

COMPONENTS:		EVALUATOR:	
(1) Fluorobenzene; C ₆ H ₅ F; [462-06-6]		A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.	
(2) Water; H ₂ O; [7732-18-5]		May 1979	
CRITICAL EVALUATION:			
<p>Four experimental measurements of the solubility of fluorobenzene in water have been reported in the literature (1-4), see Figure 1. However, only one single measurement of the solubility of water in fluorobenzene has been reported (5).</p> <p>Some of the more recent data for the solubility of fluorobenzene in water is that of Nelson and Smit (4) in the temperature range between 278 and 318 K. However, despite equilibrium periods of 24 hours (which might not have been long enough), the measured solubilities are substantially lower than those found by earlier investigators. It is not possible to establish any shortcomings of the experimental procedures from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (6). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.</p> <p>Jockers (3) reported the solubility of fluorobenzene in water at high temperatures and high pressures only. The objective of these measurements was to establish the phase equilibria and thermodynamics for fluid mixtures in which fluorobenzene and water are miscible in all proportions. The critical curve was also determined (7,8). There are no other solubility measurements in the temperature range between 546 and 562 K and in the pressure range between 96×10^5 and 114×10^5 Pa for comparison.</p> <p>The two experimental determinations by Andrews and Keefer (1) at 298.15 K and Gross et al. (2) at 303.15 K are in good agreement with respect to the errors estimated by the authors. The recommended solubility has been established as the arithmetic mean of the two solubilities and temperatures.</p> <p>Only a single solubility measurement for the solubility of water in fluorobenzene has been reported in the literature (5). This experimental determination was done by Wing in 1956 (9) at Purdue University in partial fulfillment of the requirements for the Doctor of Philosophy degree. This measurement was made by an isotopic dilution technique using tritiated water as the tracer. There are no other reported values for comparison and selection.</p> <p>Recommended solubility values are as follows (that for water in fluorobenzene is tentative):</p>			
T/K	10^2 mol(1)/dm^3	g(1)/kg	$10^4 x(1)$
300.65	1.59	1.54	2.89
T/K	10^2 mol(2)/dm^3	10g(2)/kg	$10^3 x(2)$
298.15	1.75	3.08	1.65

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CRITICAL EVALUATION: (Continued) <p style="text-align: center;">REFERENCES</p> <ol style="list-style-type: none">1. Andrews, L. J.; Keefer, R. M. <i>J. Am. Chem. Soc.</i> <u>1950</u>, <i>72</i>(7), 3113-6.2. Gross, P. M.; Saylor, J. H.; Gorman, M. A. <i>J. Am. Chem. Soc.</i> <u>1933</u>, <i>55</i>(2), 650-2.3. Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, <u>1976</u>.4. Nelson, H. D.; Smit, J. H. <i>S.-Afr. Tydskr. Chem.</i> <u>1978</u>, <i>31</i>(2), 76.5. Wing, J.; Johnston, W.H. <i>J. Am. Chem. Soc.</i> <u>1957</u>, <i>79</i>(4), 864-5.6. Nelson, H. D.; Smit, J. H., Personal Communication, <u>1979</u>.7. Götze, G.; Jockers, R.; Schneider, G. M., 4th Internat. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, <u>1975</u>, Part IV/9, 57-64.8. Jockers, R.; Schneider, G. M. <i>Ber. Bunsenges, Phys. Chem.</i> <u>1978</u>, <i>83</i>, 576-82.9. Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, <u>1956</u>.	

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CRITICAL EVALUATION: (Continued)

