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|--|---|
| <p>COMPONENTS:</p> <p>(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8]</p> <p>(2) Water; H_2O; [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:

The mutual solubility of 2-chlorophenol and water was investigated by Sidgwick and Turner (1) in 1922. While the measurements seem to be performed with care and the method, which involved classical synthetic procedures based upon gravimetry, gives relatively accurate results, there is some difficulty in resolving a solubility value at 298 K from the data. This circumstance arises because of the range of temperatures over which the measurements were made which makes the interpolation of the data inaccurate. Also, some of the data values scatter considerably in the low temperature range.

Kuroda (2) found the solubility of 2-chlorophenol in water to be in the order of 2 percent at room temperature (291 K). Better agreement is obtained when the data of Mulley and Metcalf (3) are compared with the values of Sidgwick and Turner. The 24.65 g(l)/dm^3 value of Mulley and Metcalf corresponds to a value of 25 g(l)/kg (assuming a density of 1.0 g/cm^3 for the solution).

The more recent work of Banerjee et al. (4) gives a value of $88.3 \text{ mmol(l)/dm}^3$ corresponding to approximately 11 g(l)/kg , a value that does not agree well with the earlier values. One possible reason for this lack of agreement may be associated with the use of a radiochemical method of analysis by Banerjee et al. For instance, a systematic error could have resulted from radiochemical impurities of the substrate. In any event, the lack of relevant information makes an evaluation here too speculative. The available experimental data are shown in Figure 1.

It should be mentioned that the pH of the solutions exerts a considerable influence on the solubility values of those solutes such as 2-chlorophenol capable of protolytic action. Here it is assumed that the reported solubilities refer to the pH values which prevail in the saturated solutions of 2-chlorophenol in water.

No more than a tentative value can be assigned to the solubility of 2-chlorophenol in water. The following value has been obtained from the data shown in Figure 1 by a graphical interpolation:

| T/K | 10 mol(l)/dm^3 | 10^{-1} g(l)/kg | $10^3 x(1)$ |
|--------|--------------------------|---------------------------|-------------|
| 298.15 | 1.6 | 2. | 2.9 |

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. Mulley, R. A.; Metcalf, A. D. *Sci. Pharm.* 1966, 2, 481-8.
4. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, 14(10), 1227-9.

COMPONENTS:

- (1) 2-Chlorophenol; C_6H_5ClO ;
[95-57-8]
- (2) Water; H_2O ; [7732-18-5]

EVALUATOR:

A. Vesala, Department of Chemistry and
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September 1982.

CRITICAL EVALUATION: (Continued)

