COMPONENTS:	EVALUATOR:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The earliest and most thorough investigation of the mutual solubilities of 3-chlorophenol and water was done in 1922 by Sidgwick and Turner (1). Their measurements of solubilities were accomplished using the so called synthetic method, i.e., the determination of solubilities from weighed masses of 3-chlorophenol and water at the appropriate temperatures. They reported no directly measured values for the solubilities at 298 K, the nearest measured values were obtained at temperatures relatively far from room temperature (276 K and 359 K), which makes an accurate interpolation difficult.

The solubilities of three isomers of monochlorophenols in water have been determined by Kuroda (2) who reported the magnitude of this solubility to be 2 percent. More support for the work of Sidgwick and Turner is provided by the value measured by Mulley and Metcalf (3) at 293.15 K. Their result of 22.4 g(1)/dm^3 (which corresponds to 22.4 g(1)/kg assuming a density of 1.0 for the solution) agrees quite satisfactorily with the values of Sidgwick and Turner as shown in Figure 1. There are not, however, enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative.

It should be mentioned that the pH of the solutions exerts a considerable influence on the solubility values of those solutes such as 3-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 3-chlorophenol in water.

No more than a tentative value can be assigned to the solubility of 3-chlorophenol in water 298.15 K as follows:

T/K	$10\,\mathrm{mol(1)/dm^3}$	$10^{-1}\,\mathrm{g(1)/kg}$	$10^3 x(1)$
298.15	1.7	2.2	3.2

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; B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, *2*, 481-8.

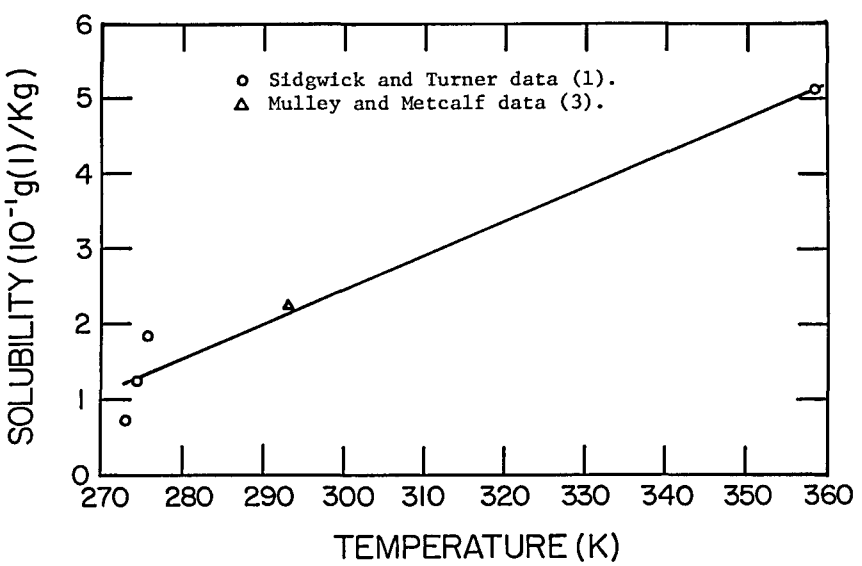

Figure 1. Solubility of 3-chlorophenol in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.
VARIABLES: Temperature: -17.0 - 130.8°C	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	10x(1) [b]
-17.0	9.223	7.1743	6.2455
-13.2	9.173	7.1354	6.0852
-8.2	9.011	7.0093	5.6080
-4.8	8.866	6.8966	5.2282
-0.9	8.487	6.6017	4.4012
-0.18	0.073	0.0568	0.0103
1.2	0.125	0.09723	0.01771
2.5	0.185	0.1439	0.02635
3.2	8.487	6.6017	4.4012
4.5	8.719	6.7822	4.8819
10.8	9.223	7.1742	6.2455
11.8	8.290	6.4485	4.0455
17.0	9.510	7.3975	7.3117

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 1-chloro-3-nitrobenzene by reduction and diazotisation. Melting point 32.5°C. H_2O: No specifications given.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....

t/°C	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	10x(1) [b]
22.2	9.711	7.5538	8.2484
23.1	8.230	6.4018	3.9453
32.5	10.00	7.7787	10.0
85.25	0.512	0.3983	0.07506
109.8	7.123	5.5407	2.5759
118.0	1.113	0.86576	0.17248
123.0	1.356	1.0548	0.21511
127.5	1.784	1.3877	0.29531
129.1	5.565	4.3288	1.4955
130.5	4.612	3.5875	1.0711
130.7	3.889	3.0251	0.81882
130.8	3.202	2.4907	0.61922

a. Reported.
b. Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

Continued ...

