COMPONENTS:	EVALUATOR:
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION:

Quantitative solubility data for 2-methylanthracene (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 2-methylanthracene.

TABLE 1: Quantitative Solubility Studies of 2-Methylanthracene (1) in Water (2)

Reference	T /K	Method
Mackay and Shiu (ref 1)	298	spectofluorometric
May *et al.* (ref 2)	279-304	chromatographic

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

At 298K, the only temperature at which comparison is possible, the datum of Mackay and Shiu (ref 1) is in only fair agreement with that of May *et al.* (ref 2). Thus all the available data, which are summarized in Table 2, must be regarded as very tentative.

TABLE 2: Tentative Solubility Values of 2-Methylanthracene (1) in Water (2)

T /K	Solubility values		
	Reported values[a] 10^6 g(1)/100 g sln	"Best values ($\pm \sigma_n$)[b] 10^6 g(1) g sln	10^9 x_1
278	0.64* (ref 2)	0.6	0.6
283	0.89* (ref 2)	0.9	0.8
293	1.60* (ref 2)	1.6	1.5
298	3.9 (ref 1), 2.16* (ref 2)	3.0 ± 0.9	2.8
303	2.93 (ref 2)	3.0	2.8

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

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

REFERENCES

1. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7] (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 2-methylanthracene in water at 25°C was reported to be 0.039 mg(1) dm^{-3} sln and $x_1 = 3.67 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 3.9×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 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. ± 0.004 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7] (2) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 175-9 and 997-1000.
VARIABLES:	**PREPARED BY:**
Temperature: 6.3-31.1°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 2-methylanthracene in water

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

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

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. stand. dev. see above

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) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7] (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 2-methylanthracene 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 = 0.336 with S_o = 0.0213.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 1.29×10^{-6} g(1)/100 g sln and 1.24×10^{-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 ± 0.006 S_o ± 0.003
	REFERENCES: