100 g sln ^a	mg (1)/L sln	g (2)/kg sln ^a	mol (2)/L sln
8.6	8.3	0.85	28.6	0.50
6.8	6.4	0.67	56.2	1.00
4.9	4.5	0.48	82.6	1.50
3.3	3.1	0.33	108.2	2.00

^aCalculated by compilers using density and other physical data for NaCl solutions from Weast.¹

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 h and then allowed to settle for 48 h. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.

Source and Purity of Materials:

(1) Fluorescence grade: from Eastman Kodak.
(2) Reagent grade: from Fisher Scientific.

Estimated Error:

Temperature: ±0.5 °C.
Solubility: ±3 relative %.

References:

¹R. C. Weast, *CRC Handbook of Chemistry and Physics*, 59th ed. (CRC, Boca Raton, FL, 1978), pp. D299–D300.

TABLE 12. Experimental values for solubility of phenanthrene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (D=doubtful, T=tentative)	Mean value for pure water g (1)/100 g sln
298	35	6.9 · 10 ⁻⁵ (R; mean from Refs. 2 and 3)	1.2 · 10 ⁻⁴
	28.6 (Ref. 1)	8.3 · 10 ⁻⁵ (T; Ref. 1)	
	56.2 (Ref. 1)	6.4 · 10 ⁻⁵ (T; Ref. 1)	
	82.6 (Ref. 1)	4.5 · 10 ⁻⁵ (T; Ref. 1)	
	108.2 (Ref. 1)	3.1 · 10 ⁻⁵ (T; Ref. 1)	
	35 (Ref. 2)	7.1 · 10 ⁻⁵ (R; Ref. 2)	
	35 (Ref. 3)	6.63 · 10 ⁻⁵ (R; Ref. 3)	
	30 (Ref. 4)	9.94 · 10 ⁻⁵ (D; Ref. 4)	

Components:

(1) Phenanthrene; C₁₄H₁₀; [85-01-8]
 (2) Artificial seawater (Lyman and Fleming¹)

Original Measurements:

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

Variables:

One temperature 25 °C;
 Salinity: 35 g/kg sln

Prepared By:

M. Kleinschmidt and W. Y. Shiu

Experimental Values

The solubility of phenanthrene in seawater is reported to be 0.71 mg/kg sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $7.1 \cdot 10^{-5}$ g (1)/100 g sln and $7.4 \cdot 10^{-8}$, respectively.

Graphical results for other salinities are also reported.

Auxiliary Information**Method/Apparatus/Procedure:**

Equilibrium was obtained in a 1 L Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ h at 215 rpm on a New Brunswick gyrotary shaker; a 24 h stationary equilibrium period followed. Hydrocarbons were extracted with twice distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard. Analysis was by gas chromatography.

Source and Purity of Materials:

Analytical grade salt for artificial seawater solution: reagent grade.

Water: doubly distilled.

Estimated Error:

Temperature: ± 0.5 °C.

Solubility: ± 0.025 (95% confidence interval).

References:

¹J. Lyman and R. H. Fleming, *J. Mar. Res.* **3**, 135 (1940).

Components:

(1) Phenanthrene; C₁₄H₁₀; [85-01-8]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [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
 Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of phenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.275$ with $S_0 = 1.002$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g (2)/kg sln, calculated by the compilers, are $6.63 \cdot 10^{-5}$ g (1)/100 g sln and $6.78 \cdot 10^{-8}$, respectively.

Graphical data for other temperatures are also reported.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

(1) Greater than 97% pure.

(2) Reagent grade.

(3) Distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.

K_S : ± 0.010 .

S_0 : ± 0.011 .

Components: (1) Phenanthrene; C ₁₄ H ₁₀ ; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: F. P. Schwarz, J. Chem. Eng. Data 22 , 273 (1977).
Variables: Temperature: 11.1–31.8 °C Salinity: 30 g (2)/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values

Solubility of phenanthrene in 0.5 g mol(2)/L

<i>t</i> /°C	10 ⁶ · mol (2)/L sln
11.1	2.88
14.0	3.2
17.5	4.07
20.2	4.51
23.2	5.75
25.0	5.72
29.3	7.2
31.8	7.9

The corresponding mass percent and mole fraction (x_1) at 25.0 °C, calculated by the compilers, are $9.94 \cdot 10^{-5}$ g (1)/100 g sln and $1.034 \cdot 10^{-7}$, respectively.

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility of phenanthrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of phenanthrene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 365 nm. The spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

(1) Phenanthrene: purity 99.9%.
Sodium chloride: reagent grade.
Water: distilled over a KMnO₄-NaOH solution and passed through a Sephadex column.
Ethanol: reagent grade.

Estimated Error:

Temperature: ± 0.1 °C (author).
Solubility: ± 8.4% (author).

2.30. Tetradecane+Seawater

Components: (1) Tetradecane; C ₁₄ H ₃₀ ; [629-59-4] (2) Seawater	Original Measurements: C. Sutton and J. A. Calder, Environ. Sci. Technol. 8 , 654 (1974).
Variables: One temperature: 25 °C One salinity: 35 g salts/kg sln	Prepared By: P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of tetradecane in seawater was reported to be $1.7 \cdot 10^{-7}$ g (1)/100 g sln and $x_1 = 1.5 \cdot 10^{-10}$.

Auxiliary Information**Method/Apparatus/Procedure:**

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+ % pure hydrocarbon. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.31. 2-Methylantracene+Seawater

Components:

- (1) 2-Methylantracene; C₁₅H₁₂; [613-12-7]
- (2) Sodium chloride; NaCl; [7647-14-5]
- (3) Water; H₂O; [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
Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of 2-methylantracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S_0 is the solubility of (1) in water (mg/L);
- S is the solubility of (1) in solution (mg/L);
- K_S is the Setschenow constant (L/mol); and
- C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.336$ with $S_0 = 0.0213$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g (2)/kg sln, calculated by the compilers, are $1.29 \cdot 10^{-6}$ g (1)/100 g sln and $1.24 \cdot 10^{-9}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.006 .
 S_0 : ± 0.003 .

2.32. 1-Methylphenanthrene+Seawater

Components:

- (1) 1-Methylphenanthrene; C₁₅H₁₂; [832-69-9]
- (2) Sodium chloride; NaCl; [7647-14-5]
- (3) Water; H₂O; [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
Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of 1-methylphenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S_0 is the solubility of (1) in water (mg/L);
- S is the solubility of (1) in solution (mg/L);
- K_S is the Setschenow constant (L/mol); and
- C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.211$ with $S_0 = 0.269$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g (2)/kg sln, calculated by the compilers, are $1.95 \cdot 10^{-5}$ g (1)/100 g sln and $1.87 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.018 .
 S_0 : ± 0.003 .

2.33. Fluoranthene+Seawater

Components: (1) Fluoranthene; C ₁₆ H ₁₀ ; [206-44-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [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 Salinity: 0–40 g (2)/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values

The solubility of fluoranthene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.399$ with $S_0 = 0.206$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g (2)/kg sln, calculated by the compilers, are $1.24 \cdot 10^{-5}$ g (1)/100 g sln and $1.14 \cdot 10^{-8}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
 K_S : ± 0.010 .
 S_0 : ± 0.002 .

2.34. Pyrene+Seawater

Components: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Seawater	Evaluators: D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.
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Critical Evaluation of Solubility of Pyrene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Krasnoshchekova <i>et al.</i> ¹	298	6
May <i>et al.</i> ²	298	35
Rossi and Thomas ³	288–298	35
Schwarz ⁴	282–304	30

Mean of selected experimental solubility data for pyrene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,⁵ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 13. At 298 K and a salinity of 35 g salts/kg sln the data of May *et al.*² and Rossi and Thomas³ are in very good agreement. Since the value reported by May *et al.*² is more precise and derived from several measurements using the Setschenow equation, it is adopted as the Recommended value for the solubility of pyrene in seawater at the temperature and salinity indicated. The value of Krasnoshchekova *et al.*,¹ Rossi and Thomas,³ and Schwarz⁴ appear slightly different and are considered Tentative. Rossi and Thomas,³ and Schwarz⁴ each report data over a range of temperatures.

References:

- ¹P. Ya. Krasnoshchekova, Yu. A. Pakhapill, and M. Ya. Gubergrits, Khim. Tverd. Topl. **11**, 133 (1977).
- ²W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).
- ³S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. **15**, 715 (1981).
- ⁴F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).
- ⁵D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated*, Part 11. C₁₃–C₃₆ Hydrocarbons with Water, J. Phys. Chem. Ref. Data **35**(2), (2005).

TABLE 13. Experimental values for solubility of pyrene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (R=recommended, T=tentative)	Mean value for pure water g (1)/100 g sln
298	6 (Ref. 1)	$7.705 \cdot 10^{-6}$ (D; Ref. 1)	$1.4 \cdot 10^{-5}$
	35 (Ref. 2)	$8.6 \cdot 10^{-6}$ (R; Ref. 2)	
	35 (Ref. 3)	$8.9 \cdot 10^{-6}$ (T; Ref. 3)	
	30 (Ref. 4)	$9.48 \cdot 10^{-6}$ (T; Ref. 4)	

Components:

(1) Pyrene; C₁₆H₁₀; [129-00-0]
 (2) Salt water

Original Measurements:

P. Ya. Krasnoschekova, Yu. A. Pakhapill, and M. Ya. Gubergrits, Khim. Tverd. Topl. **11**, 133 (1977).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Krasnoschekova and Gubergrits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of pyrene in salt water was reported to be 78.9 μg/L.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $7.705 \cdot 10^{-6}$ g (1)/100 g sln and $7.02 \cdot 10^{-9}$, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ±1 °C.
 Solubility: ±2.93; type of error not specified.

References:

¹P. Ya. Krasnoschekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Components:

(1) Pyrene; C₁₆H₁₀; [129-00-0]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [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
 Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of pyrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.286$ with $S_0 = 0.132$.

The corresponding mass percent and mole fraction (x_1) at salinity = 35 g (2)/kg sln, calculated by the compilers, are $8.60 \cdot 10^{-6}$ g (1)/100 g sln and $7.84 \cdot 10^{-9}$, respectively.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

(1) Greater than 97% pure.

(2) Reagent grade.

(3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ±0.05 °C.

K_S : ±0.003.

S_0 : ±0.001.

Components: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Seawater; natural	Original Measurements: S. S. Rossi and W. H. Thomas, Environ. Sci. Technol. 15 , 715 (1981).
Variables: Temperature: 15–25 °C Salinity: 35 g/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values
Solubility of pyrene in seawater

<i>t</i> /°C	10 ⁹ · <i>x</i> ₁ ^a	10 ⁶ · g (1)/100 g sln ^a	μg (1)/g (2)
15	5.1	5.6	0.056
20	6.5	7.1	0.071
25	8.1	8.9	0.089

^aCalculated by compilers.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solution was prepared by equilibrating seawater with an excess of pyrene for at least 24 h in a constant-temperature gyrotary shaker followed by a 12 h stationary equilibration period. A 100 mL aliquot was extracted three times with *n*-hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the pyrene concentration.

Source and Purity of Materials:

Pyrene: from Aldrich Chemical Co. and purified with 2,4,6-trinitrophenol.
n-Hexane: doubly distilled in glass.
Seawater: collected off Scripps Pier and was filtered twice through 0.22 μm membrane and twice extracted with *n*-hexane then its salinity was adjusted to 35%.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: ± 11%.

Components: (1) Pyrene; C ₁₆ H ₁₀ ; [129-00-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	Original Measurements: F. P. Schwarz, J. Chem. Eng. Data 22 , 273 (1977).
Variables: Temperature: 8.6–31.1 °C Salinity: 30 g (2)/kg sln	Prepared By: W. Y. Shiu and D. Mackay

Experimental Values
Solubility of pyrene in 0.5 g mol (2)/L sln

<i>t</i> /°C	10 ⁷ · mol(1)/L sln
8.6	2.00
12.2	2.50
15.5	2.85
18.2	3.22
20.7	3.57
23.0	3.90
25.0	4.41
28.1	5.19
31.1	5.96

The corresponding mass percent and mole fraction (*x*₁) at 25.0 °C, calculated by the compilers, are 9.48 · 10⁻⁶ g (1)/100 g sln and 7.97 · 10⁻⁹, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 365 nm. The spectrofluorimeter employed a ratio-photon counting mode where pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of pyrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

(1) Pyrene: purity >99mole %.
Sodium chloride: reagent grade.
Water: distilled over a KMnO₄-NaOH solution and passed through a Sephadex column.
Ethanol: reagent grade.

Estimated Error:

Temperature: ± 0.1 °C (author).
Solubility: ± 1.6% (author).

2.35. Hexadecane+Seawater

Components:

- (1) Hexadecane; C₁₆H₃₄; [544-76-3]
 (2) Seawater

Variables:

One temperature: 25 °C
 One salinity: 35 g salts/kg sln

Original Measurements:

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

Prepared By:

P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of hexadecane in seawater was reported to be $4 \cdot 10^{-8}$ g (1)/100 g sln and $x_1 = 3 \cdot 10^{-11}$.

Auxiliary Information

Method/Apparatus/Procedure:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+% pure hydrocarbons. Seawater collected from 25 m depth in Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.36. Benz[*a*]anthracene+Seawater

Components:

- (1) Benz[*a*]anthracene; C₁₈H₁₂; [56-55-3]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Benz[*a*]anthracene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Krasnoshchekova <i>et al.</i> ¹	298	6
May <i>et al.</i> ²	298	35

Mean of selected experimental solubility data for benz[*a*]anthracene in pure water at 298 K were reported in Part 11, Shaw and Maczynski,³ and converted by the Evaluators to g (1)/100 g sln.

The experimental data are listed in Table 14. The value reported by May *et al.*² was derived from several measurements using the Setschenow equation and is consistent with the mean value for the solubility of benz[*a*]anthracene in pure water. Therefore their value is adopted as Tentative. The value of Krasnoshchekova *et al.*¹ appears slightly low and is considered Doubtful.

References:

- ¹P. Ya. Krasnoshchekova, Yu. A. Pakhapill, and M. Ya. Gubergits, *Khim. Tverd. Topl.* **11**, 133 (1977).
²W. E. May, S. P. Wasik, and D. H. Freeman, *Anal. Chem.* **50**, 997 (1978).
³D. Shaw and A. Maczynski, Editors, *IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater-Revised and Updated, Part 11. C₁₃-C₃₆ Hydrocarbons with Water*, *J. Phys. Chem. Ref. Data* **35**(2), (2006).

TABLE 14. Experimental values for solubility of benz[*a*]anthracene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative, D=doubtful)	Mean value for pure water g (1)/100 g sln
298	6 (Ref. 1)	$6.2 \cdot 10^{-8}$ (D; Ref. 1)	$9.2 \cdot 10^{-7}$
	35 (Ref. 2)	$5.6 \cdot 10^{-7}$ (T; Ref. 2)	

Components:

- (1) Benz[*a*]anthracene; C₁₈H₁₂; [56-55-3]
 (2) Salt water

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits¹)

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhapill, and M. Ya. Gubergrits, Khim. Tverd. Topl. **11**, 133 (1977).

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benz[*a*]anthracene in salt water was reported to be 0.63 μg/L.

The corresponding mass percent and mole fraction (*x*₁), calculated by the compilers, are 6.2 · 10⁻⁸ g (1)/100 g sln and 5.2 · 10⁻¹¹, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 *g* to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
 Solubility: ± 0.075; type of error not specified.

References:

¹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Components:

- (1) Benz[*a*]anthracene; C₁₈H₁₂; [56-55-3]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Variables:

One temperature: 25 °C
 Salinity: 0–40 g (2)/kg sln

Original Measurements:

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

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of benz[*a*]anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

- S*₀ is the solubility of (1) in water (mg/L);
S is the solubility of (1) in solution (mg/L);
*K*_{*S*} is the Setschenow constant (L/mol); and
*C*_{*S*} is the concentration of sodium chloride (L/mol).

When evaluating the equation for *S* over the range of *C*_{*S*} 0–0.7 mol/L, *K*_{*S*} = 0.354 with *S*₀ = 0.0094.

The corresponding mass percent and mole fraction (*x*₁) at salinity = 35 g (2)/kg sln, calculated by the compilers, are 5.6 · 10⁻⁷ g (1)/100 g sln and 4.5 · 10⁻¹⁰, respectively.

Auxiliary Information**Method/Apparatus/Procedure:**

A saturated solution of (1) was prepared by pumping salt water through a “generator column” which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an “extractor column” packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
 (2) Reagent grade.
 (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C.
*K*_{*S*}: ± 0.002.
*S*₀: ± 0.001.

2.37. Chrysene+Seawater

Components:

- (1) Chrysene; C₁₈H₁₂; [218-01-9]
- (2) Sodium chloride; NaCl; [7647-14-5]
- (3) Water; H₂O; [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
Salinity: 0–40 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

The solubility of chrysene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_S C_S$$

where

S_0 is the solubility of (1) in water (mg/L);

S is the solubility of (1) in solution (mg/L);

K_S is the Setschenow constant (L/mol); and

C_S is the concentration of sodium chloride (L/mol).

When evaluating the equation for S over the range of C_S 0–0.7 mol/L, $K_S = 0.336$, $S_0 = 0.0018$.

The corresponding mass percent and mole fraction (x_1) at salinity=35 g (2)/kg sln, calculated by the compilers, are $1.1 \cdot 10^{-7}$ g (1)/100 g sln and $8.8 \cdot 10^{-11}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

A saturated solution of (1) was prepared by pumping salt water through a "generator column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C₁₈ stationary phase. Then a water–acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

Source and Purity of Materials:

- (1) Greater than 97% pure.
- (2) Reagent grade.
- (3) Distilled from potassium permanganate–sodium hydroxide and passed through an XAD-2 column.

Estimated Error:

Temperature: ± 0.05 °C
 K_S : ± 0.010 .
 S_0 : ± 0.0001 .

2.38. Octadecane+Seawater

Components:

- (1) Octadecane; C₁₈H₃₈; [593-45-3]
- (2) Seawater

Original Measurements:

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

Variables:

One temperature: 25 °C
Salinity: 35 g salts/kg sln

Prepared By:

P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of octadecane in seawater was reported to be $8 \cdot 10^{-8}$ g (1)/100 g sln and $x_1 = 5 \cdot 10^{-11}$.

Auxiliary Information

Method/Apparatus/Procedure:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μ m membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+ % pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of $\pm 16\%$, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.39. Benzo[a]pyrene+Seawater

Components:

- (1) Benzo[a]pyrene; C₂₀H₁₂; [50-32-8]
 (2) Salt water

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Ref. 1)

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhail, and M. Ya. Gubergits,
 Khim. Tverd. Topl. **11**, 133 (1977).

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benzo[a]pyrene in salt water was reported to be 0.13 μg/L.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $1.3 \cdot 10^{-8}$ g (1)/100 g sln and $9.5 \cdot 10^{-12}$, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
 Solubility: ± 0.008; type of error not specified.

References:

¹P. Ya. Krasnoshchekova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

2.40. Benzo[e]pyrene+Seawater

Components:

- (1) Benzo[e]pyrene; C₂₀H₁₂; [192-97-2]
 (2) Seawater

Evaluators:

D. G. Shaw, Institute of Marine Science, University of Alaska, Fairbanks, Alaska, USA.
 A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, May, 2004.

Critical Evaluation of Solubility of Benzo[e]Pyrene (1) in Seawater (2)

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

Author (s)	T/K	Salinity g salts/kg sln
Krasnoshchekova <i>et al.</i> ¹	298	6
Schwarz ²	298	30

The experimental data are listed in Table 15. The two reported values are in fair agreement and therefore both are adopted as Tentative at their respective salinities. Schwarz also provides data over the temperature range 282–303 K.

References:

¹P. Ya. Krasnoshchekova, Yu. A. Pakhapill, and M. Ya. Gubergits, Khim. Tverd. Topl. **11**, 133 (1977).

²F. P. Schwarz, J. Chem. Eng. Data **22**, 273 (1977).

TABLE 15. Experimental values for solubility of benzo[e]pyrene (1) in seawater (2)

T/K	Salinity g salts/kg sln	Experimental values g (1)/100 g sln (T=tentative)
298	6 (Ref. 1)	$1.79 \cdot 10^{-7}$ (T; Ref. 1)
	30 (Ref. 2)	$3.32 \cdot 10^{-7}$ (T; Ref. 2)

Components:

(1) Benzo[*e*]pyrene; C₂₀H₁₂; [192-97-2]
 (2) Salt water

Original Measurements:

P. Ya. Krasnoshechekova, Yu. A. Pakhaill, and M. Ya. Gubergrits, *Khim. Tverd. Topl.* **11**, 133 (1977).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Krasnoshechekova and Gubergrits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benzo[*e*]pyrene in salt water was reported to be 1.83 μg/L.

The corresponding mass percent and mole fraction (*x*₁), calculated by the compilers, are 1.79 · 10⁻⁷ g (1)/100 g sln and 1.34 · 10⁻¹⁰, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
 Solubility: ± 0.111; type of error not specified.

References:

¹P. Ya. Krasnoshechekova and M. Ya. Gubergrits, *Neftekhimiya* **13**, 885 (1973).

Components:

(1) Benzo[*e*]pyrene; C₂₀H₁₂; [192-97-2]
 (2) Sodium chloride; NaCl; [7647-14-5]
 (3) Water; H₂O; [7732-18-5]

Original Measurements:

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

Variables:

Temperature: 8.9–30.2 °C
 Salinity: 30 g (2)/kg sln

Prepared By:

W. Y. Shiu and D. Mackay

Experimental Values

Solubility of benzo[*e*]pyrene in 0.5 mol (2)/L

<i>t</i> /°C	10 ⁸ · mol (1)/L sln
8.9	0.82
10.8	0.88
15.6	1.01
17.0	1.01
19.2	1.04
21.7	1.13
25.3	1.35
27.1	1.42
30.2	1.66

The corresponding mass percent and mole fraction *x*₁ at 25.3 °C, calculated by the compilers, are 3.32 · 10⁻⁷ g(1)/100 g sln and 2.44 · 10⁻¹⁰, respectively

Auxiliary Information**Method/Apparatus/Procedure:**

The solubility of benzo[*e*]pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of benzo[*e*]pyrene to an air-tight 1 × 1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 h in a thermostatted water bath and then its fluorescence intensity was measured at 410 and 265 nm. The spectrofluorimeter employed a ratio-photon counting mode where benzo[*e*]pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[*e*]pyrene in cyclohexane therefore providing an absolute solubility scale for the fluorescence method.

Source and Purity of Materials:

(1) Benzo[*e*]pyrene: purity >99 mole %.
 Sodium chloride: reagent grade.
 Water: distilled over a KMnO₄-NaOH solution and passed through a Sephadex column.
 Cyclohexane: reagent grade.

Estimated Error:

Temperature: ± 0.1 °C (author).
 Solubility: ± 19.5% (author).

2.41. Eicosane+Seawater

Components:

- (1) Eicosane; C₂₀H₄₂; [112-95-8]
 (2) Seawater

Original Measurements:

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

Variables:

One temperature: 25 °C
 Salinity: 35 g salts/kg sln

Prepared By:

P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of eicosane in seawater was reported to be $8 \cdot 10^{-8}$ g (1)/100 g sln and $x_1 = 5 \cdot 10^{-11}$.

Auxiliary Information**Method/Apparatus/Procedure:**

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+% pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of ±16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

2.42. Benzo[ghi]perylene+Seawater

Components:

- (1) Benzo[ghi]perylene; C₂₂H₁₂; [191-24-2]
 (2) Salt water

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhail, and M. Ya. Gubergrits, Khim. Tverd. Topl. **II**, 133 (1977).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benzo[ghi]perylene in salt water was reported to be 0.21 μg/L.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $2.1 \cdot 10^{-8}$ g (1)/100 g sln and $1.4 \cdot 10^{-11}$ assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ±1 °C.
 Solubility: ±0.048; type of error not specified.