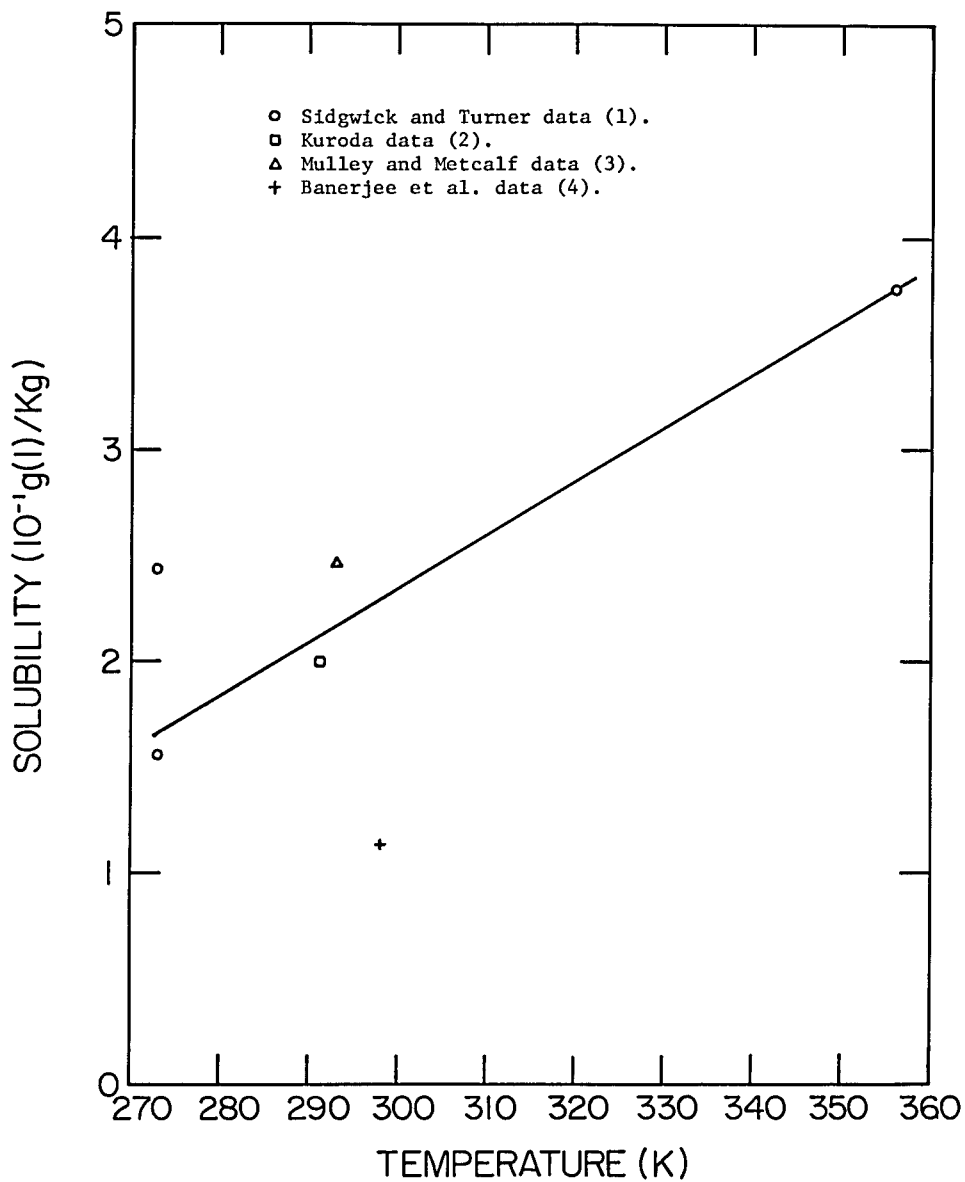


Figure 1. Solubility of 2-chlorophenol in water versus Absolute temperature.

| COMPONENTS: | | ORIGINAL MEASUREMENTS: | |
|---|---------------------------------------|---|---------------------|
| (1) 2-Chlorophenol; C ₆ H ₅ ClO; [95-57-8] (2) Water; H ₂ O; [7732-18-5] | | Sidgwick, N. V.; Turner, S. L. <i>J. Chem. Soc.</i> <u>1922</u> , <i>121</i> , Part II, 2256-63. | |
| VARIABLES: | | PREPARED BY: | |
| Temperature: -8.2 - 173.0°C | | A. Vesala | |
| EXPERIMENTAL VALUES: | | | |
| t/°C | 10 ⁻² g(1)/kg ^a | mol(1)/kg ^b | 10x(1) ^b |
| -8.2 | 9.220 | 7.1719 | 6.2357 |
| -8.0 | 9.087 | 7.0685 | 5.8243 |
| -6.0 | 9.393 | 7.3065 | 6.8440 |
| -5.0 | 8.962 | 6.9712 | 5.4750 |
| -4.0 | 8.925 | 6.9424 | 5.3778 |
| -2.0 | 8.773 | 6.8242 | 5.0050 |
| -1.5 | 9.676 | 7.5266 | 8.0714 |
| -0.30 | 0.244 | 0.1898 | 0.03493 |
| -0.20 | 0.156 | 0.1213 | 0.02216 |
| 2.0 | 9.839 | 7.6534 | 8.9544 |
| 7.0 | 10.00 | 7.7787 | 10.0 |
| 82.9 | 0.376 | 0.2925 | 0.05445 |
| 91.5 | 8.590 | 6.6819 | 4.6056 |
| 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 were reduced by successive steps. | | C ₆ H ₅ ClO: Synthesized by the chlorination of phenol in carbon tetrachloride, purified as described in Ref. 1, no criterions of the purity given. | |
| | | H ₂ O: Source and purity not specified. | |
| | | ESTIMATED ERROR: | |
| | | REFERENCES: | |
| | | 1. Wohleben, W. J. <i>Ber. Dtsch. Chem. Ges.</i> <u>1909</u> , <i>42</i> , 4370. | |

| COMPONENTS: | | ORIGINAL MEASUREMENTS: | |
|--|---------------------------------------|--|---------------------|
| (1) 2-Chlorophenol; C ₆ H ₅ ClO; [95-57-8] | | Sidgwick, N. V.; Turner, S. L. <i>J. Chem. Soc.</i> <u>1922</u> , 121, Part II, 2256-63. | |
| (2) Water; H ₂ O; [7732-18-5] | | | |
| EXPERIMENTAL VALUES: continued | | | |
| t/°C | 10 ⁻² g(1)/kg ^a | mol(1)/kg ^b | 10x(1) ^b |
| 106.3 | 0.512 | 0.3983 | 0.07506 |
| 118.9 | 8.282 | 6.4423 | 4.0319 |
| 156.6 | 7.062 | 5.4933 | 2.5197 |
| 159.1 | 1.358 | 1.0563 | 0.21547 |
| 165.8 | 1.695 | 1.3185 | 0.27806 |
| 166.2 | 6.072 | 4.7232 | 1.7806 |
| 170.1 | 5.495 | 4.2744 | 1.4598 |
| 170.7 | 2.259 | 1.7572 | 0.39289 |
| 172.9 | 4.504 | 3.5035 | 1.0301 |
| 173.0 | 3.300 | 2.5670 | 0.64568 |
| <p>a. Reported.</p> <p>b. Calculated by F. W. Getzen.</p> <p>Measurements are shown graphically in Figure 1.</p> | | | |
| Continued ... | | | |

