

<p>COMPONENTS:</p> <p>(1) Phenanthrene; C<sub>14</sub>H<sub>10</sub>; [85-01-8]</p> <p>(2) Water; H<sub>2</sub>O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.</p> <p>February 1986.</p>
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## CRITICAL EVALUATION:

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

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

Reference	T/K	Method
Davis <i>et al.</i> (ref 1)	300	nephelometric
Andrews and Keefer (ref 2)	298	spectrophotometric
Klevens (ref 3)	298	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Eganhouse and Calder (ref 5)	298	GLC
Mackay and Shiu (ref 6)	298	spectrofluorometric
Schwarz (ref 7)	282-305	spectrofluorometric
May <i>et al.</i> (ref 8)	282-303	chromatographic

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

The plethora of values reported (Table 1) at 298K for the solubility of phenanthrene (1) in water (2) enable a particularly critical assessment to be made. Thus the values of Davis *et al.* (ref 1) at 300K and of Klevens (ref 3) have been rejected as they are significantly higher than all other values. The remaining data at 298K are in good agreement enabling the average value to be Recommended.

At other temperatures where comparison is possible the data of May *et al.* (ref 8), Schwarz (ref 7) and Wauchope and Getzen (ref 4) are in excellent agreement enabling the average values to be Recommended over a reasonably wide range. At higher temperatures (> 303K) only the data of Wauchope and Getzen (ref 4) are available and must therefore be regarded as Tentative.

All the available data, except for the rejected values noted above (ref 1, 3), are summarized in Table 2 and plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
(2) Water; H <sub>2</sub> O; [7732-18-5]	February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubility Values of Phenanthrene (1) in Water (2)

T/K	Solubility values		
	Reported values <sup>a</sup> 10 <sup>4</sup> g(1)/100g sln	"Best" values (± σ <sub>n</sub> ) <sup>b</sup> 10 <sup>4</sup> g(1)/100g sln	10 <sup>7</sup> x <sub>1</sub>
273	0.39 (ref 4)	0.4	0.4
283	0.53* (ref 7), 0.46* (ref 8)	0.50 ± 0.04 ( <i>R</i> )	0.50 ( <i>R</i> )
293	0.88* (ref 7), 0.78* (ref 8)	0.85 ± 0.05 ( <i>R</i> )	0.86 ( <i>R</i> )
298	0.994 (ref 2), 1.18 (ref 4), 1.07 (ref 5), 1.29 (ref 6), 1.151 (ref 7), 1.002 (ref 8)	1.1 ± 0.1 ( <i>R</i> )	1.1 ( <i>R</i> )
303	1.50* (ref 4), 1.46* (ref 7), 1.28* (ref 8)	1.4 ± 0.1 ( <i>R</i> )	1.4 ( <i>R</i> )
313	2.45* (ref 4)	2.5	2.5
323	4.14 (ref 4)	4.1	4.1
333	7.2* (ref 4)	7.2	7.2
343	12.8* (ref 4)	13	13
348	17 (ref 4)	17	17

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

<sup>b</sup> Obtained by averaging where appropriate; σ<sub>n</sub> has no statistical significance.

