

COMPONENTS: (1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (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 Chemistry of the Polish Academy of Sciences, Warszawa, Poland. June 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for chrysene (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 chrysene.

TABLE 1. Quantitative Solubility Studies of Chrysene (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.

With the exception of Klevens (ref 2) value at 298K, which is very much higher than other studies (ref 3,4) and is therefore rejected, all the available data are summarized in Table 2 below. The solubilities are in reasonable agreement although their limited number and temperature range suggests a Tentative classification at this stage.

TABLE 2. Tentative Solubility Values for Chrysene (1) in Water (2)

T/K	Solubility values		
	Reported values 10 ⁷ g(1)/100 g sln	"Best" values ($\pm\sigma_n$) ^a 10 ⁷ g(1)/100 g sln	10 ¹⁰ x ₁
298	2.0 (ref 3), 1.8 (ref 4)	1.9 ± 0.1	1.5
300	1.5 (ref 1)	1.5	1.2
302	2.2 (ref 4)	2.2	1.7

^a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

<p>COMPONENTS:</p> <p>(1) Chrysene; $C_{18}H_{12}$; [218-01-9]</p> <p>(2) Water; H_2O; [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 Chemistry of the Polish Academy of Sciences, Warszawa, Poland.</p> <p>June 1986.</p>
<p>CRITICAL EVALUATION: (continued)</p> <p>REFERENCES</p> <ol style="list-style-type: none">1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. <i>J. Am. Chem. Soc.</i> <u>1942</u>, <i>64</i>, 108-10.2. Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u>, <i>54</i>, 283.3. Mackay, D.; Shiu, W.Y. <i>J. Chem. Eng. Data</i> <u>1977</u>, <i>22</i>, 399-402.4. May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u>, <i>50</i>, 997-1000.	

COMPONENTS: (1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (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: <div style="text-align: center;"> <table border="1"> <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;">1.5 ± 0.5</td> </tr> <tr> <td></td> <td style="text-align: center;">1.5 ± 0.2</td> </tr> </tbody> </table> </div> <p>The best value recommended by the authors is 1.5 x 10⁻⁶ g(1) L⁻¹ (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.5 x 10⁻⁷ g(1)/100 g sln and 1.2 x 10⁻¹⁰.</p>		<u>t/°C</u>	<u>10⁶ g(1) L⁻¹ (2)</u>	27	1.5 ± 0.5		1.5 ± 0.2
<u>t/°C</u>	<u>10⁶ g(1) L⁻¹ (2)</u>						
27	1.5 ± 0.5						
	1.5 ± 0.2						
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) prepared at Harvard University; m.p. range 253.2-253.8°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) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Klevens, H.B. <i>J. Phys. Chem.</i> <u>1950</u> , <i>54</i> , 283-98.
VARIABLES: Temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson
EXPERIMENTAL VALUES: The solubility of chrysene in water at 25°C was reported to be 6×10^{-6} g(1) L ⁻¹ sln and 2.76×10^{-8} mol(1) L ⁻¹ 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 6.29×10^{-7} g(1)/100 g sln and 4.98×10^{-10} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) not specified. (2) not specified. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS: (1) Chrysene; $C_{18}H_{12}$; [218-01-9] (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 chrysene in water at 25°C was reported to be 0.0020 mg(1) dm^{-3} sln and $x_1 = 1.58 \times 10^{-10}$. The corresponding mass percent calculated by the compiler is 2.0×10^{-7} 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. ± 0.00017 mg(1) dm^{-3} sln (maximum deviation from several determinations). REFERENCES:

COMPONENTS: (1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (2) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u> , <i>50</i> , 997-1000.												
VARIABLES: Temperature: 25 and 29°C	PREPARED BY: A. Maczynski												
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of chrysene 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;">10⁷ g(1)/100 g sln (compiler)</th> <th style="text-align: center;">10¹⁰ x₁ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">0.0018</td> <td style="text-align: center;">1.8</td> <td style="text-align: center;">1.4</td> </tr> <tr> <td style="text-align: center;">29</td> <td style="text-align: center;">0.0022</td> <td style="text-align: center;">2.2</td> <td style="text-align: center;">1.7</td> </tr> </tbody> </table>		<i>t</i> /°C	mg(1)/kg(2)	10 ⁷ g(1)/100 g sln (compiler)	10 ¹⁰ x ₁ (compiler)	25	0.0018	1.8	1.4	29	0.0022	2.2	1.7
<i>t</i> /°C	mg(1)/kg(2)	10 ⁷ g(1)/100 g sln (compiler)	10 ¹⁰ x ₁ (compiler)										
25	0.0018	1.8	1.4										
29	0.0022	2.2	1.7										
AUXILIARY INFORMATION													
METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) commercial product; less than 3% impurities. (2) distilled over KMnO ₄ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa). ESTIMATED ERROR: temp. ± 0.05°C soly. ± 0.001 mg(1)/kg(2) (standard deviation) REFERENCES: 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.												

COMPONENTS: (1) Chrysene; C ₁₈ H ₁₂ ; [218-01-9] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: May, W.E.; Wasik, S.P.; Freeman, D.H. <i>Anal. Chem.</i> <u>1978</u> , <i>50</i> , 997-1000.
VARIABLES: One temperature: 25°C Salinity: 0-40 g(2)/kg sln	PREPARED BY: W.Y. Shiu and D. Mackay
EXPERIMENTAL VALUES: The solubility of chrysene in aqueous sodium chloride is reported in terms of the Setschenow equation: $\log(S_0/S) = K_S C_S$ where; S ₀ is the solubility of (1) in water (mg/L) S is the solubility of (1) in saline solution (mg/L) K _S is the Setschenow constant (L/mol) C _S in the concentration of sodium chloride (mol/L) evaluating the equation for S over the range of C _S 0-0.7 mol/L, K _S = 0.336 with S ₀ = 0.0018. The corresponding mass percent and mole fraction x_1 , at salinity = 35 g(2)/kg sln calculated by the compilers are 1.1×10^{-7} g(1)/100 g sln and 8.8×10^{-11} .	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE: 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 ₁₈ 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.	SOURCE AND PURITY OF MATERIALS: (1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column. ESTIMATED ERROR: temp ± 0.05°C K _S ± 0.010 S ₀ ± 0.0001 REFERENCES: