

COMPONENTS:  (1) 1,4-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [106-46-7]  (2) Water; H <sub>2</sub> O; [7732-18-5]	EVALUATOR:  A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.  May 1979.
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## CRITICAL EVALUATION:

Two sets of experimental data have been reported in the literature for the solubility of liquid 1,4-dichlorobenzene in water (1,2). Klemenc and Low (1) reported measurements in the temperature range between 328 and 333 K while Wauchope and Getzen (2) reported data in the narrow temperature interval between 332 and 346 K, see Figure 1. There is, however, a considerable discrepancy between the two results. For example, at 333 K, the difference is about 25 percent between the reported solubility values.

While the early solubility measurements of Klemenc and Low (1) in 1930 used the volumetric determination of the excess solute, the more recent determination of Wauchope and Getzen (2) in 1972 employed the extraction method followed by spectrophotometric analysis. The reagents used in the latter investigation were of higher purity.

Klemenc and Low (1) did not state the accuracy or the reliability of their method; neither duplicate nor triplicate samples were taken. Their temperature control during the equilibration periods of their measurements was about  $\pm 1$  K. Therefore, a conservative estimate of the possible errors in their solubility determinations is about  $\pm 10$  percent. The investigation of Wauchope and Getzen (2) was done under much more controlled conditions. The time required for completion of the equilibrium was assured in the experiment and replicate samples were always withdrawn and analyzed. The shorter equilibration times in the measurements of Klemenc and Low (1) may well account for the low solubility values at 328 and 333 K.

The solubility data of Wauchope and Getzen (2) have been assigned a higher weight in the establishment of recommended solubility values. The data have been correlated against Absolute temperature using the following second degree polynomial equation:

$$S_1(\text{g(l)/kg}) = 13.974 - 8.5829 \times 10^{-2} T + 1.3365 \times 10^{-4} T^2 \quad [1]$$

Recommended solubility values calculated from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

Table 1. Solubility of 1,4-Dichlorobenzene in Water.

T/K	10 <sup>3</sup> mol(l)/dm <sup>3</sup>	10g(l)/kg	10 <sup>5</sup> x(1)
328.15	1.35	2.01	2.46
333.15	1.43	2.14	2.62
338.15	1.56	2.33	2.86
343.15	1.72	2.59	3.18
348.15	1.94	2.92	3.58

The recommended molar concentrations and mole fractions have been calculated from the g(l)/kg and the densities of the two components at the equilibrium temperatures indicated.

## REFERENCES

- Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* 1930, *49*(4), 629-40.
- Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17*(1), 38-41.

## NOTE:

The critical evaluation for *solid* 1,4-dichlorobenzene with water appears on page 103.

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; $H_2O$ ; [7732-18-5]	May 1979.

CRITICAL EVALUATION: (Continued)