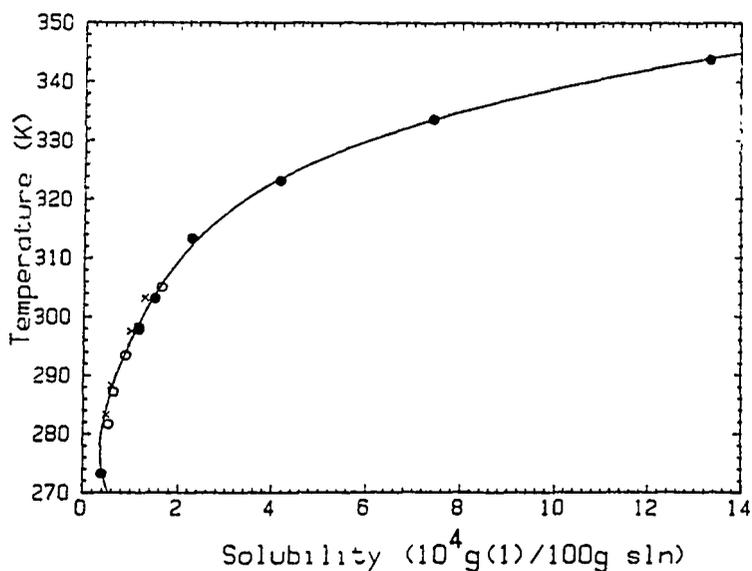


FIGURE 1. Solubility of phenanthrene in water, selected data: ref 4 (●); ref 7 (o); ref 8 (x). Solid curve plotted through "Best" values (Table 2).

(continued next page)

<p>COMPONENTS:</p> <p>(1) Phenanthrene; C<sub>14</sub>H<sub>10</sub>; [85-01-8] (2) Water; H<sub>2</sub>O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.</p> <p>February 1986.</p>
<p>CRITICAL EVALUATION: (continued)</p> <p>REFERENCES</p> <ol style="list-style-type: none"><li>1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1942</u>, <i>64</i>, 108-10.</li><li>2. Andrews, L.J.; Keefer, R.M. <i>J. Am. Chem. Soc.</i> <u>1949</u>, <i>71</i>, 3644-77.</li><li>3. Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u>, <i>54</i>, 283-298.</li><li>4. Wauchope, R.D.; Getzen, F.W. <i>J. Chem. Eng. Data</i> <u>1972</u>, <i>17</i>, 38-41.</li><li>5. Eganhouse, R.P.; Calder, J.A. <i>Geochim. Cosmochim. Acta</i> <u>1976</u>, <i>40</i>, 555-61.</li><li>6. Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 399-402.</li><li>7. Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 273-7.</li><li>8. May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u>, <i>50</i>, 997-1000.</li></ol> <p>ACKNOWLEDGEMENT</p> <p>The Evaluator thanks Dr Brian Clare for the graphics.</p>	

<b>COMPONENTS:</b>  (1) Phenanthrene; $C_{14}H_{10}$ ; [85-01-8] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.  <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 108-10.								
<b>VARIABLES:</b>  One temperature: 27°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson								
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of phenanthrene in water</p> <table style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><math>t/^\circ C</math></th> <th style="text-align: center;"><math>10^3 \text{ g(1) L}^{-1} \text{ (2)}</math></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">27</td> <td style="text-align: center;">1.55</td> </tr> <tr> <td></td> <td style="text-align: center;">1.62</td> </tr> <tr> <td></td> <td style="text-align: center;">1.65</td> </tr> </tbody> </table> <p>The best value recommended by the authors is <math>1.60 \times 10^{-3} \text{ g(1) L}^{-1} \text{ (2)}</math>. Assuming that 1.00 L sln = kg sln the corresponding mass percent and mole fraction, <math>x_1</math>, calculated by the compiler are <math>1.60 \times 10^{-4} \text{ g(1)/100 g sln}</math> and <math>1.62 \times 10^{-7}</math>.</p>		$t/^\circ C$	$10^3 \text{ g(1) L}^{-1} \text{ (2)}$	27	1.55		1.62		1.65
$t/^\circ C$	$10^3 \text{ g(1) L}^{-1} \text{ (2)}$								
27	1.55								
	1.62								
	1.65								
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Eastman Kodak Company, 599; m.p. range 100.0-100.9°C; used as received; (cf. ref 2).  (2) dust-free.  <b>ESTIMATED ERROR:</b>  temp. $\pm 3^\circ C$ soly. $\pm 0.05 \times 10^{-3} \text{ g(1) dm}^{-3} \text{ (2)}$  <b>REFERENCES:</b>  1. Davis, W.W.; Parker, Jr., T.V. <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 101. 2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1940</u> , <i>62</i> , 3086.								