COMPONENTS:

(1) 2-Chlorophenol; C_6H_5ClO ; [95-57-8](2) Water; H_2O ; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, 121, Part II, 2256-63.

EXPERIMENTAL VALUES:

Continued

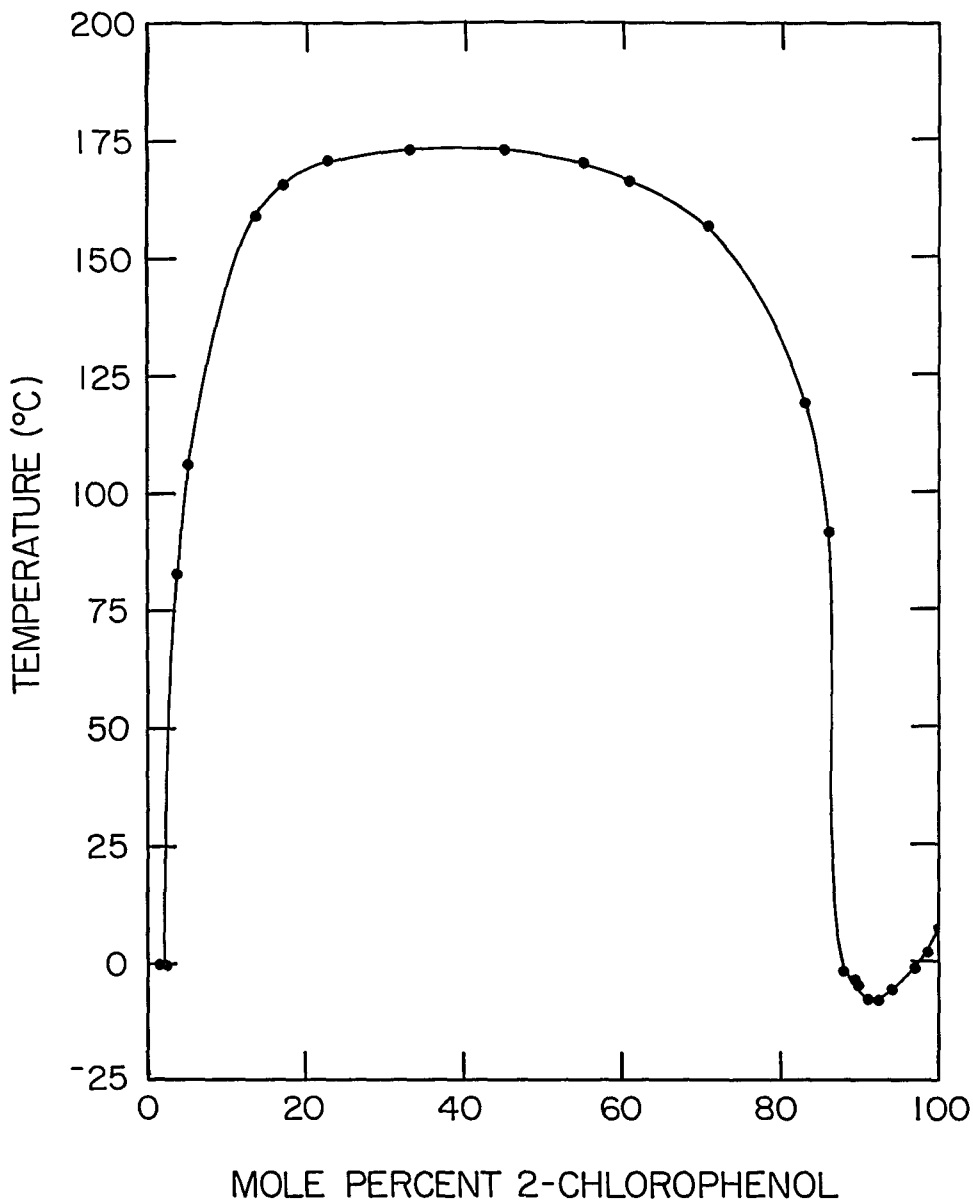


Figure 1. 2-Chlorophenol, water solubility behavior versus Centigrade temperature.

