

COMPONENTS:  (1) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3] (2) Water; H <sub>2</sub> O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland. June 1986.
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## CRITICAL EVALUATION:

Quantitative solubility data for benz[a]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 bena[a]anthracene.

TABLE 1. Quantitative Solubility Studies of  
Benz[a]anthracene (1) in Water (2)

Reference	T/K	Method
Davis <i>et al.</i> (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May <i>et al.</i> (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In general the available data are in good agreement given the very low solubility of benz[a]anthracene in water. Although the data of Mackay and Shiu is somewhat higher than all other values there are at the present time insufficient grounds for its rejection. The available data are summarized in Table 2 and may be regarded as Tentative.

TABLE 2. Tentative Solubility Values of  
Benz[a]anthracene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 <sup>6</sup> g(1)/100 g sln	"Best" values ( $\pm\sigma_n$ ) <sup>a</sup> 10 <sup>6</sup> g(1)/100 g sln	10 <sup>10</sup> x <sub>1</sub>
298	0.983 (ref 2), 1.4 (ref 3), 0.94 (ref 4)	1.1 $\pm$ 0.2	9
300	1.1 (ref 1)	1.1	9
302	1.22 (ref 4)	1.2	9

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

(continued next page)

<p>COMPONENTS:</p> <p>(1) Benz[a]anthracene; C<sub>18</sub>H<sub>12</sub>; [56-55-3]</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. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.</p> <p>June 1986.</p>
<p>CRITICAL EVALUATION:</p> <p>(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>, 283-98.</li><li>3. Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 399-402.</li><li>4. May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u>, <i>50</i>, 997-1000.</li></ol>	

<b>COMPONENTS:</b>  (1) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3]  (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 benz[a]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>5</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;">1.1</td> </tr> <tr> <td></td> <td style="text-align: center;">1.1</td> </tr> <tr> <td></td> <td style="text-align: center;">1.2</td> </tr> </tbody> </table> <hr style="width: 50%; margin: 10px auto;"/> <p>The best value recommended by the authors is <math>1.1 \times 10^{-5}</math> g(1) L<sup>-1</sup> (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are <math>1.1 \times 10^{-6}</math> g(1)/100 g sln and <math>8.7 \times 10^{-10}</math>.</p>		<u>t/°C</u>	<u>10<sup>5</sup> g(1) L<sup>-1</sup> (2)</u>	27	1.1		1.1		1.2
<u>t/°C</u>	<u>10<sup>5</sup> g(1) L<sup>-1</sup> (2)</u>								
27	1.1								
	1.1								
	1.2								
<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) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2).  (2) dust-free.  <b>ESTIMATED ERROR:</b>  temp. ± 3°C soly. ± 0.1 × 10 <sup>-5</sup> g(1) dm <sup>-3</sup> (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) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3]  (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 benz[a]anthracene in water at 25°C was reported to be 10 <sup>-5</sup> g(1) L <sup>-1</sup> sln and 4.31 x 10 <sup>-8</sup> mol(1) L <sup>-1</sup> 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 9.83 x 10 <sup>-7</sup> g(1)/100 g sln and 7.78 x 10 <sup>-10</sup> .	
<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>

<b>COMPONENTS:</b> (1) Benz[a]anthracene; $C_{18}H_{12}$ ; [56-55-3] (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>  The solubility of benz[a]anthracene in water at 25°C was reported to be 0.014 mg(1) $dm^{-3}$ sln and $x_1 = 1.1 \times 10^{-9}$ .  The corresponding mass percent calculated by the compiler is $1.4 \times 10^{-6}$ 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. $\pm 0.0002$ mg(1) $dm^{-3}$ sln (maximum deviation from several determinations).  <b>REFERENCES:</b>

<b>COMPONENTS:</b>  (1) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3]  (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> , 997-1000.												
<b>VARIABLES:</b>  Temperature: 25 and 29°C	<b>PREPARED BY:</b>  A. Maczynski												
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of benz[a]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;">mg(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>10</sup> x<sub>1</sub> (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">0.0094</td> <td style="text-align: center;">0.94</td> <td style="text-align: center;">7.4</td> </tr> <tr> <td style="text-align: center;">29</td> <td style="text-align: center;">0.0122</td> <td style="text-align: center;">1.22</td> <td style="text-align: center;">9.6</td> </tr> </tbody> </table>		<i>t</i> /°C	mg(1)/kg(2)	10 <sup>6</sup> g(1)/100 g sln (compiler)	10 <sup>10</sup> x <sub>1</sub> (compiler)	25	0.0094	0.94	7.4	29	0.0122	1.22	9.6
<i>t</i> /°C	mg(1)/kg(2)	10 <sup>6</sup> g(1)/100 g sln (compiler)	10 <sup>10</sup> x <sub>1</sub> (compiler)										
25	0.0094	0.94	7.4										
29	0.0122	1.22	9.6										
<b>AUXILIARY INFORMATION</b>													
<b>METHOD/APPARATUS/PROCEDURE:</b>  <p>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.</p>	<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 Haas, Philadelphia, Pa).  <b>ESTIMATED ERROR:</b> temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2) (stand. dev.)  <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) Benz[a]anthracene; C<sub>18</sub>H<sub>12</sub>; [55-56-3]</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 benz[a]anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10 <sup>7</sup> g(1)/100 g sln
Krasnoshchekova <i>et al.</i> (ref 1)	spectral	6	0.62
May <i>et al.</i> (ref 2)	HPLC	35	5.6

The value reported by May *et al.* was derived from several measurements using the Setschenow equation and is consistent with the recommended value for the solubility of benz[a]anthracene in pure water. Therefore their value is adopted as tentative. The value of Krasnoshchekova *et al.* appears slightly low and is considered doubtful.

SOLUBILITY OF BENZ[A]ANTHRACENE (1) IN SEAWATER (2)  
TENTATIVE VALUE

T/K	g salts/kg sln	10 <sup>7</sup> g(1)/100 g sln
298	35	5.6

## REFERENCES

1. Krasnoshchekova, R.Ya.; Pakpill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
2. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

<b>COMPONENTS:</b>  (1) Benz [a]anthracene; $C_{18}H_{12}$ ; [56-55-3]  (2) Salt Water	<b>ORIGINAL MEASUREMENTS:</b>  Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.  <i>Khim. Tverd. Topl.</i> <u>1977</u> , 11(2), 133-6.
<b>VARIABLES:</b>  One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	<b>PREPARED BY:</b>  M. Kleinschmidt and D. Shaw
<b>EXPERIMENTAL VALUES:</b>  The solubility of benz[a]anthracene in salt water was reported to be 0.63 $\mu\text{g/L}$ .  The corresponding mass percent and mole fraction, $x_1$ , calculated by the compilers are $6.2 \times 10^{-8}$ g(1)/100 g sln and $5.2 \times 10^{-11}$ assuming a solution density of 1.004 kg/L.	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  Not given.  <b>ESTIMATED ERROR:</b> temp. $\pm 1^\circ\text{C}$ soly. $\pm 0.075$ type of error not specified  <b>REFERENCES:</b> 1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> , 13, 885.



<b>COMPONENTS:</b> (1) Benz[a]anthracene; C <sub>18</sub> H <sub>12</sub> ; [56-55-3] (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 benz[a]anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:</p> $\log(S_o/S) = K_s C_s$ <p>where;</p> <p>S<sub>o</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> = 0.354 with S<sub>o</sub> = 0.0094.</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 5.6 x 10<sup>-7</sup> g(1)/100 g sln and 4.5 x 10<sup>-10</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> ± 0.002 S <sub>o</sub> ± 0.001  <b>REFERENCES:</b>