<b>COMPONENTS:</b>  (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Andrews, L.J.; Keefer, R.M.  <i>J. Am. Chem. Soc.</i> <u>1949</u> , <i>71</i> , 3644-77.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  A. Maczynski and Z. Maczynska
<b>EXPERIMENTAL VALUES:</b>  The solubility of phenanthrene in water at 25°C was reported to be $9.94 \times 10^{-5}$ g(l)/100 g sln. The corresponding mole fraction, $x_1$ , value calculated by compiler is $1.004 \times 10^{-7}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Eastman Kodak Co., best grade; recrystallized twice from ethanol; m.p. 101.0°C. (2) not specified.  <b>ESTIMATED ERROR:</b>  not specified.  <b>REFERENCES:</b>

<b>COMPONENTS:</b>  (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u> , 54, 283-98.
<b>VARIABLES:</b>  Temperature: 25°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  The solubility of phenanthrene in water at 25°C was reported to be $0.0016 \times 10^{-5}$ g(l)/L sln and $9.0 \times 10^{-6}$ mole (l)/L sln. Assuming that 1.00 dm <sup>3</sup> sln = 1.00 kg sln the corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are $1.6 \times 10^{-4}$ g(l)/100 g sln and $1.62 \times 10^{-7}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) not specified. (2) not specified.
	<b>ESTIMATED ERROR:</b>  not specified.
	<b>REFERENCES:</b>

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Water; H <sub>2</sub> O; [7732-18-5]		Wauchope, R.D.; Getzen, F.W. <i>J. Chem. Eng. Data</i> <u>1972</u> , <i>17</i> , 38-41.	
VARIABLES:		PREPARED BY:	
Temperature: 0-75°C		A. Maczynski	
EXPERIMENTAL VALUES:			
Solubility of phenanthrene in water			
<i>t</i> /°C	mg(1)/kg(2)		
	experiment	smoothed with (std dev)	10 <sup>4</sup> g(1)/100 g sln (compiler)
			10 <sup>7</sup> x <sub>1</sub> (compiler)
0.0		0.39(0.01)	0.39
24.6	1.12, 1.11	1.16	1.16
25.0		1.18(0.02)	1.18
29.9	1.49, 1.49	1.49	1.49
30.3	1.47, 1.48	1.52	1.52
38.4	2.44, 2.45	2.27	2.27
40.1	2.27, 2.28, 2.25	2.47	2.47
47.5	3.81, 3.88, 3.87	3.63	3.63
50.0		4.14(0.04)	4.14
50.1	4.30, 4.38, 4.32	4.16	4.16
50.2	4.08, 4.04, 4.11	4.19	4.19
54.7	5.66, 5.64, 5.63	5.34	5.34
59.2	7.17, 7.19, 7.21	6.85	6.85
60.5	7.2, 7.2, 7.6	7.4	7.4
65.1	9.8, 9.7, 9.8	9.6	9.6
70.7	12.4, 12.6, 12.4	13.3	13.3
71.9	12.9	14.2	14.2
73.4	18.2	15.6	15.6
75.0		17.2(0.3)	17.2
AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
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 glass-ware.		(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:	

<b>COMPONENTS:</b>  (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8]  (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Eganhouse, R.P.; Calder, J.A.  <i>Geochim. Cosmochim. Acta</i> <u>1976</u> , 40, 555-61.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  A. Maczynski
<b>EXPERIMENTAL VALUES:</b>  The solubility of phenanthrene in water at 25°C was reported to be 1.07 mg(1)/kg(2) and $6 \times 10^{-6}$ mol(1) dm <sup>-3</sup> (2).  The corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are $1.07 \times 10^{-4}$ g(1)/100 g sln and $1.08 \times 10^{-7}$ .	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) source not specified; analytical grade; used as received; no impurities by glc.  (2) doubly distilled; free of trace organics.  <b>ESTIMATED ERROR:</b>  temp. ± 0.5°C soly. ± 0.01 mg(1)/kg(2) (from eight determinations)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) Phenanthrene; $C_{14}H_{10}$ ; [85-01-8] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 399-402.
<b>VARIABLES:</b> One temperature: 25°C	<b>PREPARED BY:</b> M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b> <p>The solubility of phenanthrene in water at 25°C was reported to be 1.29 mg(1) dm<sup>-3</sup> sln and <math>x_1 = 1.3 \times 10^{-7}</math>.</p> <p>The corresponding mass percent calculated by the compiler is <math>1.29 \times 10^{-4}</math> g(1)/100 g sln.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> 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.	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received. (2) doubly distilled. <b>ESTIMATED ERROR:</b> soly. $\pm 0.07$ mg(1) dm <sup>-3</sup> sln (maximum deviation from several determinations). <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Water; H <sub>2</sub> O; [7732-18-5]		<b>ORIGINAL MEASUREMENTS:</b> Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 273-7.	
<b>VARIABLES:</b> Temperature: 8.4-31.8°C		<b>PREPARED BY:</b> A. Maczynski	
<b>EXPERIMENTAL VALUES:</b>			
Solubility of phenanthrene in water			
<i>t</i> /°C	10 <sup>6</sup> mol(1) L <sup>-1</sup>	10 <sup>5</sup> g(1)/100 g sln (compiler)	10 <sup>8</sup> x <sub>1</sub> (compiler)
8.4	2.81 ± 0.07	5.01	5.06
11.1	3.09 ± 0.07	5.51	5.57
14.0	3.59 ± 0.06	6.40	6.47
17.5	4.40 ± 0.04	7.84	7.92
20.2	4.94 ± 0.09	8.80	8.90
23.3	6.09 ± 0.07	10.85	10.97
25.0	6.46 ± 0.02	11.51	11.63
29.3	7.7 ± 0.2	13.72	13.87
31.8	9.13 ± 0.08	16.27	16.44
<b>AUXILIARY INFORMATION</b>			
<b>METHOD/APPARATUS/PROCEDURE:</b> 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.		<b>SOURCE AND PURITY OF MATERIALS:</b> (1) source not specified; better than 99 mole%, by glc; used as received.  (2) distilled over KMnO <sub>4</sub> and NaOH and passed through a Sephadex column.	
		<b>ESTIMATED ERROR:</b> temp. ± 0.1°C soly. see above	
		<b>REFERENCES:</b>	

