COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	March 1986.

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Studies of the Solubility of Acenaphthene (1) in Water (2)

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Eganhouse and Calder (ref 2)	298	GLC
Mackay and Shiu (ref 3)	298	spectrofluorometric
Banerjee *et al.* (ref 4)	298	radiotracer
Rossi and Thomas (ref 5)	298	GLC, spectrophotometric

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

At 298K, the only temperature where comparison is possible (Table 1), the data of Wauchope and Getzen (ref 1), Eganhouse and Calder (ref 2) and Mackay and Shiu (ref 3) are in excellent agreement. The values of Banerjee *et al.* (ref 4) and Rossi and Thomas (ref 5) are respectively very much higher and lower and are therefore rejected.

At other temperatures only the data of Wauchope and Getzen (ref 1) are available and must therefore be regarded as Tentative values.

The solubility values of acenaphthene in water are summarized in Table 2 and plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Solubility Values for Acenaphthene (1) in Water (2)

T/K	Solubility values		
	Reported values[a] 10^4g(1)/100g sln	"Best" values ($\pm \sigma_n$)[b] 10^4g(1)/100g sln	10^7 x_1
273	1.45 (ref 1)	1.5	1.8
293	3.2* (ref 1)	3.2	3.7
298	3.88 (ref 1), 3.47 (ref 2), 3.93 (ref 3)	3.8 ± 0.2 (R)	4.4(R)

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H_2O; [7732-18-5]	March 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values		
	Reported values[a] 10^4g(1)/100g sln	"Best" values (± σ_n)[b] 10^4g(1)/100g sln	10^7 x_1
303	4.80 (ref 1)	4.8	5.6
313	7.4* (ref 1)	7.4	8.6
323	9.2 (ref 1)	9.2	10
333	19.4* (ref 1)	19	22
343	32.0* (ref 1)	32	37
348	42.5 (ref 1)	43	50

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data.
b Obtained by averaging where appropriate; σ_n has no significance.

