

<p>COMPONENTS:</p> <p>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</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 anthracene (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 anthracene.

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

Reference	T/K	Method
Davis <i>et al.</i> (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)	282-305	spectrophotometric
May <i>et al.</i> (ref 6)	278-302	chromatographic

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

With the exception of the 300K datum of Davis *et al.* (ref 1) which is several orders of magnitude lower than all other values, all the available data on the solubility of anthracene in water are summarized in Table 2. Selected data are also plotted in Figure 1.

At 298K the data are clustered around two values (Table 2). A possible explanation for this (ref 6) is that most commercial preparations of anthracene contain about 2% phenanthrene. Although isomeric with anthracene, phenanthrene is about 20 times more soluble which could result in higher observed values for analytical methods such as spectrophotometry which do not distinguish between the two isomers. However, at the present time there are insufficient data to justify rejection of the higher values. Clearly, a careful reinvestigation of this system is justified.

At temperatures lower than 298K the data of Schwarz (ref 5) and May *et al.* (ref 6) are in good agreement. However, in view of the discrepancies at 298K these values are regarded only as Tentative.

At  $T > 298K$  only the data of Wauchope and Getzen (ref 3) are available and in view of the disagreement at 298K must also be regarded as very tentative.

(continued next page)

## COMPONENTS:

- (1) Anthracene:  $C_{14}H_{10}$ ; [120-12-7]  
 (2) Water;  $H_2O$ ; [7732-18-5]

## EVALUATOR:

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 University, Perth, W.A., Australia.

February 1986.

## CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Anthracene (1) in Water (2)

T/K	Solubility values		
	Reported values <sup>a</sup> $10^6 g(1)/100g\ sln$	"Best" values ( $\pm \sigma_n$ ) <sup>b</sup> $10^6 g(1)/100g\ sln$	$10^8 x_1$
273	2.2 (ref 3)	2.2	0.22
283	2.38* (ref 5), 1.74* (ref 6)	$2.1 \pm 0.3$	0.21
293	3.48* (ref 5), 3.23* (ref 6)	$3.4 \pm 0.1$	0.34
298	7.5 (ref 2), 7.5 (ref 3) 7.3 (ref 4), 4.46* (ref 5), 4.46 (ref 6)	$6.2 \pm 1.5^c$	$0.62^c$
303	8.0* (ref 3)	$8^c$	$8^c$
313	16* (ref 3)	$16^c$	$16^c$
323	28.6 (ref 3)	$29^c$	$29^c$
333	51* (ref 3)	$51^c$	$51^c$
343	91 (ref 3)	$91^c$	$91^c$

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

<sup>b</sup> Obtained by averaging where appropriate;  $\sigma_n$  has no statistical significance.

<sup>c</sup> See text however.

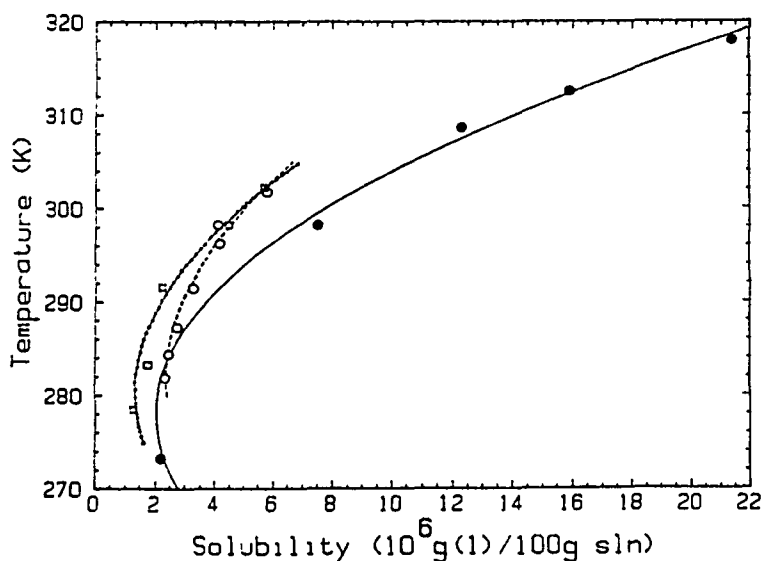


FIGURE 1. Solubility of anthracene in water, selected data: ref 3 (●), solid curve; ref 5 (○), broken curve; ref 6 (□), broken curve.

