

COMPONENTS: (1) 1-Ethynaphthalene; C ₁₂ H ₁₂ ; [1127-76-0] (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, Polish Academy of Sciences, Warszawa, Poland. April 1986.
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CRITICAL EVALUATION:

Quantitative solubility data for 1-ethynaphthalene (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 1-ethynaphthalene.

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

Reference	T/K	Method
Mackay and Shiu (ref 1)	298	spectrofluorometric
Schwarz and Wasik (ref 2)	282-305	spectrophotometric
Schwarz (ref 3)	284-298	spectrophotometric

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

The data available (Table 1) are summarized in Table 2 and plotted in Figure 1. For the purpose of this Evaluation the values of Schwarz (ref 3) are not considered as independent determinations. Nevertheless, the excellent agreement between the data of Schwarz and Wasik (ref 2,3) and Mackay and Shiu (ref 1) at 298K suggests the values of Schwarz and Wasik at other temperatures can be considered as Tentative.

TABLE 2: Recommended (R) and Tentative Solubility Values of
1-Ethynaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values ^a 10 ⁴ g(1)/100g sln	"Best" values (± σ _n) ^b 10 ⁴ g(1)/100g sln	10 ⁷ x ₁
283	8.1 (ref 2), 8.1* (ref 3)	8.1	9.4
293	10.0 (ref 2), 8.5* (ref 3)	8.5	9.8
298	10.7 (ref 1), 10.0 (ref 2), 9.5* (ref 3)	10.1 ± 0.5 (R)	11.6 (R)
303	11.0* (ref 3)	11	13

^a Values marked with an asterisk (*) were obtained by the Evaluators by graphical interpolation of the authors' original data.

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

(continued next page)

COMPONENTS:

(1) 1-Ethynaphthalene; $C_{12}H_{12}$;
[1127-76-0]

(2) Water; H_2O ; [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, Polish Academy of Sciences,
Warszawa, Poland.

April 1986.

CRITICAL EVALUATION: (continued)

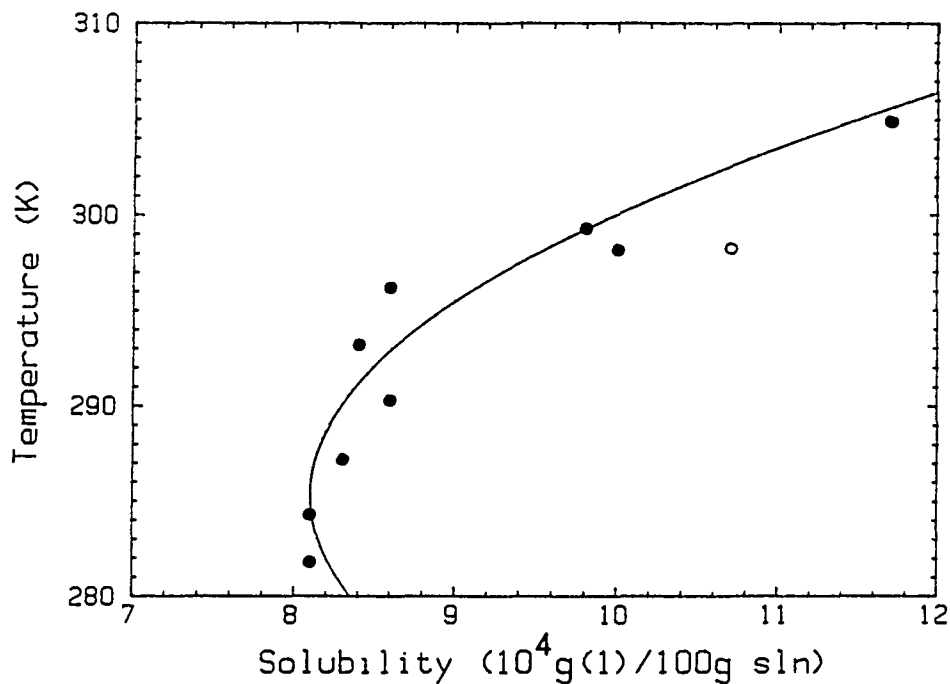


FIGURE 1. Solubility of 1-ethynaphthalene in water: ref 1(o); ref 2(●). Solid curve is a least squares line of best fit through data of ref 2.

