

<p>COMPONENTS:</p> <p>(1) 4-Chlorophenol; <math>C_6H_5ClO</math>; [106-48-9]</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>November 1979.</p>
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## CRITICAL EVALUATION:

The earliest of the published works on the solubility of 4-chlorophenol in water is that of Sidgwick and Turner (1). Even though this work has been available for more than 50 years, it still serves as a useful reference for comparison of later results. No solubility value at 298.15 K has been reported as a measured value; the nearest measurements reported have been relatively far from room temperature (274 K and 339 K by Sidgwick and Turner) making an interpolation difficult.

Kuroda (2) reported an approximate solubility of the three isomeric monochlorophenols in water in the range of 2 percent. More support for the work of Sidgwick and Turner is given by the work of Blackman et al. (3) and that of Mulley and Metcalf (4). The data reported in these two works are in good agreement. For an assumed solution density of  $1.0 \text{ g/cm}^3$ , a value of  $27 \text{ g(l)/kg}$  results from the work of Blackman et al. and a value of  $26 \text{ g(l)/kg}$  results from the work of Mulley and Metcalf.

In reviewing the work of Blackman et al. it should be stressed that the solubility was determined at a pH of 5.1, a condition being controlled by the addition of a phosphate buffer (a  $KH_2PO_4$  solution). However, the effect of the buffer solution can be minimized since the pH of a saturated 4-chlorophenol solution can be assumed to be of the same magnitude as that of the buffer and the ionic effects can be assumed to be quite low (as reported by Robinson and Stokes (5), the pK for 4-chlorophenol in water is 9.4). Even so, one should remember that the pH does exert some influence on the solubility of protolytic solutes such as 4-chlorophenol and attention should be paid to agents in the solution which change its acidity. The data are shown in Figure 1.

The solubility of 4-chlorophenol in water at normal temperatures has a reliable value as deduced from the three references. However, the mutual solubility of 4-chlorophenol and water as reported by Sidgwick and Turner over its entire temperature range must be considered tentative because of the lack of other supporting data.

The following solubility of 4-chlorophenol in water is tentative and based primarily on the reported value of Blackman et al.:

T/K	10mol(l)/dm	$10^{-1} \text{ g(l)/kg}$	$10^3 x(1)$
298.15	2.1	2.7	3.9

## REFERENCES

1. Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, 121, Part II, 2256-63.
2. Kuroda, T. cf. *Chem. Zentralbl.* 1926, I, 3610.
3. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, 54(1), 55-71.
4. Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, 2, 481-8.
5. Robinson, R. A.; Stokes, R. H. "Electrolyte Solutions"; Butterworths: London, 1970; p 533.

## COMPONENTS:

(1) 4-Chlorophenol;  $C_6H_5ClO$ ;  
[106-48-9]

(2) Water;  $H_2O$ ; [7732-18-5]

## EVALUATOR:

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

November 1979.

## CRITICAL EVALUATION: (Continued)

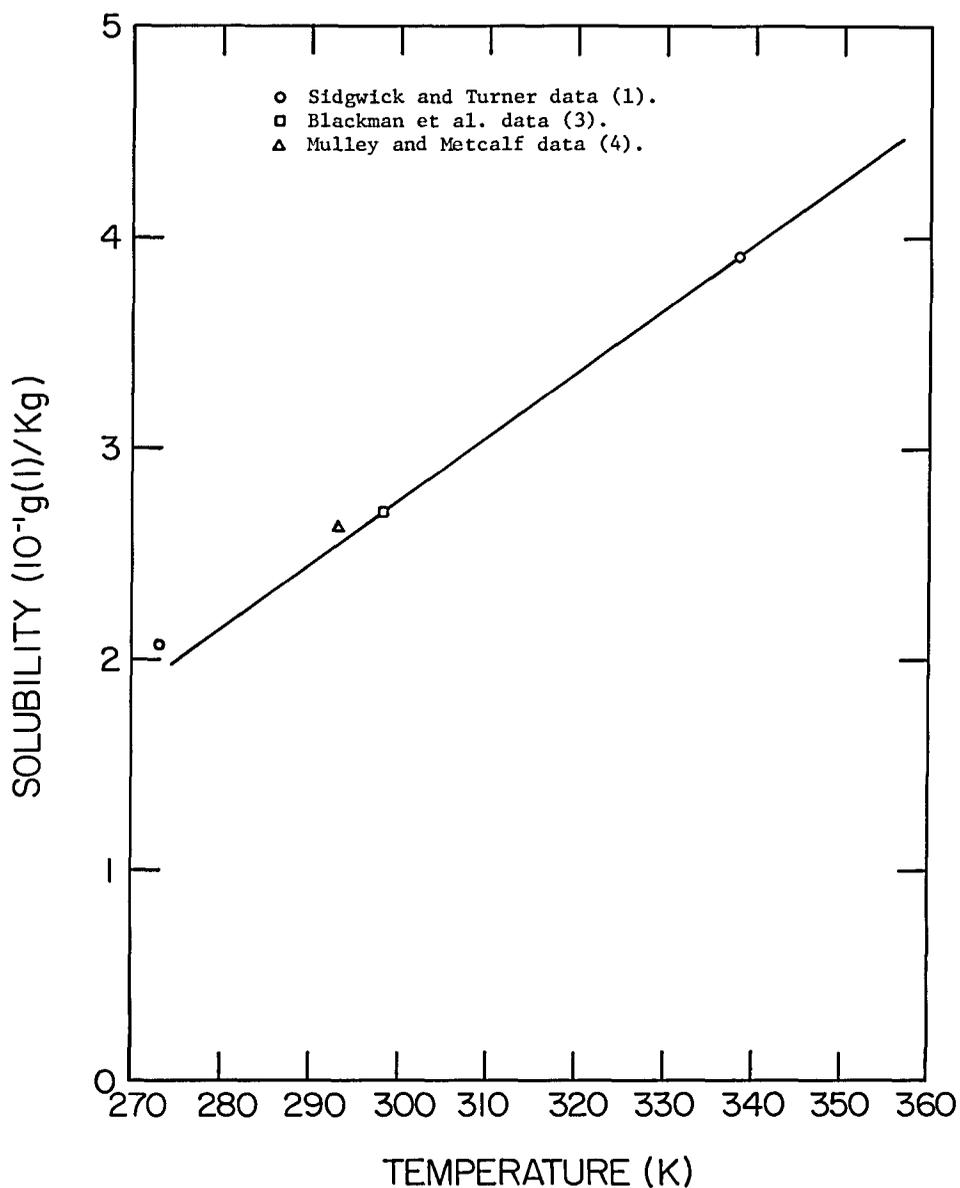


Figure 1. Solubility of 4-chlorophenol in water versus Absolute temperature.

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) 4-Chlorophenol; $C_6H_5ClO$ ; [106-48-9] (2) Water; $H_2O$ ; [7732-18-5]		Sidgwick, N. V.; Turner, S. L. <i>J. Chem. Soc.</i> <u>1922</u> , 121, Part II, 2256-63.	
VARIABLES:		PREPARED BY:	
Temperature: -0.2 - 128.7°C		A. Vesala	
EXPERIMENTAL VALUES:			
t/°C	$10^{-2}g(l)/kg$	mol(l)/kg	$10\alpha(1)$
-0.2	0.207	0.1610	0.02953
0.5	8.892	6.9168	5.2934
5.5	8.619	6.7044	4.6656
6.2	9.248	7.1937	6.3282
11.0	9.448	7.3493	7.0576
14.2	9.570	7.4442	7.5722
17.0	8.542	6.6445	4.5086
18.0	9.682	7.5313	8.1013
19.5	9.729	7.5678	8.3419
35.5	8.402	6.5356	4.2424
41.0	10.00	7.7787	10.0
65.0	0.391	0.3041	0.05670
97.0	7.403	5.7585	2.8545
Continued ...			
AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
The solubility versus temperature measurements were made by the so called synthetic method which involved the mixing of known masses of solute and solvent and the testing of miscibility with temperature. A bracketing procedure was applied. In this method, two adjustable thermostats, one above and the other below the solubility temperature, were used. The contents of sample tubes in the two thermostat baths were observed to maintain one homogeneous and the other heterogeneous as the temperature interval between the two thermostats was reduced by successive steps.		$C_6H_5ClO$ : Synthesized from 4-chloroaniline, melting point of the product 40.9°C.	
		$H_2O$ : Source and purity not specified.	
		ESTIMATED ERROR:	
		REFERENCES:	

COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) 4-Chlorophenol; $C_6H_5ClO$ ; [106-48-9]		Sidgwick, N. V.; Turner, S. L. <i>J. Chem. Soc.</i> <u>1922</u> , <i>121</i> , Part II, 2256-63.	
(2) Water; $H_2O$ ; [7732-18-5]			
EXPERIMENTAL VALUES:		Continued ....	
$t/^\circ C$	$10^{-2} g(1)/kg$	$mol(1)/kg$	$10\alpha(1)$
107.7	6.936	5.3953	2.4083
113.8	1.066	0.82920	0.16446
115.5	6.505	5.0600	2.0687
122.4	5.962	4.6376	1.7144
125.0	2.050	1.5946	0.34876
125.8	5.349	4.1608	1.3880
128.2	2.916	2.2683	0.54540
128.7	4.257	3.3114	0.94104
a. Reported.			
b. Calculated by F. W. Getzen.			
Measurements are shown graphically in Figure 1.			
Continued ...			

COMPONENTS:  (1) 4-Chlorophenol; $C_6H_5ClO$ ; [106-48-9]  (2) Water; $H_2O$ ; [7732-18-5]	ORIGINAL MEASUREMENTS:  Sidgwick, N. V.; Turner, S. L. <i>J. Chem. Soc.</i> 1922, 121, Part II, 2256-63.
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EXPERIMENTAL VALUES: Continued ....

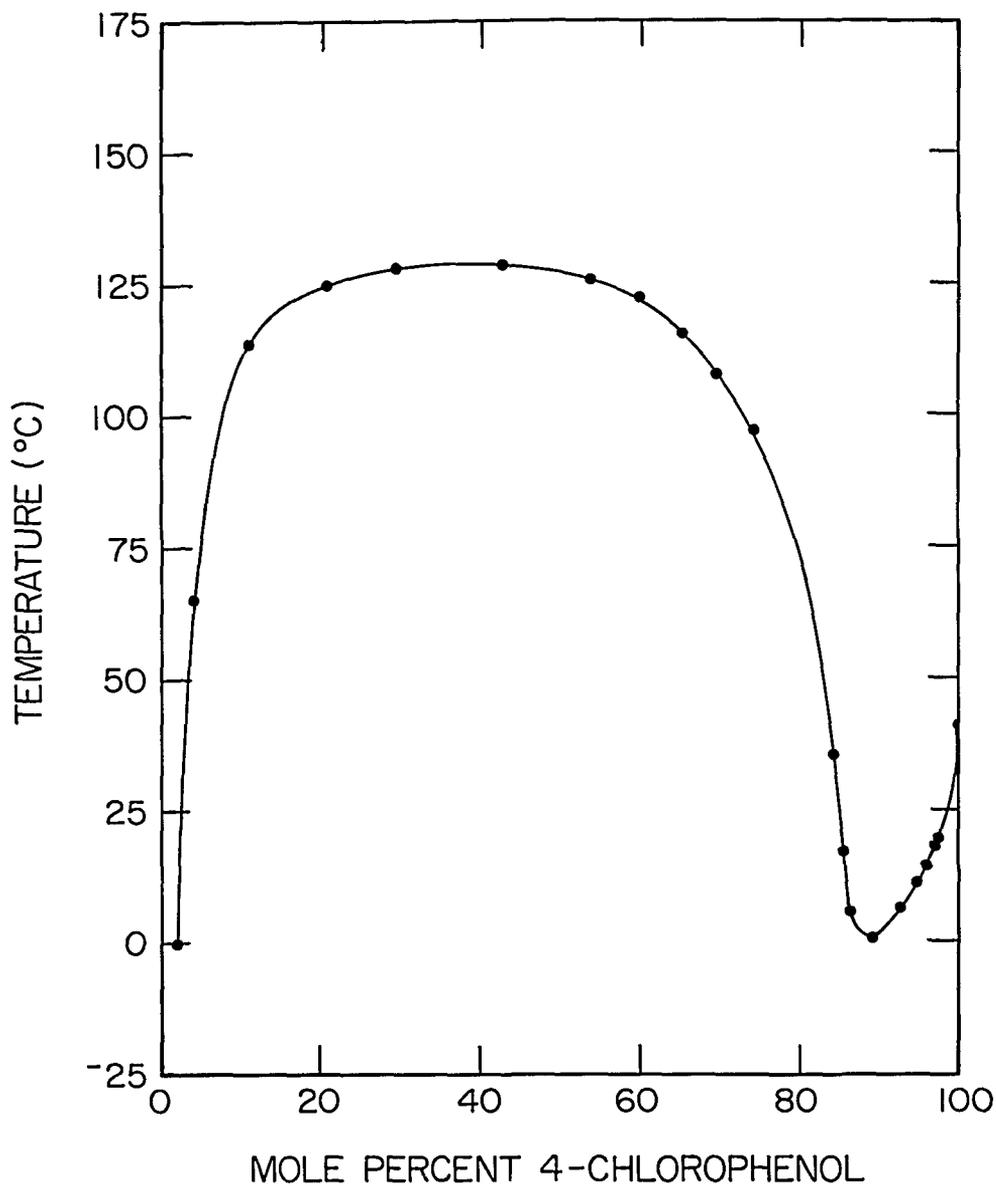


Figure 1. 4-Chlorophenol, water solubility behavior versus Centrigrade temperature.