(continued next page)

<p>COMPONENTS:</p> <p>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7] (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. Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u>, <i>54</i>, 283-298.</li><li>3. Wauchope, R.D.; Getzen, F.W. <i>J. Chem. Eng. Data</i> <u>1972</u>, <i>17</i>, 38-41.</li><li>4. Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 399-402.</li><li>5. Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 273-7.</li><li>6. 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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Water; H <sub>2</sub> O; [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 anthracene in water</p> <table 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>7</sup> g(1) L<sup>-1</sup> (2)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">27</td> <td style="text-align: center;">7.5 ± 0.8</td> </tr> <tr> <td></td> <td style="text-align: center;">7.2 ± 0.5</td> </tr> <tr> <td></td> <td style="text-align: center;">7.5 ± 0.5</td> </tr> </tbody> </table> <hr style="width: 20%; margin: 10px auto;"/> <p>The best value recommended by the authors is <math>7.5 \times 10^{-7}</math> g(1) L<sup>-1</sup> (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding values of mass percent and mole fraction, <math>x_1</math>, calculated by the compiler are <math>7.5 \times 10^{-8}</math> g(1)/100 g sln and <math>7.6 \times 10^{-11}</math>.</p>		<u>t/°C</u>	<u>10<sup>7</sup> g(1) L<sup>-1</sup> (2)</u>	27	7.5 ± 0.8		7.2 ± 0.5		7.5 ± 0.5
<u>t/°C</u>	<u>10<sup>7</sup> g(1) L<sup>-1</sup> (2)</u>								
27	7.5 ± 0.8								
	7.2 ± 0.5								
	7.5 ± 0.5								
<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, 450x; m.p. range 215.6-216.5°C; used as received; (cf. ref 2). (2) dust-free.								
	<b>ESTIMATED ERROR:</b> temp. ± 3°C soly. see above.								
	<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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (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> , <i>54</i> , 283-98.
<b>VARIABLES:</b>  Temperature: 25°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  The solubility of anthracene in water at 25°C was reported to be $7.5 \times 10^{-5} \text{ g(1) dm}^{-3} \text{ sln}$ and $4.47 \times 10^{-7} \text{ mol(1) dm}^{-3} \text{ sln}$ . Assuming that $1.00 \text{ dm}^3 \text{ sln} = 1.00 \text{ dm}^3 \text{ sln}$ the corresponding mass percent and mole fraction, $x_1$ , calculated by the compiler are $7.5 \times 10^{-6} \text{ g(1)/100 g sln}$ and $8.07 \times 10^{-9}$ .	
<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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (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 anthracene in water				
t/°C	mg(1)/kg(2)		10 <sup>5</sup> g(1)/100 g sln (compiler)	10 <sup>8</sup> x <sub>1</sub> (compiler)
	experiment	smoothed with (std dev)		
0.0		0.022(0.001)	0.22	0.22
25.0		0.075(0.002)	0.75	0.76
35.4	0.125, 0.122, 0.119	0.123	1.23	1.24
39.3	0.152, 0.151, 0.148	0.159	1.59	1.61
44.7	0.208, 0.210, 0.206	0.214	2.14	2.16
47.5	0.279	0.249	2.49	2.52
50.0		0.286(0.003)	2.86	2.89
50.1	0.301, 0.297, 0.302	0.288	2.88	2.91
54.7	0.391, 0.389, 0.402	0.372	3.72	3.76
59.2	0.480, 0.488, 0.525	0.481	4.81	4.86
64.5	0.72, 0.62, 0.64	0.66	6.6	6.7
65.1	0.67, 0.64, 0.67	0.68	6.8	6.9
69.8	0.92	0.90	9.0	9.1
70.7	0.90, 0.97, 0.96	0.95	9.5	9.6
71.9	0.91	1.02	10.2	10.3
74.7	1.19, 1.13, 1.26	1.21	12.1	12.2
75.0		1.23(0.02)	12.3	12.4
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) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Mackay, D.; Shiu, W.Y.  <i>J. Chem. Eng. Data</i> <u>1977</u> , 22, 399-402.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  M.C. Haulait-Pirson
<b>EXPERIMENTAL VALUES:</b>  The solubility of anthracene in water at 25°C was reported to be 0.073 mg(1) dm <sup>-3</sup> sln and $x_1 = 7.57 \times 10^{-9}$ .  The corresponding mass percent calculated by the compiler is $7.3 \times 10^{-6}$ g(1)/100 g sln.	
<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. $\pm$ mg(1) dm <sup>-3</sup> sln (maximum deviation from several determinations.)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) Anthracene; $C_{14}H_{10}$ ; [120-12-7] (2) Water; $H_2O$ ; [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: 8.6 - 31.3°C	<b>PREPARED BY:</b> A. Maczynski																																																								
<b>EXPERIMENTAL VALUES:</b> <p style="text-align: center;">Solubility of Anthracene in Water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: center;"><math>t/^\circ C</math></th> <th style="text-align: center;"><math>10^7 \text{ mol(l) L}^{-1}</math></th> <th style="text-align: center;"><math>10^6 \text{ g(l)/100g sln}</math> (compiler)</th> <th style="text-align: center;"><math>10^9 x_1</math> (compiler)</th> </tr> </thead> <tbody> <tr><td>8.6</td><td>1.31 ± 0.04</td><td>2.33</td><td>2.36</td></tr> <tr><td>11.1</td><td>1.37 ± 0.03</td><td>2.44</td><td>2.47</td></tr> <tr><td>12.2</td><td>1.44 ± 0.03</td><td>2.57</td><td>2.59</td></tr> <tr><td>14.0</td><td>1.54 ± 0.04</td><td>2.74</td><td>2.77</td></tr> <tr><td>15.5</td><td>1.66 ± 0.03</td><td>2.96</td><td>3.00</td></tr> <tr><td>18.2</td><td>1.81 ± 0.03</td><td>3.23</td><td>3.26</td></tr> <tr><td>20.3</td><td>2.22 ± 0.03</td><td>3.96</td><td>4.00</td></tr> <tr><td>23.0</td><td>2.34 ± 0.03</td><td>4.17</td><td>4.21</td></tr> <tr><td>23.3</td><td>2.30 ± 0.04</td><td>4.10</td><td>4.14</td></tr> <tr><td>25.0</td><td>2.30 ± 0.05</td><td>4.10</td><td>4.14</td></tr> <tr><td>26.2</td><td>2.67 ± 0.03</td><td>4.76</td><td>4.81</td></tr> <tr><td>28.5</td><td>3.25 ± 0.06</td><td>5.79</td><td>5.85</td></tr> <tr><td>31.3</td><td>3.90 ± 0.02</td><td>6.95</td><td>7.02</td></tr> </tbody> </table>		$t/^\circ C$	$10^7 \text{ mol(l) L}^{-1}$	$10^6 \text{ g(l)/100g sln}$ (compiler)	$10^9 x_1$ (compiler)	8.6	1.31 ± 0.04	2.33	2.36	11.1	1.37 ± 0.03	2.44	2.47	12.2	1.44 ± 0.03	2.57	2.59	14.0	1.54 ± 0.04	2.74	2.77	15.5	1.66 ± 0.03	2.96	3.00	18.2	1.81 ± 0.03	3.23	3.26	20.3	2.22 ± 0.03	3.96	4.00	23.0	2.34 ± 0.03	4.17	4.21	23.3	2.30 ± 0.04	4.10	4.14	25.0	2.30 ± 0.05	4.10	4.14	26.2	2.67 ± 0.03	4.76	4.81	28.5	3.25 ± 0.06	5.79	5.85	31.3	3.90 ± 0.02	6.95	7.02
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<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 74 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 $KMnO_4$ and NaOH and passed through a Sephadex column.  <b>ESTIMATED ERROR:</b> Temperature: ±0.1°C Solubility: See above.  <b>REFERENCES:</b>																																																								



