Temperature Dependence of the Aqueous Solubility of Selected Chlorobenzenes and Chlorotoluenes

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The aqueous solubilities of chlorobenzene, 1,2- and 1,3-dichlorobenzene, 1,2,4-trichlorobenzene, toluene, 2-, 3-, and 4-chlorotoluene, 2,4- and 2,6-dichlorotoluene, 2,4,5-trichlorotoluene, and pentachlorotoluene are reported over the temperature range (5−45) °C.

Introduction

In this study, the aqueous solubilities of selected chlorobenzenes and chlorotoluenes are reported over the temperature range (5−45) °C, and where possible, the enthalpies of solution can be estimated. These compounds are of interest industrially and environmentally, being among the products obtained when chlorine, used for bleaching or disinfection, reacts with aromatic substances present in natural organic (humic) matter and in process streams of the pulp and paper industry.[1] These compounds constitute a series which increases in hydrophobicity with increasing chlorination and is of interest thermodynamically and for establishing quantitative structure property relationships (QSPRs) and quantitative structure activity relationships (QSARs).

Numerous studies have reported the aqueous solubilities of the chlorobenzenes and toluene at 25 °C, but few have reported their solubilities as a function of temperature.[2−4] There are fewer data for chlorotoluenes; specifically only the solubility of 2-chlorotoluene and 4-chlorotoluene have been reported (see Table 1). The present study reports the solubility of 12 substances at five temperatures ranging from (5 to 45) °C. Data for 1,2,4-trichlorobenzene have not been reported previously, and all data for chlorotoluenes represent new measurements.

Experimental Section

Chemicals. Chlorobenzene (99%), 1,2-dichlorobenzene (98%), 1,3-dichlorobenzene (98%), 1,2,4-trichlorobenzene (99%), 2-chlorotoluene (99%), 3-chlorotoluene (98%), 4-chlorotoluene (98%), 2,4-dichlorotoluene (99%), and 2,6-dichlorotoluene (99+%) were obtained from Aldrich Chemical Co. 2,4,5-Trichlorotoluene (99.9%) and pentachlorotoluene (95+%) were purchased from Ultra Scientific, North Kingstown, RI, and were used without further purification. HPLC grade hexane and toluene were obtained from Caledon Laboratories, Georgetown, ON. ACS grade acetone was obtained from Fisher Scientific. Chromosorb 750 and Chromosorb W, 30/60 mesh (Johnson-Manville), were obtained from Chromatographic Specialties, Bellvelle, ON. Double distilled water or Milli-Q ultrapure deionized water (Millpore Corp., Milford, MA) was used for all experiments.

Methods: ***Aqueous Solubility***. Two methods were used depending on the solubility.

(1) A shake flask or batch contacting equilibration method was used for the more soluble chlorobenzenes and the mono- and dichlorotoluenes. Saturated solutions were prepared by adding an excess amount of chemical of interest to 125 mL or 250 mL Erlenmeyer flasks containing distilled water. The flasks were shaken gently by a wrist-action shaker or stirred by a magnetic stirrer for 24 h, and allowed to settle in the temperature bath, Neslab Model RTE-8, for at least 48 h at the desired temperature (±0.5 °C) before analysis by gas chromatography.

(2) A generator column method was used for the solubility determination of 2,4,5-trichlorotoluene. Saturated aqueous solutions were prepared by pumping water through 0.64 cm o.d. by 30 cm long stainless steel tubing (generator column), with an Eldex Pump Model B-100-S, at a flow rate of 2 mL/min. This column was packed with prewashed (acetone, hexane, and toluene) Chromosorb W or Chromosorb 750, 30/60 mesh, and coated with 0.5−2.0% by mass of chemical of interest. It was thermostated with an Alltech water jacket, to ±0.2 °C with a Neslab refrigerated circulating bath Model Endocal RTE-5. The saturated solution was collected in a weighed separatory funnel and extracted with hexane. The hexane extract was then analyzed by gas chromatography.

A Hewlett-Packard Model 5700A GC equipped with a flame ionization detector or a Hewlett-Packard Model 5890 series II GC equipped with an electron capture and a flame ionization detector was used for analysis of the hexane extracts. A J&W Durabond DB-1 column (30 m long by 0.53 mm o.d. Megabore fused silica capillary column) or a J&W Durabond DB-17 column (30 m long by 0.32 mm o.d. fused silica capillary column) was used. The injection port temperature was at 300 °C, the detector was at 320 °C, and the GC oven was in isothermal mode between 90 and 180 °C. Peak areas were integrated by a Hewlett-Packard Model 3300 or 3396A integrator-recorder. Calibration standards were prepared with known amounts of chemical in hexane with subsequent serial dilution.