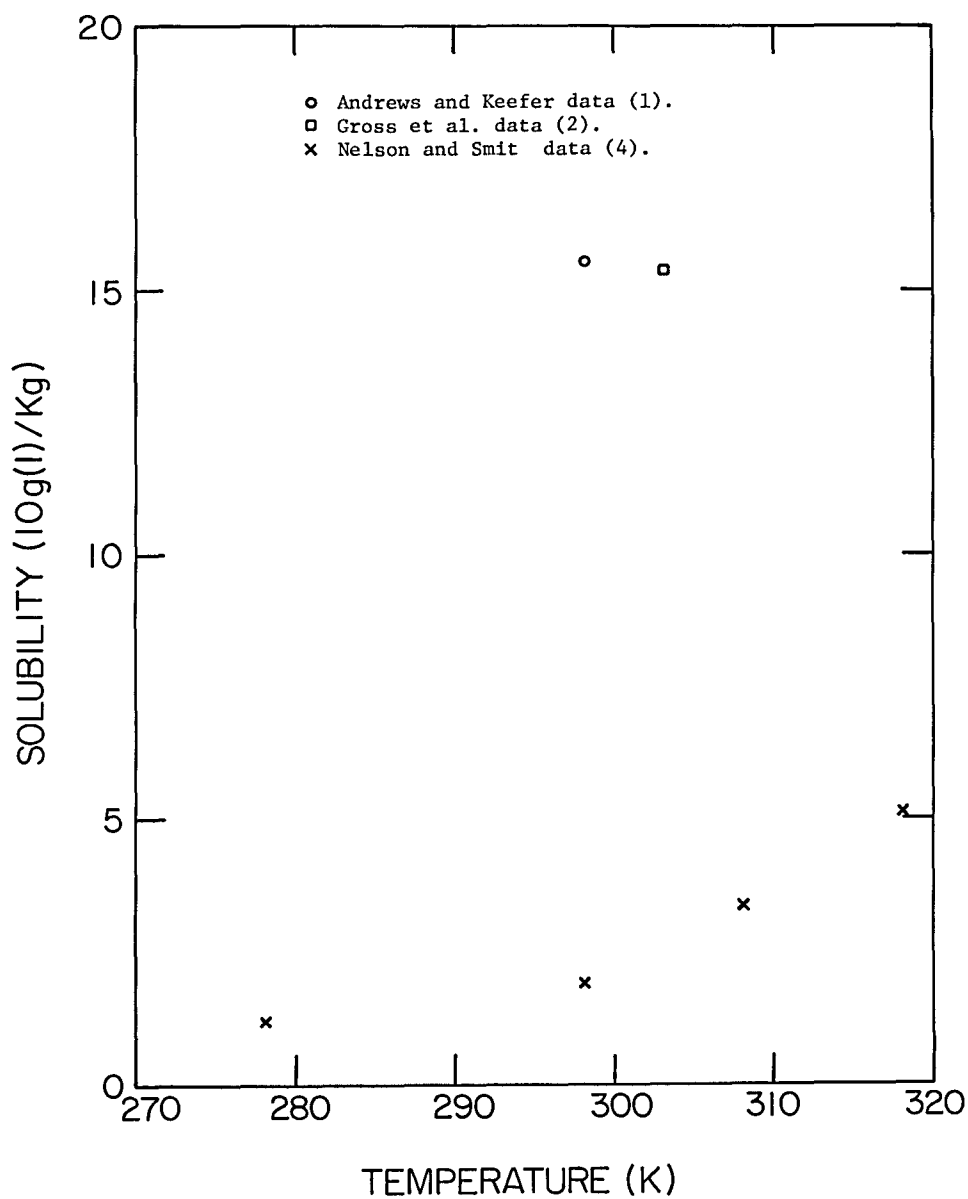


Figure 1. Solubility of fluorobenzene in water versus Absolute temperature, reported values.

COMPONENTS: (1) Fluorobenzene; C_6H_5F ; [462-06-6] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Gross, P. M.; Saylor, J. H.; Gorman, M. A. <i>J. Am. Chem. Soc.</i> <u>1933</u> , <i>55</i> (1), 650-2.								
VARIABLES: One temperature	PREPARED BY: A. L. Horvath								
EXPERIMENTAL VALUES: <table data-bbox="188 487 873 596" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th style="text-align: center;">$t/^\circ C$</th> <th style="text-align: center;">$g(1)/kg(2)^a$</th> <th style="text-align: center;">$10^2 mol(1)/kg^b$</th> <th style="text-align: center;">$10^4 \alpha(1)^c$</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">30</td> <td style="text-align: center;">1.54</td> <td style="text-align: center;">1.600</td> <td style="text-align: center;">2.886</td> </tr> </tbody> </table> <p data-bbox="188 626 564 705"> a. Reported. b. Calculated by F. W. Getzen. c. Calculated by compiler. </p>		$t/^\circ C$	$g(1)/kg(2)^a$	$10^2 mol(1)/kg^b$	$10^4 \alpha(1)^c$	30	1.54	1.600	2.886
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30	1.54	1.600	2.886						
AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: The saturated solution was prepared in a flask placed in a water thermostat bath. The samples were analyzed by means of a Zeiss combination liquid and gas interferometer as described in (1). A detailed description of the complete procedure has been included in a M.A. dissertation (2).	SOURCE AND PURITY OF MATERIALS: C_6H_5F : Eastman Kodak Co., distilled fractionally before use, b.p. range $84.55^\circ - 84.63^\circ C$. H_2O : Distilled. ESTIMATED ERROR: Solubility: $\pm 1.5\%$. Temperature: $\pm 0.02 K$. REFERENCES: 1. Gross, P. M.; Saylor, J. H. <i>J. Am. Chem. Soc.</i> <u>1931</u> , <i>53</i> (5), 1744-51. 2. Gorman, M. A., M.A. Thesis, Duke University, Durham, <u>1932</u> .								