<b>COMPONENTS:</b>  (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (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: 5.2-29.0°C	<b>PREPARED BY:</b>  A. Maczynski																																								
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of anthracene in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><i>t</i>/°C</th> <th style="text-align: center;">μg(1)/kg(2)</th> <th style="text-align: center;">10<sup>6</sup> g(1)/100 g sln (compiler)</th> <th style="text-align: center;">10<sup>9</sup> x<sub>1</sub> (compiler)</th> </tr> </thead> <tbody> <tr><td>5.2</td><td style="text-align: center;">12.7 ± 0.4</td><td style="text-align: center;">1.27</td><td style="text-align: center;">1.28</td></tr> <tr><td>10.0</td><td style="text-align: center;">17.5 ± 0.3</td><td style="text-align: center;">1.75</td><td style="text-align: center;">1.77</td></tr> <tr><td>14.1</td><td style="text-align: center;">22.2 ± 0.1</td><td style="text-align: center;">2.22</td><td style="text-align: center;">2.24</td></tr> <tr><td>18.3</td><td style="text-align: center;">29.1 ± 0.6</td><td style="text-align: center;">2.91</td><td style="text-align: center;">2.94</td></tr> <tr><td>22.4</td><td style="text-align: center;">37.2 ± 1.1</td><td style="text-align: center;">3.72</td><td style="text-align: center;">3.76</td></tr> <tr><td>24.6</td><td style="text-align: center;">43.4 ± 0.1</td><td style="text-align: center;">4.34</td><td style="text-align: center;">4.39</td></tr> <tr><td>25.0</td><td style="text-align: center;">44.6 ± 0.2</td><td style="text-align: center;">4.46</td><td style="text-align: center;">4.51</td></tr> <tr><td>28.7</td><td style="text-align: center;">55.7 ± 0.7</td><td style="text-align: center;">5.57</td><td style="text-align: center;">5.63</td></tr> <tr><td>29.0</td><td style="text-align: center;">57.0 ± 3.0</td><td style="text-align: center;">5.7</td><td style="text-align: center;">5.76</td></tr> </tbody> </table> <hr/> $\mu\text{g}(1)/\text{kg}(2) = 8.21 + 0.8861 t + 0.0097 t^2 + 0.0013 t^3$		<i>t</i> /°C	μg(1)/kg(2)	10 <sup>6</sup> g(1)/100 g sln (compiler)	10 <sup>9</sup> x <sub>1</sub> (compiler)	5.2	12.7 ± 0.4	1.27	1.28	10.0	17.5 ± 0.3	1.75	1.77	14.1	22.2 ± 0.1	2.22	2.24	18.3	29.1 ± 0.6	2.91	2.94	22.4	37.2 ± 1.1	3.72	3.76	24.6	43.4 ± 0.1	4.34	4.39	25.0	44.6 ± 0.2	4.46	4.51	28.7	55.7 ± 0.7	5.57	5.63	29.0	57.0 ± 3.0	5.7	5.76
<i>t</i> /°C	μg(1)/kg(2)	10 <sup>6</sup> g(1)/100 g sln (compiler)	10 <sup>9</sup> x <sub>1</sub> (compiler)																																						
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<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.																																								

<p>COMPONENTS:</p> <p>(1) Anthracene; C<sub>14</sub>H<sub>10</sub>; [120-12-7]</p> <p>(2) Seawater</p>	<p>EVALUATOR:</p> <p>D.G. Shaw          Institute of Marine Science          University of Alaska          Fairbanks, Alaska USA</p> <p>December 1982</p>
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## CRITICAL EVALUATION:

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

<u>Authors</u>	<u>Method</u>	<u>Salinity g salts/kg sln</u>	<u>10<sup>6</sup> g(1)/100 g sln</u>
Schwarz (ref 1)	uv spectral	30	3.55
May <i>et al.</i> (ref 2)	HPLC	35.0	3.11

The reported data are from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the tentative value for the solubility of anthracene in pure water, the data of Schwarz, and May *et al.* are adopted as tentative. Schwarz also reports data over the temperature range 281-303 K.

SOLUBILITY OF ANTHRACENE (1) IN SEAWATER (2)

TENTATIVE VALUE

<u>T/K</u>	<u>g salts/kg sln</u>	<u>10<sup>6</sup> g(1)/100 g sln</u>
298	35.0	3.11

## REFERENCES

1. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
2. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

<b>COMPONENTS:</b> (1) Anthracene; $C_{14}H_{10}$ ; [120-12-7] (2) Sodium chloride· NaCl; [7647-14-5] (3) Water: $H_2O$ ; [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: 8.2-30.2°C Salinity: 30 g(2)/kg sln	<b>PREPARED BY:</b> W.Y. Shiu, D. Mackay																				
<b>EXPERIMENTAL VALUES:</b>  Solubility of Anthracene in 0.5 mol(2)/L <table data-bbox="321 556 900 844" 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>10^7</math> mol(l)/L sln</th> </tr> </thead> <tbody> <tr><td style="text-align: center;">8.2</td><td style="text-align: center;">0.93</td></tr> <tr><td style="text-align: center;">8.6</td><td style="text-align: center;">1.01</td></tr> <tr><td style="text-align: center;">11.7</td><td style="text-align: center;">1.22</td></tr> <tr><td style="text-align: center;">19.2</td><td style="text-align: center;">1.47</td></tr> <tr><td style="text-align: center;">21.5</td><td style="text-align: center;">1.68</td></tr> <tr><td style="text-align: center;">25.0</td><td style="text-align: center;">2.04</td></tr> <tr><td style="text-align: center;">25.3</td><td style="text-align: center;">1.92</td></tr> <tr><td style="text-align: center;">27.1</td><td style="text-align: center;">2.02</td></tr> <tr><td style="text-align: center;">30.2</td><td style="text-align: center;">2.46</td></tr> </tbody> </table> The corresponding mass percent and mole fraction $x_1$ , at 25.0°C calculated by the compilers are $3.55 \times 10^{-6}$ g(l)/100 g sln and $3.69 \times 10^{-9}$ .		$t, ^\circ C$	$10^7$ mol(l)/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
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<b>AUXILIARY INFORMATION</b>																					
<b>METHOD/APPARATUS/PROCEDURE:</b> The solubility of anthracene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1x1 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 258 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 therefore provide an absolute solubility scale for the fluorescence method.	<b>SOURCE AND PURITY OF MATERIALS:</b> Anthracene: purity >99 mole % Sodium chloride: reagent grade Ethanol: reagent grade Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.  <b>ESTIMATED ERROR:</b> Solubility $\pm$ 4.3 % (author) Temperature $\pm$ 0.1°C (author)  <b>REFERENCES:</b>																				

<b>COMPONENTS:</b> (1) Anthracene; C <sub>14</sub> H <sub>10</sub> ; [120-12-7] (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> , <i>50</i> , 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 anthracene 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> is 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> = 0.238 with S<sub>0</sub> = 0.0446.</p> <p>The corresponding mass percent and mole fraction x<sub>1</sub>, at salinity = 35 g(2)/kg sln calculated by the compilers are 3.11 x 10<sup>-6</sup> g(1)/kg sln and 3.22 x 10<sup>-9</sup>.</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> ± 0.004 S <sub>0</sub> ± 0.0002  <b>REFERENCES:</b>