REFERENCES

1. Mackay, C.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
2. Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
3. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

ACKNOWLEDGEMENT

The Evaluators thank Dr Brian Clare for the graphics.

COMPONENTS: (1) 1-Ethyl-naphthalene; C ₁₂ H ₁₂ ; [1127-76-0] (2) Water; H ₂ O; [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: <p>The solubility of 1-ethyl-naphthalene in water at 25°C was reported to be 10.7 mg(1) dm⁻³ sln and $x_1 = 1.24 \times 10^{-6}$.</p> <p>The corresponding mass percent calculated by the compiler is 0.00107 g(1)/100 g sln.</p>	
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. ± 0.3 mg(1) dm ⁻³ sln (maximum deviation from several determinations). REFERENCES:

COMPONENTS: (1) 1-Ethyl-naphthalene; $C_{12}H_{12}$; [1127-76-0] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 273-7.																																								
VARIABLES: Temperature: 8.6-31.7°C	PREPARED BY: A. Maczynski																																								
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of 1-ethyl-naphthalene in water</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">$t/^\circ C$</th> <th style="text-align: center;">$10^5 \text{ mol(1) L}^{-1}$</th> <th style="text-align: center;">$10^4 \text{ g(1)/100 g sln}$ (compiler)</th> <th style="text-align: center;">$10^7 x_1$ (compiler)</th> </tr> </thead> <tbody> <tr><td>8.6</td><td style="text-align: center;">5.2 ± 0.3</td><td style="text-align: center;">8.1</td><td style="text-align: center;">9.4</td></tr> <tr><td>11.1</td><td style="text-align: center;">5.2 ± 0.2</td><td style="text-align: center;">8.1</td><td style="text-align: center;">9.4</td></tr> <tr><td>14.0</td><td style="text-align: center;">5.3 ± 0.1</td><td style="text-align: center;">8.3</td><td style="text-align: center;">9.5</td></tr> <tr><td>17.1</td><td style="text-align: center;">5.5 ± 0.1</td><td style="text-align: center;">8.6</td><td style="text-align: center;">9.9</td></tr> <tr><td>20.0</td><td style="text-align: center;">5.4 ± 0.1</td><td style="text-align: center;">8.4</td><td style="text-align: center;">9.7</td></tr> <tr><td>23.0</td><td style="text-align: center;">5.5 ± 0.1</td><td style="text-align: center;">8.6</td><td style="text-align: center;">9.9</td></tr> <tr><td>25.0</td><td style="text-align: center;">6.4 ± 0.1</td><td style="text-align: center;">10.0</td><td style="text-align: center;">11.5</td></tr> <tr><td>26.1</td><td style="text-align: center;">6.3 ± 0.1</td><td style="text-align: center;">9.8</td><td style="text-align: center;">11.3</td></tr> <tr><td>31.7</td><td style="text-align: center;">7.5 ± 0.2</td><td style="text-align: center;">11.7</td><td style="text-align: center;">13.5</td></tr> </tbody> </table>		$t/^\circ C$	$10^5 \text{ mol(1) L}^{-1}$	$10^4 \text{ g(1)/100 g sln}$ (compiler)	$10^7 x_1$ (compiler)	8.6	5.2 ± 0.3	8.1	9.4	11.1	5.2 ± 0.2	8.1	9.4	14.0	5.3 ± 0.1	8.3	9.5	17.1	5.5 ± 0.1	8.6	9.9	20.0	5.4 ± 0.1	8.4	9.7	23.0	5.5 ± 0.1	8.6	9.9	25.0	6.4 ± 0.1	10.0	11.5	26.1	6.3 ± 0.1	9.8	11.3	31.7	7.5 ± 0.2	11.7	13.5
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METHOD/APPARATUS/PROCEDURE: 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.	SOURCE AND PURITY OF MATERIALS: (1) source not specified; better than 99.9 mole%, by glc; used as received. (2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column. ESTIMATED ERROR: temp. ± 0.1°C soly. see above REFERENCES:																																								

COMPONENTS: (1) 1-Ethyl-naphthalene; $C_{12}H_{12}$; [1127-76-0] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Schwarz, F.P.; Wasik, S.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 270-3.																				
VARIABLES: Temperature: 10-25°C	PREPARED BY: A. Maczynski																				
EXPERIMENTAL VALUES: <div style="text-align: center;">Solubility of 1-ethyl-naphthalene in water</div> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">$t/^\circ C$</th> <th style="text-align: center;">$10^5 \text{ mol(1) L}^{-1}$</th> <th style="text-align: center;">$10^4 \text{ g(1)/100 g sln}$ (compiler)</th> <th style="text-align: center;">$10^7 x_1$ (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: left;">10</td> <td style="text-align: center;">5.2 ± 0.2</td> <td style="text-align: center;">8.1</td> <td style="text-align: center;">9.4</td> </tr> <tr> <td style="text-align: left;">14</td> <td style="text-align: center;">5.2 ± 0.1</td> <td style="text-align: center;">8.1</td> <td style="text-align: center;">9.4</td> </tr> <tr> <td style="text-align: left;">20</td> <td style="text-align: center;">6.4 ± 0.1</td> <td style="text-align: center;">10.0</td> <td style="text-align: center;">11.5</td> </tr> <tr> <td style="text-align: left;">25</td> <td style="text-align: center;">6.4 ± 0.1</td> <td style="text-align: center;">10.0</td> <td style="text-align: center;">11.5</td> </tr> </tbody> </table>		$t/^\circ C$	$10^5 \text{ mol(1) L}^{-1}$	$10^4 \text{ g(1)/100 g sln}$ (compiler)	$10^7 x_1$ (compiler)	10	5.2 ± 0.2	8.1	9.4	14	5.2 ± 0.1	8.1	9.4	20	6.4 ± 0.1	10.0	11.5	25	6.4 ± 0.1	10.0	11.5
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AUXILIARY INFORMATION																					
METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.	SOURCE AND PURITY OF MATERIALS: (1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%. (2) distilled from $KMnO_4$ and passed through a Sephadex column. ESTIMATED ERROR: temp. $\pm 0.1^\circ C$ soly. see above REFERENCES:																				

COMPONENTS: (1) 1-Ethynaphthalene; C ₁₂ H ₁₂ ; [1127-76-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 273-7.																		
VARIABLES: Temperature: 8.1-28.5°C Salinity: 30 g(2)/kg sln	PREPARED BY: W.Y. Shiu, D. Mackay																		
EXPERIMENTAL VALUES: <p style="text-align: center;">Solubility of 1-ethynaphthalene in 0.5 mol(2)/L sln</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>10⁵ mol(1)/L sln</u></th> </tr> </thead> <tbody> <tr><td style="text-align: center;">8.1</td><td style="text-align: center;">3.65</td></tr> <tr><td style="text-align: center;">11.1</td><td style="text-align: center;">3.87</td></tr> <tr><td style="text-align: center;">17.4</td><td style="text-align: center;">4.23</td></tr> <tr><td style="text-align: center;">20.3</td><td style="text-align: center;">4.45</td></tr> <tr><td style="text-align: center;">23.3</td><td style="text-align: center;">4.38</td></tr> <tr><td style="text-align: center;">25.0</td><td style="text-align: center;">4.67</td></tr> <tr><td style="text-align: center;">26.2</td><td style="text-align: center;">4.53</td></tr> <tr><td style="text-align: center;">28.5</td><td style="text-align: center;">4.82</td></tr> </tbody> </table> <p>The corresponding mass percent and mole fraction x_1, at 25.0°C calculated by the compilers are 7.12×10^{-4} g(1)/100 g sln and 8.44×10^{-7}.</p>		<u>t/°C</u>	<u>10⁵ mol(1)/L sln</u>	8.1	3.65	11.1	3.87	17.4	4.23	20.3	4.45	23.3	4.38	25.0	4.67	26.2	4.53	28.5	4.82
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AUXILIARY INFORMATION																			
METHOD/APPARATUS/PROCEDURE: <p>The solubility of 1-ethynaphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of 1-ethynaphthalene 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 nm. The Spectrofluorimeter employed a ratio-photon counting mode where 1-ethynaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of 1-ethynaphthalene in ethanol solution therefore provide an absolute solubility scale for the fluorescence method.</p>	SOURCE AND PURITY OF MATERIALS: 1-Ethynaphthalene: purity >99 mole % Sodium chloride: reagent grade Water: distilled over a KMnO ₄ - NaOH solution and passed through a Sephadex column Ethanol: reagent grade ESTIMATED ERROR: Solubility ± 2.0% (author) Temperature ± 0.1°C (author) REFERENCES:																		