<b>COMPONENTS:</b>  (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  May, W.E.; Wasik, S.P.; Freeman, D.H.  <i>Anal. Chem.</i> <u>1978</u> , <i>50</i> , 175-9 and 997-1000.																																								
<b>VARIABLES:</b>  Temperature: 8.5-29.9°C	<b>PREPARED BY:</b>  A. Maczynski																																								
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of phenanthrene in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><u>t/°C</u></th> <th style="text-align: center;"><u>µg(1)/kg(2)</u></th> <th style="text-align: center;"><u>10<sup>4</sup> g(1)/100 g sln (compiler)</u></th> <th style="text-align: center;"><u>10<sup>8</sup> x<sub>1</sub> (compiler)</u></th> </tr> </thead> <tbody> <tr><td>8.5</td><td style="text-align: center;">423 ± 4</td><td style="text-align: center;">0.423</td><td style="text-align: center;">0.427</td></tr> <tr><td>10.0</td><td style="text-align: center;">468 ± 2</td><td style="text-align: center;">0.468</td><td style="text-align: center;">0.473</td></tr> <tr><td>12.5</td><td style="text-align: center;">512 ± 1</td><td style="text-align: center;">0.512</td><td style="text-align: center;">0.517</td></tr> <tr><td>15.0</td><td style="text-align: center;">601 ± 7</td><td style="text-align: center;">0.601</td><td style="text-align: center;">0.607</td></tr> <tr><td>21.0</td><td style="text-align: center;">816 ± 8</td><td style="text-align: center;">0.816</td><td style="text-align: center;">0.825</td></tr> <tr><td>24.3</td><td style="text-align: center;">995 ± 1</td><td style="text-align: center;">0.995</td><td style="text-align: center;">1.006</td></tr> <tr><td>25.0</td><td style="text-align: center;">1002 ± 11</td><td style="text-align: center;">1.002</td><td style="text-align: center;">1.013</td></tr> <tr><td>29.0</td><td style="text-align: center;">1220 ± 13</td><td style="text-align: center;">1.220</td><td style="text-align: center;">1.233</td></tr> <tr><td>29.9</td><td style="text-align: center;">1277 ± 11</td><td style="text-align: center;">1.277</td><td style="text-align: center;">1.291</td></tr> </tbody> </table> $\mu\text{g}(1)/\text{kg}(2) = 324.0 + 5.413 t + 0.8059 t^2 + 0.0025 t^3$		<u>t/°C</u>	<u>µg(1)/kg(2)</u>	<u>10<sup>4</sup> g(1)/100 g sln (compiler)</u>	<u>10<sup>8</sup> x<sub>1</sub> (compiler)</u>	8.5	423 ± 4	0.423	0.427	10.0	468 ± 2	0.468	0.473	12.5	512 ± 1	0.512	0.517	15.0	601 ± 7	0.601	0.607	21.0	816 ± 8	0.816	0.825	24.3	995 ± 1	0.995	1.006	25.0	1002 ± 11	1.002	1.013	29.0	1220 ± 13	1.220	1.233	29.9	1277 ± 11	1.277	1.291
<u>t/°C</u>	<u>µg(1)/kg(2)</u>	<u>10<sup>4</sup> g(1)/100 g sln (compiler)</u>	<u>10<sup>8</sup> x<sub>1</sub> (compiler)</u>																																						
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29.9	1277 ± 11	1.277	1.291																																						
<b>AUXILIARY INFORMATION</b>																																									
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) commercial product; less than 3% impurities.  (2) distilled over KMnO <sub>4</sub> and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).  <b>ESTIMATED ERROR:</b>  temp. ± 0.05°C soly. stand. dev. see above  <b>REFERENCES:</b>  1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. <i>J. Chromatogr. Sci.</i> <u>1975</u> , <i>13</i> , 535.																																								

<b>COMPONENTS:</b>  (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Seawater	<b>EVALUATOR:</b>  D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA  December 1982
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**CRITICAL EVALUATION:**

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

<u>Authors</u>	<u>Method</u>	<u>Salinity g salts/kg sln</u>	<u>10<sup>5</sup> g(1)/100 g sln</u>
Eganhouse and Calder (ref 1)	GLC	35	7.1
Schwarz (ref 2)	uv spectral	30	9.94
May <i>et al.</i> (ref 3)	HPLC	35	6.63
Aquan-Yuen <i>et al.</i> (ref 4)	uv spectral	28.6	8.3

At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder and of May *et al.* are in very good agreement. Therefore their mean,  $6.9 \times 10^{-5}$  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.* appears consistent with the data discussed above and with the recommended value for the solubility of phenanthrene in pure water and is adopted at tentative. The value of Schwarz appears slightly high and is considered doubtful.

THE SOLUBILITY OF PHENANTHRENE (1) IN SEAWATER (2)

RECOMMENDED VALUE

<u>T/K</u>	<u>g salts/kg sln</u>	<u>10<sup>5</sup> g(1)/100 g sln</u>
298	35	6.9

**REFERENCES**

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
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. Aquan-Yuen, M.; Mackay, D.; Shui, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.