<b>COMPONENTS:</b> (1) 4-Chlorophenol; $C_6H_5ClO$ ; [106-48-9] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Mulley, B. A.; Metcalf, A. D. <i>Sci. Pharm.</i> <u>1966</u> , 2, 481-8.								
<b>VARIABLES:</b> One temperature	<b>PREPARED BY:</b> A. Vesala								
<b>EXPERIMENTAL VALUES:</b> <table data-bbox="241 483 967 579" 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^{-1}g(1)/dm^3</math> <sup>a</sup></th> <th style="text-align: center;"><math>10mol(1)/dm^3</math> <sup>b</sup></th> <th style="text-align: center;"><math>10^3x(1)</math> <sup>b</sup></th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">2.625</td> <td style="text-align: center;">2.0418</td> <td style="text-align: center;">3.7705</td> </tr> </tbody> </table> <p data-bbox="241 608 618 666">           a. Reported.            b. Calculated by F. W. Getzen.         </p>		$t/^\circ C$	$10^{-1}g(1)/dm^3$ <sup>a</sup>	$10mol(1)/dm^3$ <sup>b</sup>	$10^3x(1)$ <sup>b</sup>	20	2.625	2.0418	3.7705
$t/^\circ C$	$10^{-1}g(1)/dm^3$ <sup>a</sup>	$10mol(1)/dm^3$ <sup>b</sup>	$10^3x(1)$ <sup>b</sup>						
20	2.625	2.0418	3.7705						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> The sample preparation and equilibration procedures were not specified. Saturated solutions were prepared and analyzed spectrophotometrically. Also, duplicate determinations were probably made by a synthetic method described in (1).	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_5ClO$ : Commercial reagent, manufacturer not specified, suitably purified until physical constants corresponded with literature values. The reagent was dried in a desiccator for two days before use.  $H_2O$ : Source and purity not specified.								
<b>ESTIMATED ERROR:</b> Solubility: <4% (estimated here on the basis of the deviations in the reported values).									
<b>REFERENCES:</b> 1. Mulley, B. A.; Metcalf, A. D. <i>J. Pharm. Pharmacol.</i> <u>1956</u> , 8, 774.									

<b>COMPONENTS:</b> (1) 4-Chlorophenol; $C_6H_5ClO$ ; [106-48-9] (2) Water; $H_2O$ ; [7732-18-5]	<b>ORIGINAL MEASUREMENTS:</b> Blackman, G. E.; Parke, M. H.; Garton, G. <i>Arch. Biochem. Biophys.</i> 1955, 54(1), 55-71.								
<b>VARIABLES:</b> One temperature One pH: 5.1	<b>PREPARED BY:</b> A. Vesala								
<b>EXPERIMENTAL VALUES:</b> <table border="1" data-bbox="188 487 907 586"> <thead> <tr> <th><math>t/^\circ C</math></th> <th><math>10^{-1}g(1)/dm^3</math> <sup>a</sup></th> <th><math>10mol(1)/dm^3</math> <sup>b</sup></th> <th><math>10^3x(1)</math> <sup>a</sup></th> </tr> </thead> <tbody> <tr> <td>25</td> <td>2.70</td> <td>2.1</td> <td>3.89</td> </tr> </tbody> </table> <p data-bbox="188 626 651 675">           a. Calculated by F. W. Getzen.            b. Reported value measured at pH 5.1.         </p>		$t/^\circ C$	$10^{-1}g(1)/dm^3$ <sup>a</sup>	$10mol(1)/dm^3$ <sup>b</sup>	$10^3x(1)$ <sup>a</sup>	25	2.70	2.1	3.89
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25	2.70	2.1	3.89						
<b>AUXILIARY INFORMATION</b>									
<b>METHOD/APPARATUS/PROCEDURE:</b> The samples were equilibrated in a thermostat bath with temporary shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	<b>SOURCE AND PURITY OF MATERIALS:</b> $C_6H_5ClO$ : Probably a commercial reagent, source and purity not specified. $H_2O$ : Distilled.  <b>ESTIMATED ERROR:</b> Solubility: <5% (evaluated on the basis of the reported results of the two techniques of analysis).  <b>REFERENCES:</b>								