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.
(2) Water; H_2O; [7732-18-5]	

EXPERIMENTAL VALUES: Continued ....

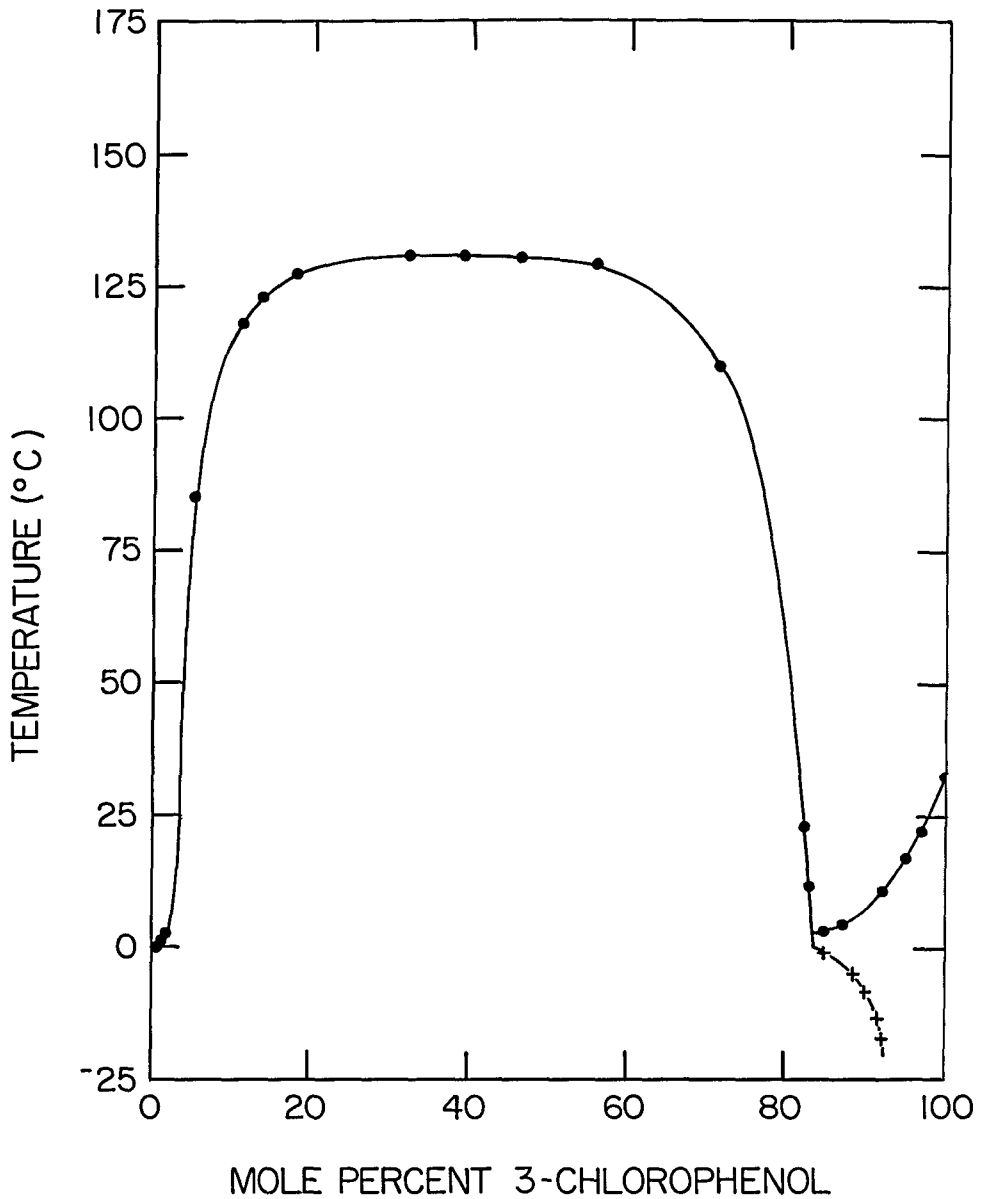

Figure 1. 3-Chlorophenol, water solubility behavior versus Centrigrade temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-01] (2) Water; H_2O; [7732-18-5]	Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, *2*, 481-8.
VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^{-1}g(1)/dm^3 a	10mol(1)/dm^3 b	$10^3 x$(1) b
20	2.242	1.7439	3.2095

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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).

SOURCE AND PURITY OF MATERIALS:

C_6H_5ClO: Commercial reagent, 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.

ESTIMATED ERROR:

Solubility: <4% (estimated here on the basis of the deviations in the values reported for the solubility of this phenol in cetomacrogol solns).

REFERENCES:

1. Mulley, B. A.; Metcalf, A. D. *J. Pharm. Pharmacol.* 1956, *8*, 774.