| COMPONENTS: (1) 2-Chlorophenol; C_6H_5ClO ; [95-57-8] (2) Water; H_2O ; [7732-18-5] | ORIGINAL MEASUREMENTS: Mulley, B. A.; Metcalf, A. D. <i>Sci. Pharm.</i> <u>1966</u> , 2, 481-8. | | | | | | | | |
|---|--|-------------------|----------------------|-------------------|--------------|----|-------|--------|--------|
| VARIABLES: One temperature | PREPARED BY: A. Vesala | | | | | | | | |
| EXPERIMENTAL VALUES: <table data-bbox="229 479 948 566" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">t/°C</th> <th style="text-align: center;">$10^{-1}g(1)/dm^3$ a</th> <th style="text-align: center;">$10mol(1)/dm^3$ b</th> <th style="text-align: center;">$10^3x(1)$ b</th> </tr> </thead> <tbody> <tr> <td style="text-align: center;">20</td> <td style="text-align: center;">2.465</td> <td style="text-align: center;">1.9174</td> <td style="text-align: center;">3.5357</td> </tr> </tbody> </table> <p data-bbox="229 614 606 658"> a. Reported. b. Calculated by F. W. Getzen. </p> | | t/°C | $10^{-1}g(1)/dm^3$ a | $10mol(1)/dm^3$ b | $10^3x(1)$ b | 20 | 2.465 | 1.9174 | 3.5357 |
| t/°C | $10^{-1}g(1)/dm^3$ a | $10mol(1)/dm^3$ b | $10^3x(1)$ b | | | | | | |
| 20 | 2.465 | 1.9174 | 3.5357 | | | | | | |
| AUXILIARY INFORMATION | | | | | | | | | |
| METHOD/APPARATUS/PROCEDURE: <p>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).</p> | SOURCE AND PURITY OF MATERIALS: <p>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.</p> <p>H_2O: Source and purity not specified.</p> ESTIMATED ERROR: <p>Solubility: <4% (estimated here on the basis of the deviations in the reported values).</p> REFERENCES: <p>1. Mulley, B. A.; Metcalf, A. D. <i>J. Pharm. Pharmacol.</i> <u>1956</u>, 8, 774.</p> | | | | | | | | |

| COMPONENTS: (1) 2-Chlorophenol; C ₆ H ₅ ClO; [95-57-8] (2) Water; H ₂ O; [7732-18-5] | ORIGINAL MEASUREMENTS: Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. <i>Environm. Sci. Techn.</i> <u>1980</u> , <i>14</i> (10), 1227-9. | | | | | | | | |
|---|--|--|---|--|------------------------|----|-------|------|-------|
| VARIABLES: One temperature | PREPARED BY: A. Vesala | | | | | | | | |
| EXPERIMENTAL VALUES: <table style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">t/°C</th> <th style="text-align: center;">10⁻¹g(1)/dm³ a</th> <th style="text-align: center;">10²mol(1)/dm³ b</th> <th style="text-align: center;">10³x(1) a</th> </tr> </thead> <tbody> <tr> <td style="text-align: left;">25</td> <td style="text-align: center;">1.135</td> <td style="text-align: center;">8.83</td> <td style="text-align: center;">1.611</td> </tr> </tbody> </table> <p>a. Calculated by F. W. Getzen. b. Reported.</p> | | t/°C | 10 ⁻¹ g(1)/dm ³ a | 10 ² mol(1)/dm ³ b | 10 ³ x(1) a | 25 | 1.135 | 8.83 | 1.611 |
| t/°C | 10 ⁻¹ g(1)/dm ³ a | 10 ² mol(1)/dm ³ b | 10 ³ x(1) a | | | | | | |
| 25 | 1.135 | 8.83 | 1.611 | | | | | | |
| AUXILIARY INFORMATION | | | | | | | | | |
| METHOD/APPARATUS/PROCEDURE: The equilibrations were performed in sealed stainless steel centrifuge tubes with constant or intermittent shaking. The equilibration was generally complete within 1 week. The mixture was then centrifuged for 60 minutes after which aliquots of the solution were removed for analysis either by a pipet or a syringe. Liquid scintillation counting with ¹⁴ C-labeled solute was employed in solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate. | SOURCE AND PURITY OF MATERIALS: C ₆ H ₅ ClO: Commercial reagent, the ¹⁴ C-labeled compound was purchased by NEN, the nonlabeled one by Aldrich. H ₂ O: Distilled. ESTIMATED ERROR: Solubility: ±0.5% (std. deviation estimated by authors). Temperature: ±0.2 K (equilibration) ±0.3 K (centrifugation)† REFERENCES: | | | | | | | | |