Results

The solubility data for chlorobenzenes (CBs) and chlorotoluenes (CTs) at 25 °C are given in Table 1 with the

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Table 1. Aqueous Solubilities ($g \cdot m^{-3}$) and Standard Deviations of Selected Chlorobenzenes and Chlorotoluenes at 25 °C

compound	shake flask	literature values at 25 °C
chlorobenzene	496 ± 23	488(30°);[9] 500;[10] 463;[11] 472.2;[12] 503;[13] (420, 480, 450);[14] 295;[15,16] 499;[17] 502;[18] 348;[19] 428[20]
1,2-dichlorobenzene	149 ± 8.2	145;[21] 79;[22] 148 (20 °C);[23] 92.8;[13] 128;[14] 155.8;[24,25] 99.1;[26] 154;[27] 92.3;[15,16] 137;[18] 169[19]
1,3-dichlorobenzene	126 ± 6.1	123;[21] 103;[11] 119.5;[13] 131;[23] (123, 144, 149);[14] 133.5;[24] 134;[27] 124.5;[15,16] 143;[18] 150[19]
1,2,4-trichlorobenzene	36.5 ± 0.36	34.7;[13] 19.4;[26] 48.8;[27] 46.1;[15,16] 31.4;[18] 34.6[28]
toluene	519 ± 5.0	570 (30 °C);[9] 530;[29] 500;[30] 627;[6] 546;[31] 538;[32] 515;[33] 573;[34] 517;[35] 627;[11] 520;[36] 535;[37] 554;[38] 488;[39] 534;[40] 670 (23.5 °C);[41] 507;[42] 557;[43] 526;[44] 579;[15,16] 521;[45] 580;[17] 524;[18] 521;[46] 520;[19] 538;[47] (501, 527, 538−21 °C)[48]
2-chlorotoluene	117 ± 5.1	101;[b] 25.2[51]
3-chlorotoluene	117 ± 2.1	
4-chlorotoluene	123 ± 6.2	106[50,52]
2,4-dichlorotoluene	26.2 ± 2.1	
	25.7 ± 2.16[a]	
2,6-dichlorotoluene	23.3 ± 0.81	
2,4,5-trichlorotoluene	2.33 ± 0.22	
pentachlorotoluene	0.028 ± 0.001	

[a] Data determined by the generator column method. [b] References 49 and 50 and calculated.

Table 2. Aqueous Solubilities of Selected Chlorobenzenes and Chlorotoluenes in the Range (5−45) °C

	aqueous solubility, $S_W/g \cdot m^{-3}$				
compound	5 °C	15 °C	25 °C	35 °C	45 °C
chlorobenzene	496 ± 16	429 ± 13	470 ± 23	538 ± 24	546 ± 33
1,2-dichlorobenzene	127 ± 5.4	132 ± 6.6	149 ± 8.2	162 ± 2.1	204 ± 4.8
1,3-dichlorobenzene	114 ± 6.3	108 ± 2.7	126 ± 6.1	134 ± 2.5	141 ± 7.3
1,2,4-trichlorobenzene	32.9 ± 0.88	28.5 ± 1.40	36.5 ± 0.36	39.8 ± 0.82	46.5 ± 2.1
toluene	540 ± 29	516 ± 16	519 ± 5.0	555 ± 30	632 ± 21
2-chlorotoluene	89.4 ± 3.8	97.1 ± 4.0	117 ± 5.1	128 ± 6.5	132 ± 5.2
3-chlorotoluene	101 ± 7.1	99.3 ± 2.5	117 ± 2.1	113 ± 3.1	128 ± 5.2
4-chlorotoluene	99.0 ± 5.9	103 ± 2.6	123 ± 6.1	136 ± 2.3	153 ± 1.5
2,4-DCT, SF		18.9 ± 0.78	26.2 ± 2.1	30.7 ± 1.1	37.0 ± 1.7
2,4-DCT, Gen.col.	22.3 ± 0.84	23.1 ± 0.14	25.9 ± 2.2	32.0 ± 0.64	36.6 ± 3.4
2,6-DCT	16.7 ± 0.90	19.8 ± 1.3	23.3 ± 0.81	30.1 ± 0.66	33.0 ± 0.012
2,4,5-TCT	1.10 ± 0.063	1.38 ± 0.063	2.33 ± 0.22	3.33 ± 0.26	5.63 ± 0.26
penta-CT			0.028 ± 0.001	0.047 ± 0.004	-

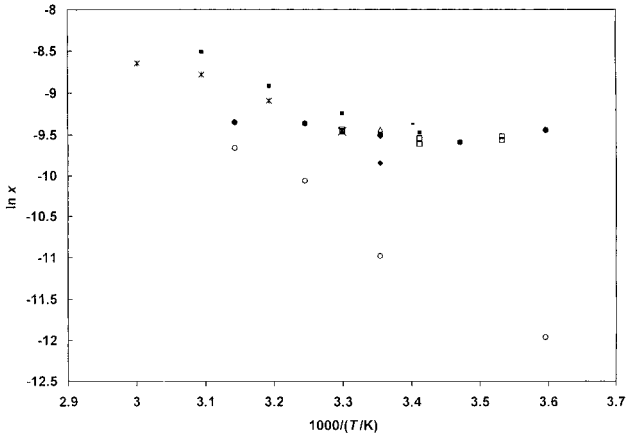

Figure 1. Van't Hoff plot of logarithm mole fraction solubility x of chlorobenzene from this work and previous studies: (●) this work; (×) Gross and Sayler;[9] (△) Andrews and Keefer;[10] (∗) Kisarov;[53] (−) Chey and Calder;[54] (◇) Vesala;[11] (○) Nelson and Smit;[5] (+) Aquan-Yuen et al.;[12] (□) Schwarz and Miller;[14] (■) Cooling et al.;[55] (◆) Boyd et al.[56]

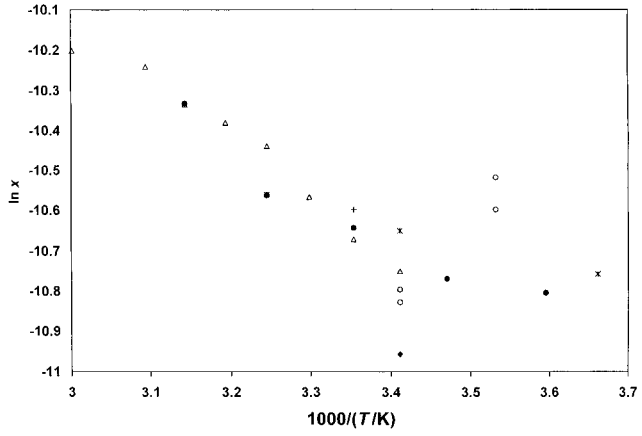

Figure 2. Van't Hoff plot of logarithm mole fraction solubility x of 1,2-dichlorobenzene from this and previous studies: (●) this work; (△) Klemenc and Löw;[21] (∗) Chiou et al.;[23] (○) Schwarz;[41] (+) Banerjee;[18] (◆) Boyd et al.[56]

reported literature values. Table 2 gives the solubilities at various temperatures; the data are also depicted in Figures 1−6. All experimental data points are the mean of more than nine determinations. The estimated precision expressed as a standard deviation is ±5%.

Discussion

The solubilities are generally in good agreement with more recent determinations reported in the literature for chlorobenzenes. The data of Nelson and Smit[5] for chlorobenzene in the temperature range between (5 and 45) °C were found to be lower than those of the other investigators, as discussed by Shaw.[3] There is considerable scatter of the data at low temperature. A minimum in solubility was observed at (18−22) °C for all of the liquid compounds analyzed, indicating a zero enthalpy of solution at that temperature. This well-known phenomenon has been observed for several liquid hydrocarbons. For example, benzene and its alkylated derivatives exhibit a minimum at (18−22) °C.[6−8]

Inspection of the van't Hoff plots shows appreciable curvature. Although enthalpies of solution could be estimated for certain temperature intervals in which a degree of linearity is observed, it is potentially misleading to

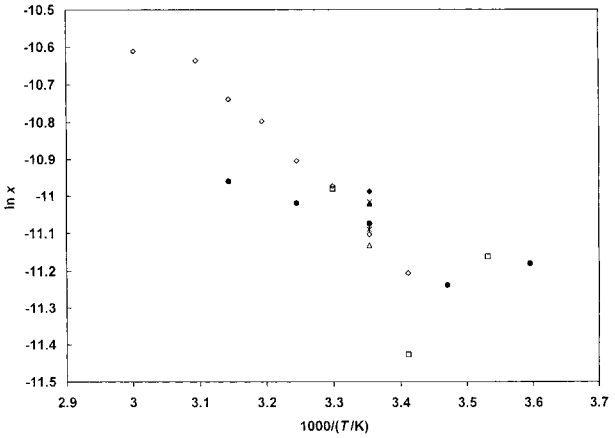

Figure 3. Van't Hoff plot of logarithm mole fraction solubility x of 1,3-dichlorobenzene from this and previous studies: (●) this work; (◇) Klemenc and Löw;[21] (△) Yalkowsky et al.;[13] (□) Schwarz;[14] (▲) Banerjee et al.;[24] (×) Chiou et al.;[27] (∗) Miller et al.;[16] (◆) Boyd et al.[56]

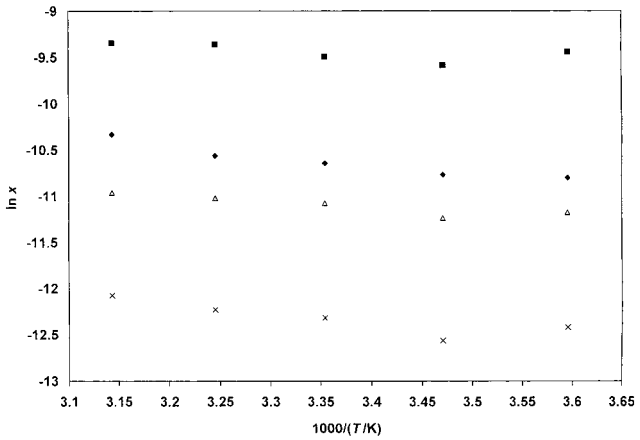

Figure 4. Van't Hoff plot of logarithm mole fraction solubility x of chlorobenzenes: (■) chlorobenzene; (◆) 1,2-dichlorobenzene; (△) 1,3-dichlorobenzene; (×) 1,2,4-trichlorobenzene.

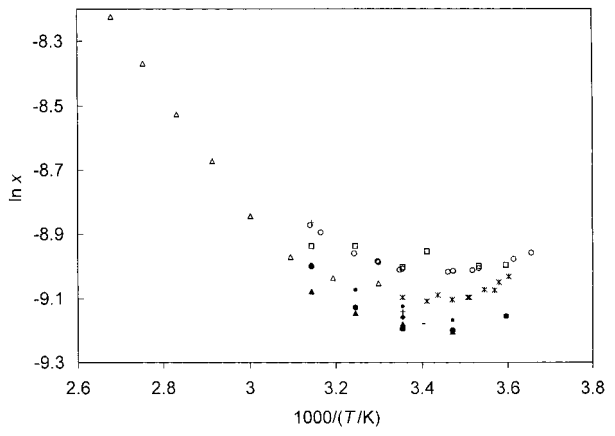

Figure 5. Van't Hoff plot of logarithm mole fraction solubility x of toluene from this and previous studies: (•) this work; (○) Bohon and Claussen;[6] (□) Pierotti and Liabastre;[57] (+) Bradley et al.;[58] (∗) Brown and Wasik;[59] (●) Sanemasa et al.;[43] (▲) Sanemasa et al.;[44] (■) Banerjee;[18] (×) Lo et al.;[19] (◆) Coutant and Keigley;[47] (△) Chen and Wagner;[60] (—) Yang et al.[48]

deduce and report these enthalpies, since they are so variable. No enthalpies of solution are thus reported; however, the data provide a direct estimate of the magnitude of the effect of temperature on solubility.

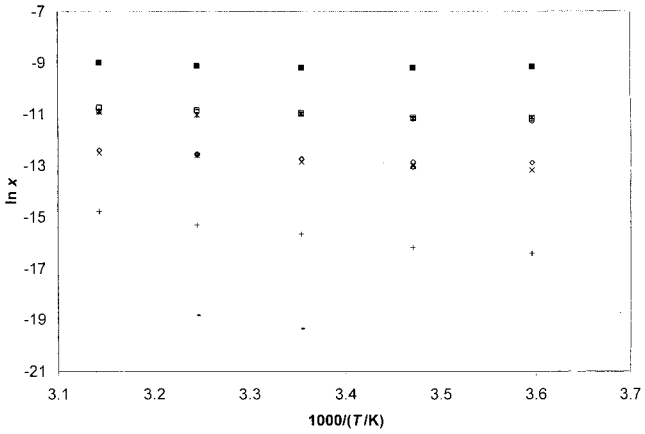

Figure 6. Van't Hoff plot of logarithm mole fraction solubility x of chlorotoluenes: (■) toluene; (○) 2-chlorotoluene; (∗) 3-chlorotoluene; (□) 4-chlorotoluene; (◇) 2,4-dichlorotoluene; (×) 2,6-dichlorotoluene; (+) 2,4,5-trichlorotoluene; (—) pentachlorotoluene.

Conclusion

Data have been reported for the solubilities in water, and their temperature dependence, of a series of chlorobenzenes and chlorotoluenes which will contribute to a more accurate assessment of the environmental partitioning behavior of these and related substances over a range of temperatures.

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