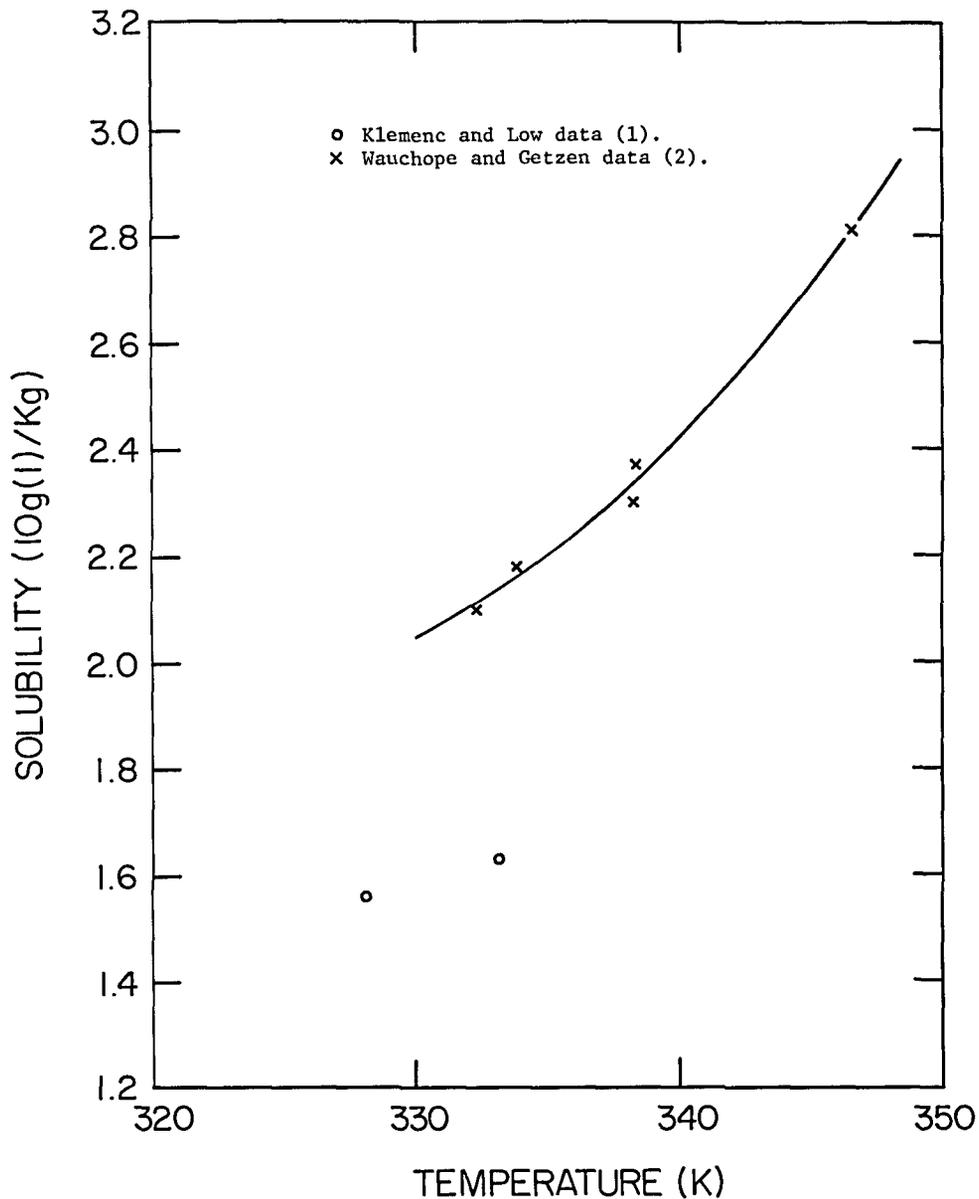


Figure 1. Solubility of 1,4-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Klemenc, A.; Löw, M. <i>Rec. trav. chim. Pays-Bas</i> <u>1930</u> , 49(4), 629-40.												
<b>VARIABLES:</b> Temperature	<b>PREPARED BY:</b> A. L. Horvath												
<b>EXPERIMENTAL VALUES:</b> <table border="1" data-bbox="131 490 855 646"> <thead> <tr> <th><math>t/^\circ C</math></th> <th>10g(1)/kg(2) <sup>a</sup></th> <th><math>10^3 \text{ mol}(1)/\text{kg}</math> <sup>b</sup></th> <th><math>10^5 x(1)</math> <sup>c</sup></th> </tr> </thead> <tbody> <tr> <td>55</td> <td>1.56</td> <td>1.061</td> <td>1.912</td> </tr> <tr> <td>60</td> <td>1.63</td> <td>1.109</td> <td>1.998</td> </tr> </tbody> </table> <p data-bbox="131 666 526 754">           a. Reported.            b. Calculated by F. W. Getzen.            c. Calculated by compiler.         </p>		$t/^\circ C$	10g(1)/kg(2) <sup>a</sup>	$10^3 \text{ mol}(1)/\text{kg}$ <sup>b</sup>	$10^5 x(1)$ <sup>c</sup>	55	1.56	1.061	1.912	60	1.63	1.109	1.998
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<b>AUXILIARY INFORMATION</b>													
<b>METHOD/APPARATUS/PROCEDURE:</b> The determination of the solubility was based upon volumetric principles applied to the measurement of excess solute in a calibrated apparatus as described by Rex (1).	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Cl_2$ : Prepared by chlorination of benzene using iodine as catalyst. The prepurate was recrystallized several times in ethanol before use, m.p. = 52.7°C. $H_2O$ : Distilled. <table border="1" data-bbox="631 1538 1171 1675"> <tr> <td colspan="2"><b>ESTIMATED ERROR:</b></td> </tr> <tr> <td>Solubility:</td> <td>±10% (compiler).</td> </tr> <tr> <td>Temperature:</td> <td>±1 K (compiler).</td> </tr> </table> <b>REFERENCES:</b> 1. Rex, A. <i>Z. Phys. Chem.</i> <u>1906</u> , 55(A), 355-70.	<b>ESTIMATED ERROR:</b>		Solubility:	±10% (compiler).	Temperature:	±1 K (compiler).						
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<p>EXPERIMENTAL VALUES:</p> <table border="1" data-bbox="257 517 943 791"> <thead> <tr> <th>t/°C</th> <th>10g(1)/kg<sup>a</sup></th> <th>10<sup>3</sup>mol(1)/kg<sup>b</sup></th> <th>10<sup>5</sup>x(1)<sup>c</sup></th> </tr> </thead> <tbody> <tr> <td>59.2</td> <td>2.10</td> <td>1.429</td> <td>2.574</td> </tr> <tr> <td>60.7</td> <td>2.18</td> <td>1.483</td> <td>2.672</td> </tr> <tr> <td>65.1</td> <td>2.30</td> <td>1.565</td> <td>2.819</td> </tr> <tr> <td>65.2</td> <td>2.37</td> <td>1.612</td> <td>2.905</td> </tr> <tr> <td>73.4</td> <td>2.81</td> <td>1.911</td> <td>3.445</td> </tr> </tbody> </table> <p>a. Reported (ppm(1) in original work).  b. Calculated by F. W. Getzen.  c. Calculated by compiler.</p>		t/°C	10g(1)/kg <sup>a</sup>	10 <sup>3</sup> mol(1)/kg <sup>b</sup>	10 <sup>5</sup> x(1) <sup>c</sup>	59.2	2.10	1.429	2.574	60.7	2.18	1.483	2.672	65.1	2.30	1.565	2.819	65.2	2.37	1.612	2.905	73.4	2.81	1.911	3.445
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<p>AUXILIARY INFORMATION</p>																									
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>An excess of 1,4-dichlorobenzene, 20 g, in water was shaken gently for one week in a water bath at constant temperature. Replicate samples were filtered through a glass-wool plug. Then, the aqueous solution was extracted with cyclohexane which was then analyzed spectrophotometrically for organic solute using a Cary 14 spectrometer.</p> <p>The article was based upon a Ph.D. dissertation (1).</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p><math>C_6H_4Cl_2</math>: Recrystallized three times and vacuum-sublimed twice of Matheson, Coleman, and Bell reagent.</p> <p><math>H_2O</math>: Distilled and deionized.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: ±3%.</p> <p>Temperature: ±0.5 K.</p> <p>REFERENCES:</p> <p>1. Vauchope, R. D., Ph.D. Dissertation, North Carolina State Univ., Raleigh, <u>1970</u>.</p>																								

<p>COMPONENTS:</p> <p>(1) 1,4-Dichlorobenzene; <math>C_6H_4Cl_2</math>; [106-46-7]</p> <p>(2) Water; <math>H_2O</math>; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>A. Vesala, Department of Chemistry and Biochemistry, University of Turku.</p> <p>September 1982.</p>
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## CRITICAL EVALUATION:

There have been eight published sets of data on the solubility of 1,4-dichlorobenzene in water at ordinary temperatures. Accordingly, the evaluation of the solubility data for this system lies on a firmer base than in the cases of the other solid halogenated benzenes in water.

The oldest data involving this system, determined by Klemenc and Low (1) in 1930, appear to be low and are imprecise because of the method used for saturation of water. There is, however, some evidence that the method allows the separation of the solubilities of the two crystallographic forms of 1,4-dichlorobenzene although the experimental values give no distinct temperature for the conversion from the  $\alpha$ -form to the  $\beta$ -form. The solubility measured by Gross and Saylor (2) at 308.2 K is probably too low because of the short time periods involved in the equilibrations. For the same reason, the value determined by Andrews and Keefer (3) must be rejected as doubtful. Booth and Everson (4) have applied a residue-volume method of Vaughn and Nutting (5) and found the solubility of 1,4-dichlorobenzene in water to be less than 0.5 g(1)/dm<sup>3</sup>(2). Their method is rapid but insensitive giving only rough values for substances having low solubilities.

More reliable data have been produced by Wauchope and Getzen (6) who reported errors to be in the range of 2 percent. These data are supported by the solubility values obtained by Vesala (7) as part of a study of the transfer free energies of certain nonelectrolytes from  $H_2O$  to  $D_2O$ . The recent data of Aquan-Yuen et al. (8) of the solubilities of 1,4-dichlorobenzene in aqueous electrolyte solutions produce a value for the solubility in water that agrees well with the above values. Banerjee et al. (9) report a solubility that is somewhat different from the former ones. The reason for the differences may be attributed to the radiochemical method of analysis used. For instance, the radiochemical purity of the substrate and the quenching of the samples in the scintillation analysis remain open to question. Their value can thus be regarded only as a slight support to the other data - even in cases of a full agreement.

The recommended solubility values are calculated on the basis of the data given by Wauchope and Getzen (6). However, instead of their smoothed equation, the calculations are done using an equation of simpler form. This, in turn, suggests that the magnitude of the reported errors is too optimistic. (In the work of Wauchope and Getzen, the meaning of the term "av.% dev.obsd. smoothed solubility" is somewhat unclear.) The values calculated from the simpler equation and the experimental data allow a fairly good estimate of precision. A standard deviation for a single value established in this fashion is of the order of 4.0 mg(1)/kg(2) or 0.027 mmol(1)/kg(2). The existence of the two crystallographic forms of the solute in the range of temperatures where the solubilities were measured is probably one reason for the deviations. However, this brings about no greater effect in the lower temperature range which suggests that the value for 298.2 K, for instance, is quite reliable. The simplified equation for concentration, g(1)/kg(2), in terms of Absolute temperature, T, is as follows:

$$\log_{10}(S_1(g(1))/kg(2)) = 2.86294 - 1176/T \quad [1]$$

The observed values from the seven relevant data are shown in Figure 1 together with the calculated behavior (shown as a solid line) from the simpler equation discussed above. The densities of pure water and the saturated solutions were assumed to be equal for the determination of the reported molarity values from the calculated g(1)/kg(2) values.

The recommended g(1)/kg solubility values for solid 1,4-dichlorobenzene in water calculated from values obtained from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1.

## COMPONENTS:

- (1) 1,4-Dichlorobenzene;  $C_6H_4Cl_2$ ;  
[106-46-7]
- (2) Water;  $H_2O$ ; [7732-18-5]

## EVALUATOR:

A. Vesala, Department of Chemistry and  
Biochemistry, University of Turku.

September 1982.

## CRITICAL EVALUATION: (Continued)

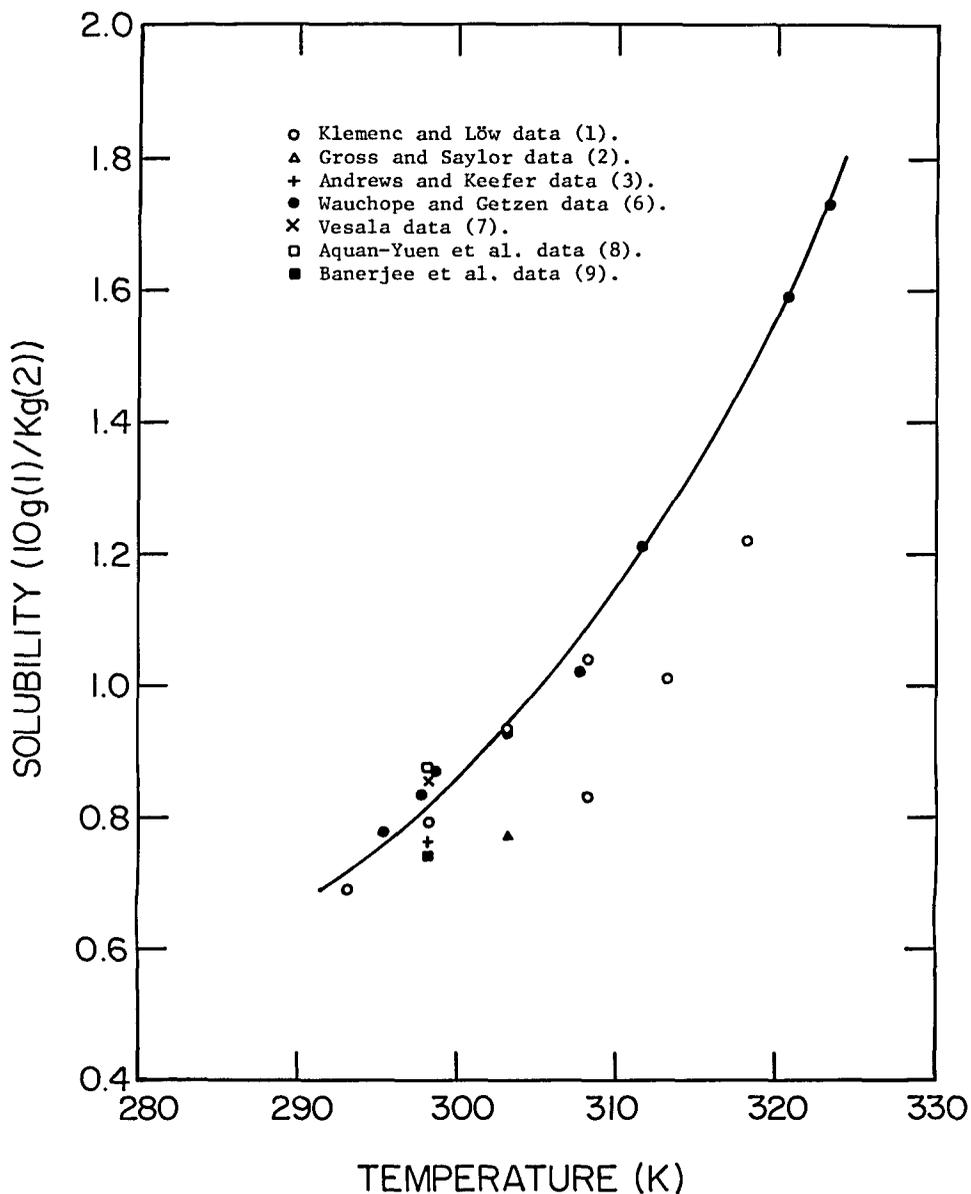


Figure 1. Solubility of solid 1,4-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS: (1) 1,4-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [106-46-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	EVALUATOR: A. Vesala, Department of Chemistry and Biochemistry, University of Turku. September 1982.
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## CRITICAL EVALUATION: (Continued)

Table 1. Solubility of 1,4-Dichlorobenzene in Water.

T/K	10 <sup>4</sup> mol(1)/dm <sup>3</sup>	10 <sup>2</sup> g(1)/kg	10 <sup>5</sup> x(1)
283.15	3.48	5.12	0.628
288.15	4.11	6.05	0.741
293.15	4.82	7.10	0.870
298.15	5.62	8.29	1.016
303.15	6.52	9.63	1.18
308.15	7.53	11.13	1.36
313.15	8.65	12.8	1.57
318.15	9.88	14.7	1.80
323.15	11.25	16.7	2.05
328.15	12.4	19.0	2.33

a. Std. dev. 0.027 mmol(1)/kg

b. Std. dev. 4.0 mg(1)/kg

The recommended molar concentrations, g(2)/kg concentrations, and mole fractions have been determined from calculated g(1)/kg(2) values and the densities of the two components at the equilibrium temperatures indicated.

## REFERENCES

- Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* 1930, *49*(4), 629-40.
- Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53*(5), 1744-51.
- Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72*(7), 3113-6.
- Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40*(8), 1491-3.
- Vaughn, T. H.; Nutting, E. G. *Ind. Eng. Chem. Anal. Ed.* 1942, *14*(6), 454-6.
- Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17*(1), 38-41.
- Vesala, A. *Acta Chem. Scand.* 1974, *28A*(8), 839-45.
- Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1979, *24*(1), 30-4.
- Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14*(10), 1227-9.

<p>COMPONENTS:</p> <p>(1) 1,4-Dichlorobenzene; <math>C_6H_4Cl_2</math>; [106-46-7]</p> <p>(2) Water; <math>H_2O</math>; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Andrews, L. J.; Keefer, R. M. <i>J. Am. Chem. Soc.</i> <u>1950</u>, <i>72</i>(7), 3113-6.</p>								
<p>VARIABLES:</p> <p>One temperature</p>	<p>PREPARED BY:</p> <p>A. Vesala</p>								
<p>EXPERIMENTAL VALUES:</p> <table data-bbox="201 502 913 598"> <thead> <tr> <th><math>t/^\circ C</math></th> <th><math>10g(1)/dm^3</math> <sup>a</sup></th> <th><math>10^4 mol(1)/dm^3</math> <sup>b</sup></th> <th><math>10^6 x(1)</math> <sup>b</sup></th> </tr> </thead> <tbody> <tr> <td>25.0</td> <td>7.6</td> <td>5.17</td> <td>9.34</td> </tr> </tbody> </table> <p>a. Reported. b. Calculated by F. W. Getzen.</p>		$t/^\circ C$	$10g(1)/dm^3$ <sup>a</sup>	$10^4 mol(1)/dm^3$ <sup>b</sup>	$10^6 x(1)$ <sup>b</sup>	25.0	7.6	5.17	9.34
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25.0	7.6	5.17	9.34						
<p>AUXILIARY INFORMATION</p>									
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>Water was saturated with 1,4-dichlorobenzene in a sealed Erlenmeyer flask by rotating the flask in a constant temperature bath for 20 hours. Measured volumes of the saturated solution were extracted with measured volumes of n-hexane for analysis. The optical density of the extract was measured against a n-hexane standard at 234 nm using a Beckman spectrophotometer (1).</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p><math>C_6H_4Cl_2</math>: Commercial product (Eastman Kodak Co.), used as received.</p> <p><math>H_2O</math>: Distilled.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: &gt;10% (compiler). Temperature: <math>\pm 0.2</math> 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>								