References:

¹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

2.43. Benzo[*b*]triphenylene+Seawater

Components:

- (1) Benzo[*b*]triphenylene; C₂₂H₁₄; [215-58-7]
(2) Salt water

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhail, and M. Ya. Gubergrits, *Khim. Tverd. Topl.* **11**, 133 (1977).

Variables:

One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of benzo[*b*]triphenylene in salt water was reported to be 27.84 μ g/L.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $2.719 \cdot 10^{-6}$ g (1)/100 g sln and $1.841 \cdot 10^{-9}$, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
Solubility: ± 1.48; type of error not specified.

References:

¹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, *Neftekhimiya* **13**, 885 (1973).

2.44. Dibenz[*a,h*]anthracene+Seawater

Components:

- (1) Dibenz[*a,h*]anthracene; C₂₂H₁₄; [53-70-3]
(2) Salt water

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhail, and M. Ya. Gubergrits, *Khim. Tverd. Topl.* **11**, 133 (1977).

Variables:

One temperature: 25 °C
Salinity: 6 g/kg sln (Krasnoshchekova and Gubergrits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of dibenz[*a,h*]anthracene in salt water was reported to be 21.13 μ g/L.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers, are $2.064 \cdot 10^{-6}$ g (1)/100 g sln and $1.397 \cdot 10^{-9}$, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
Solubility: ± 1.14; type of error not specified.

References:

¹P. Ya. Krasnoshchekova and M. Ya. Gubergrits, *Neftekhimiya* **13**, 885 (1973).

2.45. Dibenz[*a,j*]anthracene+Seawater**Components:**

- (1) Dibenz[*a,j*]anthracene; C₂₂H₁₄; [224-41-9]
 (2) Salt water

Original Measurements:

P. Ya. Krasnoshchekova, Yu. A. Pakhail, and M. Ya. Gubergits, Khim. Tverd. Topl. **11**, 133 (1977).

Variables:

One temperature: 25 °C
 Salinity: 6 g/kg sln (Krasnoshchekova and Gubergits¹)

Prepared By:

M. Kleinschmidt and D. G. Shaw

Experimental Values

The solubility of dibenz[*a,j*]anthracene in salt water was reported to be 10.544 μg/L.

The corresponding mass percent and mole fraction (*x*₁), calculated by the compilers, are 1.029 · 10⁻⁶ g (1)/100 g sln and 6.970 · 10⁻¹⁰, respectively, assuming a solution density of 1.004 kg/L.

Auxiliary Information**Method/Apparatus/Procedure:**

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1 L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water (or salt water) was added to the dried residue, and the solution was stirred for 6 h and allowed to settle for 16–18 h. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

Source and Purity of Materials:

Not given.

Estimated Error:

Temperature: ± 1 °C.
 Solubility: ± 1.05; type of error not specified.

References:

- ¹P. Ya. Krasnoshchekova and M. Ya. Gubergits, Neftekhimiya **13**, 885 (1973).

2.46. Hexacosane+Seawater

Components:

- (1) Hexacosane; C₂₆H₅₄; [630-01-3]
 (2) Seawater

Original Measurements:

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

Variables:

One temperature: 25 °C
 Salinity: 35 g salts/kg sln

Prepared By:

P. A. Meyers and D. G. Shaw

Experimental Values

The solubility of hexacosane in seawater was reported to be 10⁻⁸ g (1)/100 g sln and *x*₁ = 6 · 10⁻¹².

Auxiliary Information**Method/Apparatus/Procedure:**

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 h at 25.0 ± 0.1 °C. The mixture was then allowed to stand for 24 h. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

Source and Purity of Materials:

Analabs, Inc., North Haven, Conn. 99+ % pure hydrocarbons. Seawater collected from 25 m depth in the Gulf of Mexico, poisoned with HgCl₂ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural *n*-alkane levels too low to cause interference.

Estimated Error:

Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

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