<b>COMPONENTS:</b>  (1) Phenanthrene; $C_{14}H_{10}$ ; [85-01-8] (2) Artificial seawater (ref. 1)	<b>ORIGINAL MEASUREMENTS:</b>  Eganhouse, R.P.; Calder, J.A. <i>Geochim. Cosmochim. Acta</i> <u>1976</u> , 40, 555-61.
<b>VARIABLES:</b> One temperature: 25.0°C Salinity: 35 g/kg sln	<b>PREPARED BY:</b> M. Kleinschmidt and W. Shiu
<b>EXPERIMENTAL VALUES:</b>  The solubility of phenanthrene in seawater is reported to be 0.71 mg/kg the corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are $7.1 \times 10^{-5}$ g(1)/100 g sln and $7.4 \times 10^{-8}$ .  Graphical results for other salinities are also reported.	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  Equilibrium flask: 1-dm <sup>3</sup> Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ hr at 215 rpm on a New Brunswick gyrotary shaker; a 24 hr 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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) analytical grade salt for artificial seawater solution, reagent grade. Water: doubly distilled.  <b>ESTIMATED ERROR:</b> temperature: $\pm 0.5^\circ\text{C}$ soly: $\pm 0.025$ (95% confidence interval)  <b>REFERENCES:</b> 1. Lyman, J.; Fleming, R.H.; <i>J. Mar. Res.</i> <u>1940</u> , 3, 135.

<b>COMPONENTS:</b> (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 273-7.																		
<b>VARIABLES:</b> Temperature: 11.1 - 31.8°C Salinity: 30 g(2)/kg sln	<b>PREPARED BY:</b> W.Y. Shiu, D. Mackay																		
<b>EXPERIMENTAL VALUES:</b>  Solubility of phenanthrene in 0.5 mol(2)/L <table data-bbox="322 594 837 856" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><u>t/°C</u></th> <th style="text-align: center;"><u>10<sup>6</sup> mol(1)/L sln</u></th> </tr> </thead> <tbody> <tr><td style="text-align: center;">11.1</td><td style="text-align: center;">2.88</td></tr> <tr><td style="text-align: center;">14.0</td><td style="text-align: center;">3.2</td></tr> <tr><td style="text-align: center;">17.5</td><td style="text-align: center;">4.07</td></tr> <tr><td style="text-align: center;">20.2</td><td style="text-align: center;">4.51</td></tr> <tr><td style="text-align: center;">23.2</td><td style="text-align: center;">5.75</td></tr> <tr><td style="text-align: center;">25.0</td><td style="text-align: center;">5.72</td></tr> <tr><td style="text-align: center;">29.3</td><td style="text-align: center;">7.2</td></tr> <tr><td style="text-align: center;">31.8</td><td style="text-align: center;">7.9</td></tr> </tbody> </table> <p data-bbox="251 897 1133 1018">The corresponding mass percent and mole fraction <math>x_1</math> at 25.0°C calculated by the compilers are <math>9.94 \times 10^{-5}</math> g(1)/100 g sln and <math>1.034 \times 10^{-7}</math>.</p>		<u>t/°C</u>	<u>10<sup>6</sup> mol(1)/L sln</u>	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
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<b>METHOD/APPARATUS/PROCEDURE:</b> The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluorescence method, an excess amount of phenanthrene was added to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of 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 365 and 320 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.	<b>SOURCE AND PURITY OF MATERIALS:</b> Phenanthrene: purity 99.9% Sodium chloride: reagent grade Water: distilled over a KMnO <sub>4</sub> - NaOH solution and passed through a Sephadex column. Ethanol: reagent grade  <b>ESTIMATED ERROR:</b> Solubility ± 8.4% (author) Temperature ± 0.1°C (author)  <b>REFERENCES:</b>																		

<b>COMPONENTS:</b> (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u> , 50, 997-1000.
<b>VARIABLES:</b> One temperature: 25°C Salinity: 0-40 g(2)/kg sln	<b>PREPARED BY:</b> W.Y. Shiu and D. Mackay
<b>EXPERIMENTAL VALUES:</b> <p>The solubility of phenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:</p> $\log(S_0/S) = K_S C_S$ <p>where;</p> <p>S<sub>0</sub> is the solubility of (1) in water (mg/L)          S is the solubility of (1) in saline solution (mg/L)          K<sub>S</sub> is the Setschenow constant (L/mol)          C<sub>S</sub> in the concentration of sodium chloride (mol/L)</p> <p>evaluating the equation for S over the range of C<sub>S</sub> 0-0.7 mol/L,          K<sub>S</sub> = 0.275 with S<sub>0</sub> = 1.002.</p> <p>The corresponding mass percent and mole fraction <math>x_1</math>, at salinity = 35 g(2)/kg sln calculated by the compilers are <math>6.63 \times 10^{-5}</math> g(1)/100 g sln and <math>6.78 \times 10^{-8}</math>.</p> <p>Graphical data for other temperatures are also presented.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b> 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 <sub>18</sub> 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.	<b>SOURCE AND PURITY OF MATERIALS:</b> (1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column. <b>ESTIMATED ERROR:</b> temp ± 0.05°C K <sub>S</sub> ± 0.010 S <sub>0</sub> ± 0.011 <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) Phenanthrene; C <sub>14</sub> H <sub>10</sub> ; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y.  <i>J. Chem. Eng. Data</i> <u>1979</u> , <i>24</i> , 30-4.																									
<b>VARIABLES:</b> One temperature: 25°C Salinity: 29-108 g(2)/kg sln	<b>PREPARED BY:</b> M. Kleinschmidt and W. Shiu																									
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of phenanthrene in aqueous NaCl</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;">mol(2)/L sln</th> <th style="text-align: center;">g(2)/kg sln<sup>a</sup></th> <th style="text-align: center;">mg(1)/L sln</th> <th style="text-align: center;">10<sup>5</sup>mass%(1)<sup>a</sup></th> <th style="text-align: center;">10<sup>8</sup>x<sub>1</sub><sup>a</sup></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0.50</td> <td style="text-align: center;">28.6</td> <td style="text-align: center;">0.85</td> <td style="text-align: center;">8.3</td> <td style="text-align: center;">8.6</td> </tr> <tr> <td style="text-align: center;">1.00</td> <td style="text-align: center;">56.2</td> <td style="text-align: center;">0.67</td> <td style="text-align: center;">6.4</td> <td style="text-align: center;">6.8</td> </tr> <tr> <td style="text-align: center;">1.50</td> <td style="text-align: center;">82.6</td> <td style="text-align: center;">0.48</td> <td style="text-align: center;">4.5</td> <td style="text-align: center;">4.9</td> </tr> <tr> <td style="text-align: center;">2.00</td> <td style="text-align: center;">108.2</td> <td style="text-align: center;">0.33</td> <td style="text-align: center;">3.1</td> <td style="text-align: center;">3.3</td> </tr> </tbody> </table> <p>'a' calculated by compilers using density and other physical data for NaCl solutions from ref 1.</p>		mol(2)/L sln	g(2)/kg sln <sup>a</sup>	mg(1)/L sln	10 <sup>5</sup> mass%(1) <sup>a</sup>	10 <sup>8</sup> x <sub>1</sub> <sup>a</sup>	0.50	28.6	0.85	8.3	8.6	1.00	56.2	0.67	6.4	6.8	1.50	82.6	0.48	4.5	4.9	2.00	108.2	0.33	3.1	3.3
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<b>METHOD/APPARATUS/PROCEDURE:</b>  Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) fluorescence grade, from Eastman Kodak. (2) reagent grade, from Fisher Scientific.  <b>ESTIMATED ERROR:</b> temp ± 0.5°C soly ± 3 relative %  <b>REFERENCES:</b> 1. Weast, R.C.; <i>CRC Handbook of Chemistry and Physics</i> , 59th Edition; 1978; CRC Press pp. D299-D300.																									