COMPONENTS:		ORIGINAL MEASUREMENTS:			
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7]		Klemenc, A.; Low, M. <i>Recl. Trav. Chim. Pays-Bas</i> 1930, 49(4), 629-40.			
(2) Water; $H_2O$ ; [7732-18-5]					
VARIABLES:		PREPARED BY:			
Temperature		A. Vesala			
EXPERIMENTAL VALUES:					
$t/^\circ C$	$10^2 g(1)/kg(2)^a$	$10^4 mol(1)/kg^b$	$10^6 x(1)^b$		
20	6.89	4.687	8.444		
25	7.91	5.380	9.694		
30	9.33	6.346	11.04		
35 <sup>c</sup>	10.4	8.30	7.074	5.646	12.75 10.17
40		10.1		6.870	12.38
45		12.2		8.298	14.95
<p>a. Reported (mean values from at least two measurements).  b. Calculated by F. W. Getzen.  c. The system reported not stable at this temperature.</p>					
Measurements are shown graphically in Figure 1.					
Continued ...					
AUXILIARY INFORMATION					
METHOD/APPARATUS/PROCEDURE:			SOURCE AND PURITY OF MATERIALS:		
<p>The equilibrations were done over periods from 2 to 17 days (average 7-10 days). Gravimetric analysis was the basis for the concentration determinations. The solute was placed in a spiral tube and weighed. Then, a known amount of water was passed through the tube and it was re-weighed. The weight loss and the mass of the water passed through the tube gave the solubility value directly.</p>			$C_6H_4Cl_2$ : Synthesized from benzene and chlorine, recrystallized from abs. ethanol, m.p. 53°C. The purity of the product was checked by elemental analysis.		
			$H_2O$ : Source and purity not specified.		
			ESTIMATED ERROR:		
			Solubility: >10% (evaluated on the basis of deviations from the averages).		
			Temperature: $\pm 0.5$ K.		
			REFERENCES:		

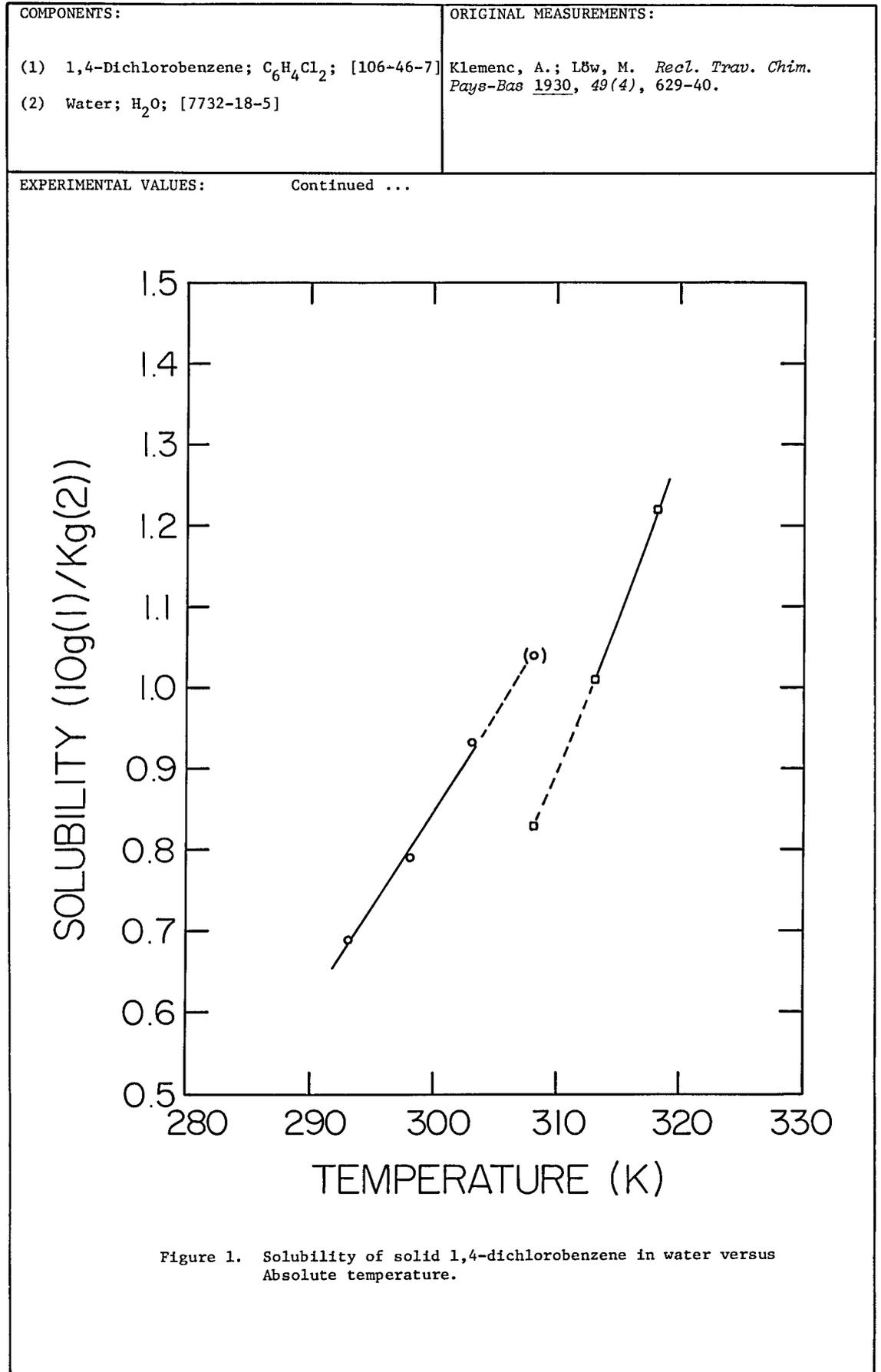


Figure 1. Solubility of solid 1,4-dichlorobenzene in water versus Absolute temperature.

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Wauchope, R. D.; Getzen, F. W. <i>J. Chem. Eng. Data</i> <u>1972</u> , 17(1), 38-41.																																				
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<b>EXPERIMENTAL VALUES:</b> <table border="1" data-bbox="181 491 901 911"> <thead> <tr> <th><math>t/^\circ C</math></th> <th><math>10g(1)/kg(2)^a</math></th> <th><math>10^4 mol(1)/kg^b</math></th> <th><math>10^5 x(1)^b</math></th> </tr> </thead> <tbody> <tr><td>22.2</td><td>0.778</td><td>5.292</td><td>0.9535</td></tr> <tr><td>24.6</td><td>0.834</td><td>5.673</td><td>1.022</td></tr> <tr><td>25.5</td><td>0.869</td><td>5.911</td><td>1.065</td></tr> <tr><td>30.0</td><td>0.926</td><td>6.298</td><td>1.135</td></tr> <tr><td>34.5</td><td>1.02</td><td>6.938</td><td>1.250</td></tr> <tr><td>38.4</td><td>1.21</td><td>8.230</td><td>1.483</td></tr> <tr><td>47.5</td><td>1.59</td><td>10.81</td><td>1.949</td></tr> <tr><td>50.1</td><td>1.73</td><td>11.77</td><td>2.120</td></tr> </tbody> </table> <p data-bbox="181 950 559 999">           a. Reported.            b. Calculated by F. W. Getzen.         </p> <p data-bbox="181 1038 756 1068">Measurements are shown graphically in Figure 1.</p> <p data-bbox="1046 1107 1217 1136" style="text-align: right;">Continued ...</p>		$t/^\circ C$	$10g(1)/kg(2)^a$	$10^4 mol(1)/kg^b$	$10^5 x(1)^b$	22.2	0.778	5.292	0.9535	24.6	0.834	5.673	1.022	25.5	0.869	5.911	1.065	30.0	0.926	6.298	1.135	34.5	1.02	6.938	1.250	38.4	1.21	8.230	1.483	47.5	1.59	10.81	1.949	50.1	1.73	11.77	2.120
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<b>METHOD/APPARATUS/PROCEDURE:</b> Equilibrium was established by allowing the mixtures to stand in glass stoppered flasks, with occasional shaking, for 1-3 week periods at constant temperature. Samples of the saturated aqueous solutions were withdrawn with pipettes through glass-wool plugs and transferred to separatory funnels for weighing. An extraction with cyclohexane was then performed after which the extracts were analyzed spectrophotometrically at 273 nm. The concentrations were established from previously obtained absorbance values of standard reference solutions (which were observed to obey Beer's law).	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Cl_2$ : Commercial product (Matheson, Coleman and Bell), recrystallized three times from abs. ethanol, vacuum sublimed twice, UV-spectrum and melting point were determined and were identical to published data. $H_2O$ : Distilled and deionized water.																																				
<b>ESTIMATED ERROR:</b> Solubility: $\pm 2.3\%$ (authors). Temperature: $\pm 0.5$ K (authors).																																					
<b>REFERENCES:</b>																																					

<b>COMPONENTS:</b>  (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7]  (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b>  Wauchope, R. D.; Getzen, F. W. <i>J. Chem. Eng. Data</i> <u>1972</u> , <i>17</i> (1), 38-41.
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EXPERIMENTAL VALUES: Continued ...

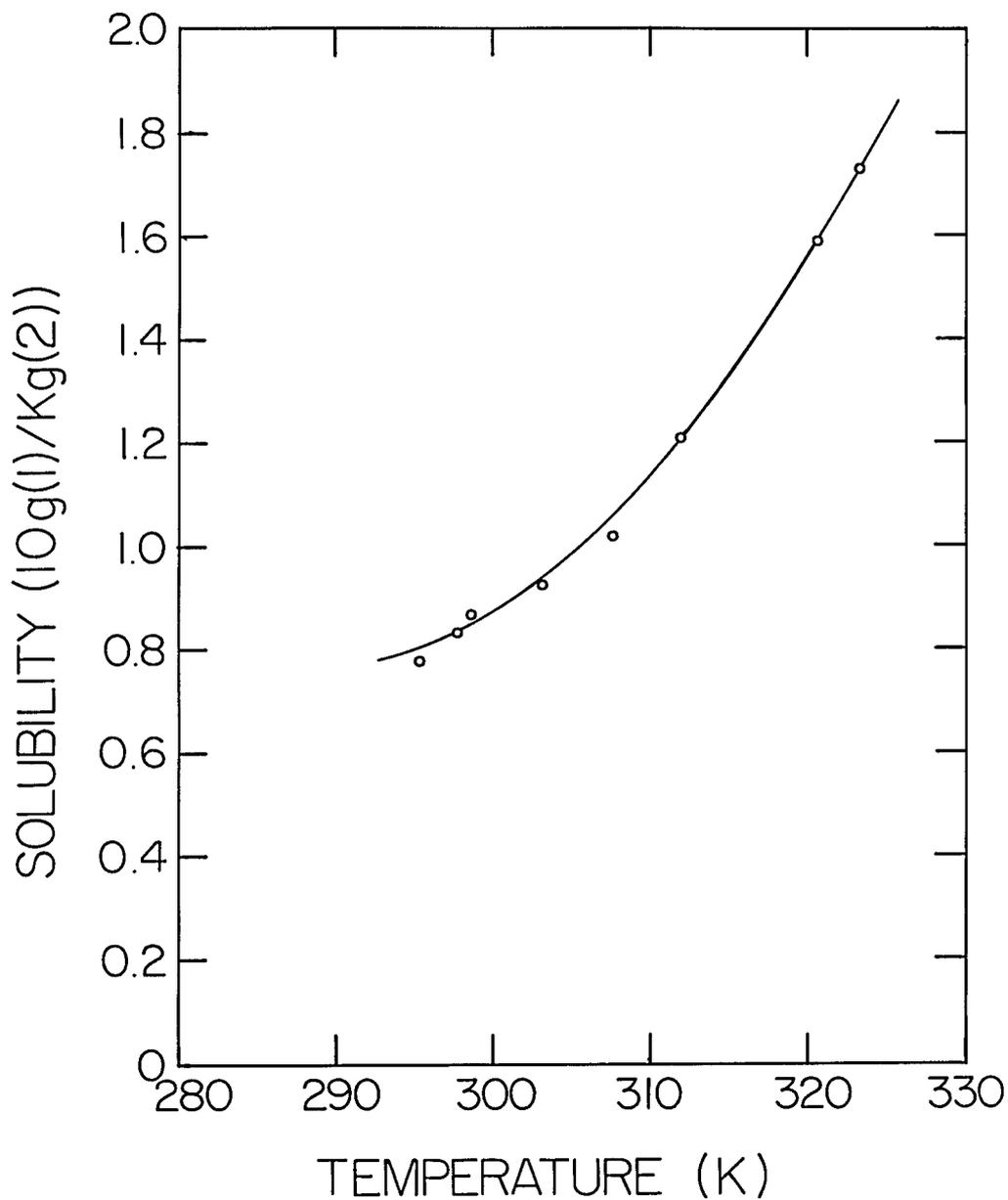


Figure 1. Solubility of solid 1,4-dichlorobenzene in water versus Absolute temperature.

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Vesala, A. <i>Acta Chem. Scand.</i> <u>1974</u> , <i>28A</i> (8), 839-45.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> H. Lonnberg								
<b>EXPERIMENTAL VALUES:</b>  <table data-bbox="194 486 921 572"> <thead> <tr> <th><math>t/^\circ C</math></th> <th><math>10^2 g(1)/kg(2)</math> <sup>a</sup></th> <th><math>10^4 mol(1)/kg</math> <sup>b</sup></th> <th><math>10^5 x(1)</math> <sup>b</sup></th> </tr> </thead> <tbody> <tr> <td>25.0</td> <td>8.55</td> <td>5.816</td> <td>1.048</td> </tr> </tbody> </table> <p data-bbox="194 615 571 662">           a. Reported.            b. Calculated by F. W. Getzen.         </p>		$t/^\circ C$	$10^2 g(1)/kg(2)$ <sup>a</sup>	$10^4 mol(1)/kg$ <sup>b</sup>	$10^5 x(1)$ <sup>b</sup>	25.0	8.55	5.816	1.048
$t/^\circ C$	$10^2 g(1)/kg(2)$ <sup>a</sup>	$10^4 mol(1)/kg$ <sup>b</sup>	$10^5 x(1)$ <sup>b</sup>						
25.0	8.55	5.816	1.048						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> Saturation of the 1,4-dichlorobenzene in water was established by shaking the mixture in a sealed tube suspended in a thermostat water bath for 1-2 weeks. The sealed tube was allowed to stand for two to three days without shaking before analysis. Samples from the saturated solution were extracted with 2,2,4-trimethylpentene. Then, the optical densities of the liquid extracts were determined spectrophotometrically. The concentration was established from optical density using a previously prepared standard calibration curve.	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Cl_2$ : Commercial product (E. Merck AG), recrystallized twice from abs. ethanol. $H_2O$ : Distilled, deionized and degassed.  <b>ESTIMATED ERROR:</b> Solubility: $\pm 1.5\%$ (author). Temperature: $\pm 0.05$ K (author).  <b>REFERENCES:</b>								

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Gross, P. M.; Saylor, J. H. <i>J. Am. Chem. Soc.</i> <u>1931</u> , <i>53</i> (5), 1744-51.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> A. Vesala								
<b>EXPERIMENTAL VALUES:</b> <table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; padding: 5px;"><math>t/^\circ C</math></th> <th style="text-align: center; padding: 5px;"><math>10^2 g(1)/kg(2)</math> <sup>a</sup></th> <th style="text-align: center; padding: 5px;"><math>10^4 mol(1)/kg</math> <sup>b</sup></th> <th style="text-align: center; padding: 5px;"><math>10^6 x(1)</math> <sup>b</sup></th> </tr> </thead> <tbody> <tr> <td style="text-align: left; padding: 5px;">30</td> <td style="text-align: center; padding: 5px;">7.7</td> <td style="text-align: center; padding: 5px;">5.24</td> <td style="text-align: center; padding: 5px;">9.44</td> </tr> </tbody> </table> <p style="margin-left: 20px;">a. Reported. b. Calculated by F. W. Getzen.</p>		$t/^\circ C$	$10^2 g(1)/kg(2)$ <sup>a</sup>	$10^4 mol(1)/kg$ <sup>b</sup>	$10^6 x(1)$ <sup>b</sup>	30	7.7	5.24	9.44
$t/^\circ C$	$10^2 g(1)/kg(2)$ <sup>a</sup>	$10^4 mol(1)/kg$ <sup>b</sup>	$10^6 x(1)$ <sup>b</sup>						
30	7.7	5.24	9.44						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> <p>The saturated solution was prepared by shaking the substances in a thermostat bath for at least 12 hours. An interferometric method was used for the analysis of the saturated solution (1). Samples were withdrawn from several saturation flasks and read against a pure water sample in an interferometer. The concentration was established from a calibration obtained from previous measurements made with a reference solution.</p>	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Cl_2$ : Commercial product (Eastman Kodak Co.), recrystallized twice from ethanol, m.p. 52.84°C. $H_2O$ : Distilled water "of good quality". <b>ESTIMATED ERROR:</b> Solubility: $\pm 5\%$ (authors). Temperature: $\pm 0.01$ K (authors). <b>REFERENCES:</b> 1. Gross, P. M. <i>J. Am. Chem. Soc.</i> <u>1929</u> , <i>51</i> (8), 2362-6.								

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$ ; [106-46-7] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. <i>J. Chem. Eng. Data</i> <u>1979</u> , <i>24</i> (1), 30-4.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> A. Vesala								
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$t/^\circ C$	$10^2 g(1)/dm^3$ <sup>a</sup>	$10^4 mol(1)/dm^3$ <sup>b</sup>	$10^5 x(1)$ <sup>b</sup>						
25	8.715	5.9283	1.0713						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> Saturated solutions were prepared by adding an excess of solute to water in a closed flask with standing for 24 hours. Then, the sample was allowed to settle at 25°C in a thermostat bath for at least 48 hours before analysis. The solubility was determined by solvent extraction followed by gas chromatographic analysis using a Hewlett Packard Model 5750 apparatus (equipped with a flame ionization detector and a 10 ft stainless steel column packed with 10% SE 30 ultra-phase on high performance Chromosorb P, 60/80 mesh).	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_4Cl_2$ : Commercial product (BDH), evidently used as received. $H_2O$ : Source and purity not specified.  <b>ESTIMATED ERROR:</b> Solubility: $\pm 3\%$ (authors, the value is based on the std. error of the least squares fit on the solubility of 1,4-dichlorobenzene in water and aqueous electrolyte solutions. Temperature: $\pm 0.2$ K (compiler).  <b>REFERENCES:</b>								

<p>COMPONENTS:</p> <p>(1) 1,4-Dichlorobenzene; <math>C_6H_4Cl_2</math>; [106-46-7]</p> <p>(2) Water; <math>H_2O</math>; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Booth, H. S.; Everson, H. E. <i>Ind. Eng. Chem.</i> <u>1948</u>, <i>40(8)</i>, 1491-3.</p>								
<p>VARIABLES:</p> <p>One temperature</p>	<p>PREPARED BY:</p> <p>A. Vesala</p>								
<p>EXPERIMENTAL VALUES:</p> <table data-bbox="212 498 934 579"> <thead> <tr> <th><math>t/^\circ C</math></th> <th><math>10g(1)/kg(2)^a</math></th> <th><math>10^3 mol(1)/kg^b</math></th> <th><math>10^5 x(1)^b</math></th> </tr> </thead> <tbody> <tr> <td>25.4</td> <td>&lt;5</td> <td>&lt;3.4</td> <td>&lt;6.1</td> </tr> </tbody> </table> <p>a. Reported. b. Calculated by F. W. Getzen.</p>		$t/^\circ C$	$10g(1)/kg(2)^a$	$10^3 mol(1)/kg^b$	$10^5 x(1)^b$	25.4	<5	<3.4	<6.1
$t/^\circ C$	$10g(1)/kg(2)^a$	$10^3 mol(1)/kg^b$	$10^5 x(1)^b$						
25.4	<5	<3.4	<6.1						
<p>AUXILIARY INFORMATION</p>									
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>The composition analysis was based upon a volumetric method described in (1). In this method, further addition of solute to a volume of solution yielded, upon saturation, proportional amounts of undissolved solute residue which could be measured volumetrically. A plot of added solute mass versus volume of residue gave a straight line the intercept of which gave the solubility.</p> <p>Stoppered tubes with capillaries graduated in steps of 0.05 ml were used for the measurements. A known volume of solvent (50 ml) was added to the tube in a constant temperature bath and weighted quantities of the solid solute were added to the liquid. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes, and centrifuged for 5 minutes. Then, the volume of residue was read. The procedures were repeated to ensure that the equilibrium had been reached.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p><math>C_6H_4Cl_2</math>: Commercial reagents of highest grade, probably used as received.</p> <p><math>H_2O</math>: Source and purity not specified.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: Within 0.1 g as reported in Ref. (1).</p> <p>Temperature: <math>\pm 0.2</math> K (compiler).</p> <p>REFERENCES:</p> <p>1. Vaughn, T.H.; Nutting, E. G. <i>Ind. Eng. Chem., Anal. Ed.</i> <u>1942</u>, <i>14(6)</i>, 454-6.</p>								

<b>COMPONENTS:</b> (1) 1,4-Dichlorobenzene; C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> ; [106-46-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. <i>Environm. Sci. Techn.</i> <u>1980</u> , <i>14</i> (10), 1227-9.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> A. Vesala								
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t/°C	10 <sup>2</sup> g(1)/dm <sup>3</sup> <sup>a</sup>	10 <sup>4</sup> mol(1)/dm <sup>3</sup> <sup>b</sup>	10 <sup>6</sup> x(1) <sup>a</sup>						
25	7.380	5.02	9.071						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> The equilibrium was performed in sealed stainless steel centrifugre tubes with constant or intermittent shaking. The equilibrium was generally complete within 1 week. The mixture was then centrifugred for 60 minutes after which aliquots of the solution were removed either by pipet or syringe for analysis. Liquid scintillation counting with <sup>14</sup> C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	<b>SOURCE AND PURITY OF MATERIALS:</b> C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> : Commercial reagent. the <sup>14</sup> C-labeled compound was purchaed by NEN, the nonlabeled one by Aldrich. H <sub>2</sub> O: Distilled.  <b>ESTIMATED ERROR:</b> Solubility: ±6.0% (std. deviation estimated by authors). Temperature: ±0.2 K (equilibration), ±0.3 K (centrifugation).  <b>REFERENCES:</b>								