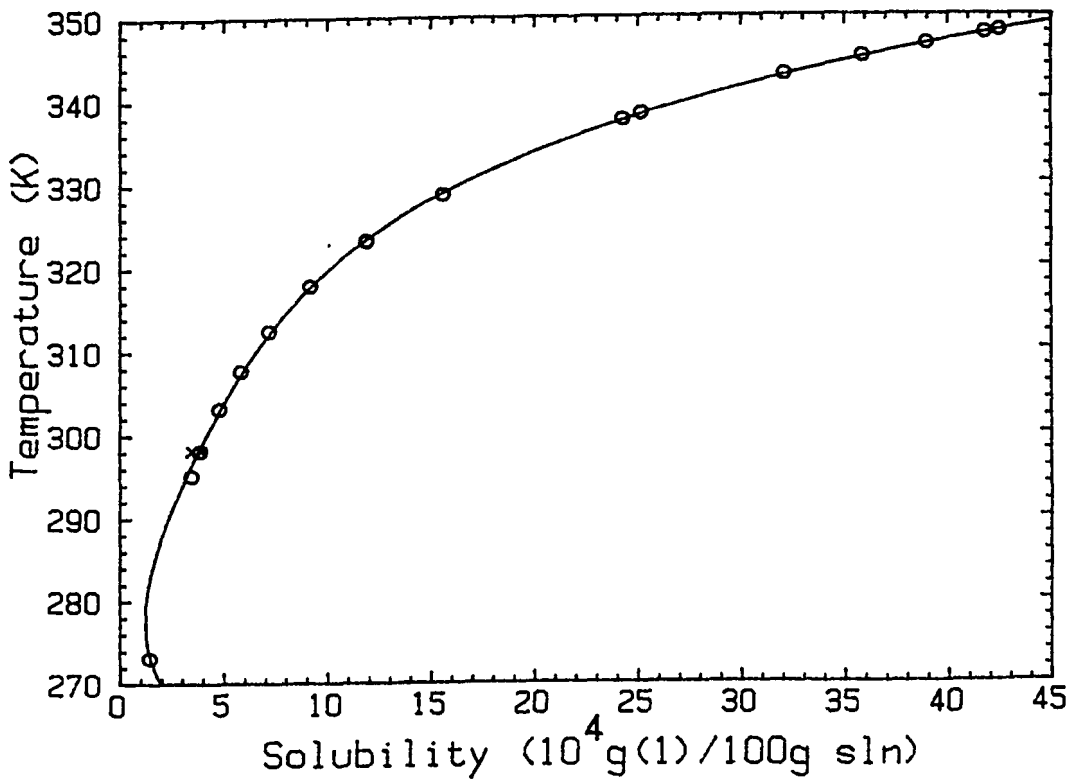

FIGURE 1. Solubility of acenaphthene in water: ref 1 (o); ref 2,3 (x).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
2. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
5. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	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 acenaphthene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^4 g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
0.0		1.45(0.04)	1.45	1.69
22.0	3.57	3.46	3.46	4.04
25.0		3.88(0.07)	3.88	4.53
30.0	4.76, 4.60, 4.72	4.80	4.80	5.61
34.5	6.00, 5.68, 5.73	5.83	5.83	6.81
39.3	6.8, 7.1, 7.0	7.2	7.2	8.4
44.7	9.4, 9.4, 9.3	9.2	9.2	10.7
50.0		11.9(0.1)	11.9	13.9
50.1	12.5, 12.4, 12.4	11.9	11.9	13.9
55.6	15.8, 16.3, 15.9	15.6	15.6	18.2
64.5	25.9, 27.8	24.3	24.3	28.4
65.2	23.7, 23.4, 22.8	25.2	25.2	29.4
69.8	30.1, 34.3, 33.6	32.1	32.1	37.5
71.9	35.2	35.9	35.9	41.9
73.4	39.1, 40.1	39.0	39.0	45.6
74.7	40.8, 39.3	41.8	41.8	48.8
75.0		42.5(0.7)	42.5	49.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from 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) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water at 25°C was reported to be 3.47 mg(1)/kg(2) and 2.2 x 10^{-5} mol(1) dm^{-3}(2).

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.	(1) source not specified; analytical grade; used as received; no impurities by glc. (2) doubly distilled; free of trace organics.
	ESTIMATED ERROR: temp. ± 0.5°C soly. ± 0.06 mg(1)/kg(2) (from eight determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	Mackay, D.; Shiu, W.Y.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water at 25°C was reported to be 3.93 mg(1) dm^{-3} sln and $x_1 = 4.59 \times 10^{-7}$.

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 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. ± 0.014 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water was reported to be 4.78×10^{-5} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction (x_1) solubilities, calculated by the compiler, are 7.37×10^{-4} g(1)/100 g sln and 8.60×10^{-7} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of acenaphthene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) ^{14}C-labelled: New England Nuclear, purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2°C

Solubility: ±4.1% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	Rossi, S.S.; Thomas, W.H.
(2) Water; H_2O; [7732-18-5]	*Environ. Sci. Technol.* 1981, *15*, 715-6.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acenaphthene in distilled water at 25°C was reported to be 2.42 μg/g, corresponding to a mole fraction, x_1, of 1.6×10^{-8}. The corresponding mass per cent calculated by the compiler is 2.42×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; 99.9% purity; recryst. twice from dist. MeOH.

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

ESTIMATED ERROR:

Temperature: ±0.1°C

Solubility: ±0.02 μg/g (std. dev. for 6 determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Seawater; natural	Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.
VARIABLES:	**PREPARED BY:**
Temperature: 15-25°C Salinity: 35 g/kg sln	W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

Solubility of Acenaphthene in Seawater

t/°C	µg(1)/g(2)	10^5 Mass %[a] g(1)/100 g sln	$10^8 x_1$[a]
15	0.214	2.14	2.56
20	0.55	5.5	6.6
25	1.84	18.4	22.0

[a]Calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solution was prepared by equilibrating seawater with an excess of hydrocarbon for 24 hrs in a constant temperature gyrotary shaker followed by 12 hr stationary 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 hydrocarbon concentration.

SOURCE AND PURITY OF MATERIALS:

Acenaphthene: from Aldrich Chemical Co. of 99% purity and doubly distilled from distilled methanol,

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 adjusted to 35 ‰.

ESTIMATED ERROR:

Temp. ±0.1°K

Soly. ±2%

REFERENCES: