

COMPONENTS: (1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8] (2) Water; H ₂ 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 Sciences, Warszawa, Poland. June 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for benzo[a]pyrene (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 benzo[a]pyrene.

TABLE 1. Quantitative Solubility Studies of Benzo[a]pyrene (1) in Water (2)

Reference	T/K	Method
Davis <i>et al.</i> (ref 1)	300	nephelometric
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. It can be seen from Table 2 that the reported solubility values are in good agreement, given that they have been measured at slightly different temperatures. However, further studies are required before any data can be Recommended.

TABLE 2. Tentative Solubility Values of Benzo[a]pyrene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁷ g(1)/100 g sln	"Best" values 10 ⁷ g(1)/100 sln	"Best" values 10 ¹⁰ x ₁
298	3.8 (ref 2)	3.8	2.7
300	4.0 (ref 1)	4.0	2.9

REFERENCES

- Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* **1942**, *64*, 108-10.
- Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* **1977**, *22*, 399-402.

COMPONENTS: (1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1942</u> , <i>64</i> , 108-10.												
VARIABLES: One temperature: 27°C	PREPARED BY: M.C. Haulait-Pirson												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of benzo[a]pyrene 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>10⁶ g(1) L⁻¹ (2)</u></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">27</td> <td style="text-align: center;">3.0 ± 0.5</td> </tr> <tr> <td></td> <td style="text-align: center;">4.5 ± 0.5</td> </tr> <tr> <td></td> <td style="text-align: center;">4.0 ± 0.1</td> </tr> <tr> <td></td> <td style="text-align: center;">4.0 ± 0.5</td> </tr> <tr> <td></td> <td style="text-align: center;">3.5 ± 0.5</td> </tr> </tbody> </table> <hr style="width: 50%; margin: 10px auto;"/> <p>The best value recommended by the authors is 4.0 x 10⁻⁶ g(1) L⁻¹ (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are 4.0 x 10⁻⁷ g(1)/100 g sln and 2.9 x 10⁻¹⁰.</p>		<u>t/°C</u>	<u>10⁶ g(1) L⁻¹ (2)</u>	27	3.0 ± 0.5		4.5 ± 0.5		4.0 ± 0.1		4.0 ± 0.5		3.5 ± 0.5
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27	3.0 ± 0.5												
	4.5 ± 0.5												
	4.0 ± 0.1												
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	3.5 ± 0.5												
AUXILIARY INFORMATION													
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2). (2) dust-free. ESTIMATED ERROR: temp. ± 3°C soly. see above REFERENCES: 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.												

COMPONENTS: (1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 399-402.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of benzo[a]pyrene in water at 25°C was reported to be 0.0038 mg(l) dm^{-3} sln and $x_1 = 2.73 \times 10^{-10}$. The corresponding mass percent calculated by the compiler is 3.8×10^{-7} g(l)/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. ± 0.00031 mg(l) dm^{-3} sln (maximum deviation from several determinations). REFERENCES:

COMPONENTS: (1) Benzo[a]pyrene; C ₂₀ H ₁₂ ; [50-32-8] (2) Salt Water	ORIGINAL MEASUREMENTS: Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. <i>Khim. Tverd. Topl.</i> <u>1977</u> , 11, 133-6.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	PREPARED BY: M. Kleinschmidt and D. Shaw
EXPERIMENTAL VALUES: The solubility of benzo[a]pyrene in salt water was reported to be 0.13 µg/L. The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 1.3×10^{-8} g(1)/100 g sln and 9.5×10^{-12} assuming a solution density of 1.004 kg/L.	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: Not given. ESTIMATED ERROR: temp. ± 1°C soly. ± 0.008 type of error not specified REFERENCES: 1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. <i>Neftekhimiya</i> <u>1973</u> ,