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<p>METHOD/APPARATUS/PROCEDURE:</p> <p>The water was saturated with fluorobenzene in a glass-stoppered Erlenmeyer flask rotated in a constant temperature bath for 20 hours. The saturated solution was extracted with n-hexane. The optical density of the extract was measured against a standard n-hexane blank with a Beckman spectrophotometer (1).</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>C₆H₅F: Eastman Kodak Co., commercial reagent, b.p. 84.4°C, fractionated before use.</p> <p>H₂O: Not specified.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: ±10% (compiler).</p> <p>Temperature: ±0.1 K (compiler).</p> <p>REFERENCES:</p> <p>1. Andrews, L. J.; Keefer, R. M. <i>J. Am. Chem. Soc.</i> <u>1949</u>, <i>71</i>(11), 3644-7.</p>								

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AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: Tritiated water was equilibrated with 20 ml fluorobenzene for two hours in a flask placed in a constant temperature bath. The sample was stirred throughout the equilibration period. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. The tritium activities in the tritiated water were determined by the acetylene method (1,2). At least four independent experiments were done. The article was based upon work reported in a Ph.D. dissertation (2).	SOURCE AND PURITY OF MATERIALS: H ₂ O: Tracerlab Inc., tritiated water, used as received. C ₆ H ₅ F: Source not specified, chemical grade, redistilled before use. ESTIMATED ERROR: Solubility: ±2.8%. Temperature: ±0.02 K. REFERENCES: 1. Wing, J.; Johnston, W. H. <i>Science</i> <u>1955</u> , <i>121</i> , 674-6. 2. Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, <u>1956</u> .								

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<p>VARIABLES:</p> <p>Temperature and pressure</p>	<p>PREPARED BY:</p> <p>A. L. Horvath</p>																									
<p>EXPERIMENTAL VALUES:</p> <table border="1" data-bbox="225 484 1022 710"> <thead> <tr> <th>t/°C</th> <th>P/bar</th> <th>10⁻²g(1)/kg^a</th> <th>mol(1)/kg^b</th> <th>10x(1)^c</th> </tr> </thead> <tbody> <tr> <td>284.0</td> <td>100</td> <td>4.9130</td> <td>5.1123</td> <td>1.533</td> </tr> <tr> <td>289.5</td> <td>114</td> <td>5.6684</td> <td>8.8985</td> <td>1.970</td> </tr> <tr> <td>279.0</td> <td>103</td> <td>5.6684</td> <td>8.8985</td> <td>1.970</td> </tr> <tr> <td>273.5</td> <td>96</td> <td>5.6684</td> <td>8.8985</td> <td>1.970</td> </tr> </tbody> </table> <p>a. Calculated by compiler. b. Calculated by F. W. Getzen. c. Reported.</p>		t/°C	P/bar	10 ⁻² g(1)/kg ^a	mol(1)/kg ^b	10x(1) ^c	284.0	100	4.9130	5.1123	1.533	289.5	114	5.6684	8.8985	1.970	279.0	103	5.6684	8.8985	1.970	273.5	96	5.6684	8.8985	1.970
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<p>METHOD/APPARATUS/PROCEDURE:</p> <p>The measurements were made using a high temperature, high pressure optical cell made from stainless steel with an internal stirrer. Predetermined mixtures of fluorobenzene in water were introduced into the cell and homogenized at various temperatures and pressures. The phase transitions were observed through a sapphire window at the appropriate temperatures and pressures. Further details have been included in (1,2).</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>C₆H₅F: Fluka AG., Buchs, Schweiz, 99.5% pure, redistilled before use.</p> <p>H₂O: Boiled with KMnO₄ and redistilled before use.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: ±1%. Temperature: ±0.5 K. Pressure: ±2 bar.</p> <p>REFERENCES:</p> <ol style="list-style-type: none"> Götze, G.; Jockers, R.; Schneider, G. M. 4th Inter. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, <u>1975</u>, Part IV/9, pp 57-64. Jockers, R.; Schneider, G. M. <i>Ber. Bunsenges. Phys. Chem.</i> <u>1978</u>, <i>83</i>, 576-82. 																									

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METHOD/APPARATUS/PROCEDURE: Water was saturated through the vapor phase with fluorobenzene in a special flask (1) using a shaker in a thermostat bath for 24 hours. A gas chromatographic analysis of the samples was done by injection into a 5% Apiezon M stainless steel column with Celite as the supporter. The column length was 1.5 m and the temp. was $120^\circ C$. The chromatograph was equipped with a flame ionization detector. Three samples were analyzed from each flask.	SOURCE AND PURITY OF MATERIALS: C_6H_5F : Not specified. H_2O : Not specified.																				
ESTIMATED ERROR: Solubility: $\pm 1.9\%$ (compiler). Temperature: ± 0.1 K (compiler).																					
REFERENCES: 1. Nelson, H. D.; de Ligny, C. L. <i>Rec. Trav. Chim.</i> <u>1968</u> , <i>87</i> , 528-44.																					