COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in pyrene.

TABLE 1. Quantitative Solubility Studies of Pyrene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Wauchope and Getzen (ref 3)	273-348	spectrophotometric
Mackay and Shiu (ref 4)	298	spectrofluorometric
Schwarz (ref 5)	285-304	spectrofluorometric
May *et al.* (ref 6)	298-302	chromatographic
Rossi and Thomas (ref 7)	298	GLC, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. At 298 K the values of Mackay and Shiu (ref 4), Schwarz (ref 5), May *et al.* (ref 6) and Rossi and Thomas (ref 7) are in excellent agreement and their average is Recommended. The values of Wauchope and Getzen (ref 3) and especially Klevens (ref 2) are signifigantly higher ($>3\sigma_n$) than the other studies and are thus rejected. At 303 K the values of Wauchope and Getzen (ref 3) are in good agreement with those of Schwarz (ref 5) and May *et al.* (ref 6). At other temperatures the data are mainly those of Wauchope and Getzen and must therefore be regarded as Tentative.

With the exception of the rejected values noted above and the 300 K datum of Davis *et al.* (ref 1) which is omitted for representational convenience, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

(continued)

TABLE 2. Recommended (R) and Tentative Solubility Values of Pyrene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values ($\pm\sigma_n$)[b]	
	10^5 g(1)/100 g sln	10^5 g(1)/100 g sln	10^8 x_1
273	0.49 (ref 3)	0.5	0.4
293	0.91* (ref 5)	0.9	0.8
298	1.35 (ref 4), 1.295 (ref 5), 1.32 (ref 6), 1.3 (ref 7)	1.32 ± 0.02(R)	1.17(R)
303	1.80* (ref 3), 1.76* (ref 5), 1.70* (ref 6)	1.75 ± 0.04(R)	1.56(R)
313	3.30* (ref 3)	3	3
323	5.32 (ref 3)	5	4
333	9.4* (ref 3)	9	8
343	16.9 (ref 3)	17	15
348	23.1 (ref 3)	23	20

a Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.

b Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

(continued)

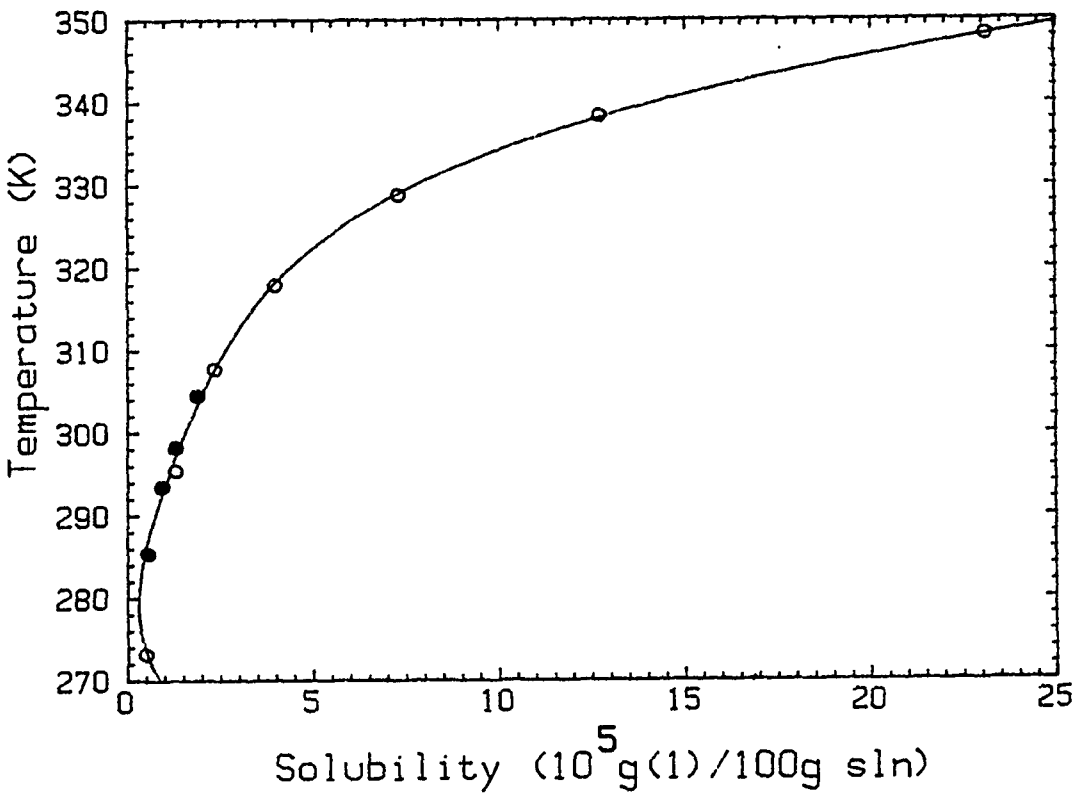

FIGURE 1. Solubility of pyrene in water, selected data: ref 3 (o); ref 5 (●).

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54* , 283-98.
3. Wauchope, R.D.; Getzen,F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
4. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
5. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
6. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
7. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
VARIABLES:	PREPARED BY:
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pyrene in water

t/°C	10^4 g(1) L^{-1} (2)
27	1.60 ± 0.10
	1.65 ± 0.05

The best value recommended by the authors is 1.65×10^{-4} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.65×10^{-5} g(1)/100 g sln and 1.45×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.	(1) prepared at Harvard University; m.p. range 149.6-150.5°C; (cf. ref 2). (2) dust-free.
	ESTIMATED ERROR: temp. ± 3°C soly. see above

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pyrene in water at 25°C was reported to be 1.75×10^{-4} g(1) L^{-1} sln and 7.7×10^{-7} mol(1) L^{-1} sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.75×10^{-5} g(1)/ 100 g sln and 1.39×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]	Wauchope, R.D.; Getzen, F.W.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1972, *17*, 38-41.
VARIABLES:	**PREPARED BY:**
Temperature: 0-75°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. see experimental values above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pyrene in water at 25°C was reported to be 0.135 mg(1) dm^{-3} sln and $x_1 = 1.2 \times 10^{-8}$.

The corresponding mass percent calculated by the compiler is 0.0000135 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.005 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0]	Schwarz, F.P.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES:	**PREPARED BY:**
Temperature: 12.2-31.3°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
VARIABLES:	**PREPARED BY:**
Temperature: 25 and 29°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

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

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.01 mg(1)/kg(2) (standard deviation)

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	Rossi, S.S.; Thomas W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.
VARIABLES: One temperature: 25°C	**PREPARED BY:** G.T. Hefter

EXPERIMENTAL VALUES:

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; purified by derivatization with 2,4,6-trinitrophenol

(2) Doubly distilled in all-glass apparatus; free of trace organics.

ESTIMATED ERROR:

Temperature: ±0.1°C

Solubility: ±0.01 μg/g (std. dev. for 6 determinations)

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of pyrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Methods	Salinity g salts/kg sln	10^6 g(1)100 g sln
Krasnoshchekova *et al.* (ref 1)	spectral	6	7.705
Schwarz (ref 2)	uv spectral	30	9.48
May *et al.* (ref 3)	HPLC	35	8.60
Rossi and Thomas (ref 4)	GLC	35	8.9

At 298 K and a salinity of 35 g salts/kg sln the data of May *et al.* and Rossi and Thomas are in very good agreement. Since the value reported by May *et al.* 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. Rossi and Thomas and Schwarz each report data over a range of temperatures.

SOLUBILITY OF PYRENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

T/K	g salts/kg sln	10^6 g(1)/100 g sln
298	35	8.60

REFERENCES

1. Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.

2. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

3. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

4. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Salt Water	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	**PREPARED BY:** M. Kleinschmidt and D. 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 7.705×10^{-6} g(1)/100 g sln and 7.02×10^{-9} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 hr and allowed to settle for 16-18 hr. 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.	Not given.
	ESTIMATED ERROR: temp. ± 1°C soly. ± 2.93 type of error not specified
	REFERENCES: 1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES: Temperature: 8.6-31.1°C Salinity: 30 g(2)/kg sln	PREPARED BY: W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of pyrene in 0.5 g-mol(2)/dm^3

t/°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}.

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 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 395 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 therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Pyrene: purity > 99 mole %,

Sodium chloride: reagent grade,

Ethanol: reagent grade,

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

ESTIMATED ERROR:

Solubility ± 1.6% (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

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

$$\log(S_o/S) = K_s C_s$$

where;

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

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

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, K_s = 0.286 with S_o = 0.132.

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.	(1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.
	ESTIMATED ERROR: temp ± 0.05°C K_s ± 0.003 S_o ± 0.001
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Seawater; natural	Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.
VARIABLES: Temperature: 15 - 25°C Salinity: 35 g/kg sln	**PREPARED BY:** W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of pyrene in seawater

t/°C	μg(1)/g(2)	10^6Mass%[a] g(1)/100 g sln	10^9 x_1[a]
15	0.056	5.6	5.1
20	0.071	7.1	6.5
25	0.089	8.9	8.1

[a] calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solution was prepared by equilibrating seawater with an excess of pyrene for at least 24 hr. in a constant-temperature gyrotary shaker followed by a 12 hr 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:

Solubility ± 11%

Temperature ± 0.1°C

REFERENCES: