

COMPONENTS: (1) 1-Methylnaphthalene; $C_{11}H_{10}$ ; [90-12-0] (2) Water; $H_2O$ ; [7732-18-5]		EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.  February 1986.	
CRITICAL EVALUATION:			
Quantitative solubility data for the 1-methylnaphthalene (1) - water (2) system have been reported in the publications listed in Table 1.			
<u>TABLE 1: Quantitative Solubility Studies of the 1-Methylnaphthalene (1) - Water (2) System</u>			
Reference	T/K	Solubility	Method
Englin <i>et al.</i> (ref 1)	273-323	(2) in (1)	analytical
Eganhouse and Calder (ref 2)	298	(1) in (2)	GLC
Mackay and Shiu (ref 3)	298	(1) in (2)	spectrofluorometric
Schwarz and Wasik (ref 4)	283-298	(1) in (2)	spectrofluorometric
Schwarz (ref 5)	282-305	(1) in (2)	spectrophotometric
The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.			
For further convenience further discussion of this system is divided into two parts.			
1. SOLUBILITY OF 1-METHYLNAPHTHALENE (1) IN WATER (2)			
All the available data on the solubility of 1-methylnaphthalene in water are summarized in Table 1 with the exception of those of Schwarz and Wasik which have been rejected as they are much more scattered than those in the paper by Schwarz (ref 5). There are insufficient data to warrant plotting.			
At 298K, the only temperature where comparison is possible, the data are in excellent agreement and the average value can be Recommended. At other temperatures only the data of Schwarz (ref 5) are available and must thus be considered as Tentative only.			
<u>TABLE 2: Recommended (R) and Tentative Values of the Solubility of 1-Methylnaphthalene (1) in Water (2)</u>			
T/K	Solubility values		
	Reported values <sup>a</sup> $10^3 g(1)/100g sln$	"Best" values ( $\pm \sigma_n$ ) <sup>b</sup> $10^3 g(1)/100g sln$ $10^6 x_1$	
283	2.05* (ref 5)	2.1	2.7
293	2.56* (ref 5)	2.6	3.3
(Table 2 continued next page)			

COMPONENTS: (1) 1-Methylnaphthalene, C <sub>11</sub> H <sub>10</sub> ; [90-12-0] (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.  February 1986.
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CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values		
	Reported values <sup>a</sup> 10 <sup>3</sup> g(1)/100g sln	"Best" values (± σ <sub>n</sub> ) <sup>b</sup> 10 <sup>3</sup> g(1)/100g sln	10 <sup>6</sup> x <sub>1</sub>
298	2.58 (ref 2), 2.85 (ref 3) 2.95* (ref 5)	2.8 ± 0.2 (R)	3.5 (R)
303	3.35* (ref 5)	3.4	4.3

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

<sup>b</sup> Obtained by averaging where relevant; σ<sub>n</sub> has no statistical significance.

## 2. SOLUBILITY OF WATER (2) IN 1-METHYLNAPHTHALENE (1)

As only the data of Englin *et al.* (ref 1) are available on the solubility of water in 1-methylnaphthalene no Critical Evaluation is possible. However, it may be noted that the solubility values of Englin *et al.* are generally reliable for  $T < 300\text{K}$  but are larger than Recommended values at higher temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

## REFERENCES

- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
- Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
- Mackay, D.; Shui, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
- Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
- Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

<b>COMPONENTS:</b>  (1) 1-Methylnaphthalene; $C_{11}H_{10}$ ; [90-12-0]  (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.  <i>Khim. Tekhnol. Topl. Masel</i> <u>1965</u> , 10, 42-6.																					
<b>VARIABLES:</b>  Temperature: 0-50°C	<b>PREPARED BY:</b>  A. Maczynski and Z. Maczynska																					
<b>EXPERIMENTAL VALUES:</b>  <p style="text-align: center;">Solubility of Water in 1-Methylnaphthalene</p> <table border="1" 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>g(2)/100\text{ g sln}</math></th> <th style="text-align: center;"><math>10^3 x_2</math> (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">0</td> <td style="text-align: center;">0.0202</td> <td style="text-align: center;">1.59</td> </tr> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">0.0282</td> <td style="text-align: center;">2.22</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">0.0377</td> <td style="text-align: center;">2.97</td> </tr> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">0.0485</td> <td style="text-align: center;">3.82</td> </tr> <tr> <td style="text-align: center;">40</td> <td style="text-align: center;">0.0619</td> <td style="text-align: center;">4.87</td> </tr> <tr> <td style="text-align: center;">50</td> <td style="text-align: center;">0.0760</td> <td style="text-align: center;">5.97</td> </tr> </tbody> </table>		$t/^\circ C$	$g(2)/100\text{ g sln}$	$10^3 x_2$ (compiler)	0	0.0202	1.59	10	0.0282	2.22	20	0.0377	2.97	30	0.0485	3.82	40	0.0619	4.87	50	0.0760	5.97
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<b>AUXILIARY INFORMATION</b>																						
<b>METHOD/APPARATUS/PROCEDURE:</b>  Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	<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) 1-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [90-12-0] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Eganhouse, R.P.; Calder, J.A.  <i>Geochim. Cosmochim. Acta</i> <u>1976</u> , 40, 555-61.
<b>VARIABLES:</b>  One temperature: 25°C	<b>PREPARED BY:</b>  A. Maczynski
<b>EXPERIMENTAL VALUES:</b>  <p>The solubility of 1-methylnaphthalene in water at 25°C was reported to be 25.8 mg(1)/kg(2) and <math>1.81 \times 10^{-4}</math> mol(1) L (2).</p> <p>The corresponding mass percent and mole fraction, <math>x_1</math>, calculated by the compiler are <math>2.58 \times 10^{-3}</math> g(1)/100 g sln and <math>3.27 \times 10^{-6}</math>.</p>	
<b>AUXILIARY INFORMATION</b>	
<b>METHOD/APPARATUS/PROCEDURE:</b>  A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) source not specified; analytical grade; used as received; no impurities by glc.  (2) doubly distilled; free of trace organics.  <b>ESTIMATED ERROR:</b>  temp. $\pm$ 0.5°C soly. $\pm$ 1.2 mg(1)/kg(2) (from eight determinations)  <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 1-Methylnaphthalene; $C_{11}H_{10}$ ; [90-12-0] (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> <p>The solubility of 1-methylnaphthalene in water at 25°C was reported to be 28.5 mg(1) <math>dm^{-3}</math> sln and <math>x_1 = 3.55 \times 10^{-6}</math>.</p> <p>The corresponding mass percent calculated by the compiler is 0.00285 g(1)/100 g sln.</p>	
<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. $\pm 0.3$ mg(1) $dm^{-3}$ sln (maximum deviation from several determinations). <b>REFERENCES:</b>

<b>COMPONENTS:</b> (1) 1-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [90-12-0] (2) Water; H <sub>2</sub> O; [7732-18-5]		<b>ORIGINAL MEASUREMENTS:</b> Schwarz, F.P. <i>J. Chem. Eng. Data</i> <u>1977</u> , 22, 273-7.	
<b>VARIABLES:</b> Temperature: 8.6-31.7°C		<b>PREPARED BY:</b> A. Maczynski	
<b>EXPERIMENTAL VALUES:</b> Solubility of 1-methylnaphthalene in water			
<i>t</i> /°C	10 <sup>4</sup> mol(1) L <sup>-1</sup>	10 <sup>3</sup> g(1)/100 g sln (compiler)	10 <sup>6</sup> x <sub>1</sub> (compiler)
8.6	1.40 ± 0.03	1.99	2.52
14.0	1.59 ± 0.03	2.26	2.86
17.1	1.61 ± 0.03	2.29	2.90
20.0	1.78 ± 0.02	2.53	3.21
23.0	1.94 ± 0.02	2.76	3.49
25.0	2.11 ± 0.07	3.00	3.80
26.1	2.14 ± 0.02	3.04	3.85
29.2	2.34 ± 0.05	3.33	4.21
31.7	2.55 ± 0.04	3.27	4.59
<b>AUXILIARY INFORMATION</b>			
<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 72 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 99.9 mole%, by glc; used as received.  (2) distilled over KMnO <sub>4</sub> and NaOH and passed through a Sephadex column.	
		<b>ESTIMATED ERROR:</b> temp. ± 0.1°C soly. see above	
		<b>REFERENCES:</b>	

<b>COMPONENTS:</b>  (1) 1-Methylnaphthalene; $C_{11}H_{10}$ ; [90-12-0]  (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Schwarz, F.P.; Wasik, S.P.  <i>J. Chem. Eng. Data</i> <u>1977</u> , <i>22</i> , 270-3.																				
<b>VARIABLES:</b>  Temperature: 10-25°C	<b>PREPARED BY:</b>  A. Maczynski																				
<b>EXPERIMENTAL VALUES:</b>  <div style="text-align: center;">Solubility of 1-methylnaphthalene in water</div> <table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;"><math>t/^\circ C</math></th> <th style="text-align: center;"><math>10^4 \text{ mol(1) L}^{-1}</math></th> <th style="text-align: center;"><math>10^3 \text{ g(1)/100 g sln}</math> (compiler)</th> <th style="text-align: center;"><math>10^6 x_1</math> (compiler)</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">10</td> <td style="text-align: center;">1.6</td> <td style="text-align: center;">2.3</td> <td style="text-align: center;">2.9</td> </tr> <tr> <td style="text-align: center;">14</td> <td style="text-align: center;">2.0</td> <td style="text-align: center;">2.8</td> <td style="text-align: center;">3.6</td> </tr> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">2.0</td> <td style="text-align: center;">2.8</td> <td style="text-align: center;">3.6</td> </tr> <tr> <td style="text-align: center;">25</td> <td style="text-align: center;">2.1</td> <td style="text-align: center;">3.0</td> <td style="text-align: center;">3.8</td> </tr> </tbody> </table>		$t/^\circ C$	$10^4 \text{ mol(1) L}^{-1}$	$10^3 \text{ g(1)/100 g sln}$ (compiler)	$10^6 x_1$ (compiler)	10	1.6	2.3	2.9	14	2.0	2.8	3.6	20	2.0	2.8	3.6	25	2.1	3.0	3.8
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<b>AUXILIARY INFORMATION</b>																					
<b>METHOD/APPARATUS/PROCEDURE:</b>  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.	<b>SOURCE AND PURITY OF MATERIALS:</b>  (1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.  (2) distilled from $KMnO_4$ and passed through a Sephadex column.  <b>ESTIMATED ERROR:</b>  temp. $\pm 0.1^\circ C$ soly. $\pm 2 \times 10^{-5} \text{ mol(1) dm}^{-3}$  <b>REFERENCES:</b>																				

<b>COMPONENTS:</b> (1) 1-Methylnaphthalene; C <sub>11</sub> H <sub>10</sub> ; [90-12-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H <sub>2</sub> O; [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: 8.1-28.5°C Salinity: 30 g(2)/kg sln	<b>PREPARED BY:</b> W.Y. Shiu, D. Mackay																				
<b>EXPERIMENTAL VALUES:</b> <p style="text-align: center;">Solubility of 1-methylnaphthalene in 0.5 mol(2)/L</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;"><i>t</i>/°C</th> <th style="text-align: center;"><u>10<sup>4</sup> mol(1)/L sln</u></th> </tr> </thead> <tbody> <tr><td style="text-align: center;">8.1</td><td style="text-align: center;">1.23</td></tr> <tr><td style="text-align: center;">11.1</td><td style="text-align: center;">1.35</td></tr> <tr><td style="text-align: center;">15.5</td><td style="text-align: center;">1.49</td></tr> <tr><td style="text-align: center;">17.4</td><td style="text-align: center;">1.53</td></tr> <tr><td style="text-align: center;">18.2</td><td style="text-align: center;">1.54</td></tr> <tr><td style="text-align: center;">20.7</td><td style="text-align: center;">1.54</td></tr> <tr><td style="text-align: center;">23.3</td><td style="text-align: center;">1.63</td></tr> <tr><td style="text-align: center;">25.0</td><td style="text-align: center;">1.69</td></tr> <tr><td style="text-align: center;">28.5</td><td style="text-align: center;">1.81</td></tr> </tbody> </table> <p>The corresponding mass percent and mole fraction, <math>x_1</math>, at 25.0°C calculated by the compilers are <math>2.34 \times 10^{-3}</math> g(1)/100 g sln and <math>3.06 \times 10^{-6}</math>.</p>		<i>t</i> /°C	<u>10<sup>4</sup> mol(1)/L sln</u>	8.1	1.23	11.1	1.35	15.5	1.49	17.4	1.53	18.2	1.54	20.7	1.54	23.3	1.63	25.0	1.69	28.5	1.81
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<b>AUXILIARY INFORMATION</b>																					
<b>METHOD/APPARATUS/PROCEDURE:</b> <p>The solubility of 1-methylnaphthalene 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-methylnaphthalene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of 1-methylnaphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.</p>	<b>SOURCE AND PURITY OF MATERIALS:</b> 1-Methylnaphthalene: purity > 99%, Sodium chloride: reagent grade, Ethanol: reagent grade, Water: distilled over a KMnO <sub>4</sub> - NaOH solution and passed through a Sephadex column. <b>ESTIMATED ERROR:</b> Solubility ± 3.6% (author) Temperature ± 0.1°C (author) <b>REFERENCES:</b>																				