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Solubility of Trioxane in Water

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The solubility of trioxane in water was determined from 20 to 55 °C. The experimental data have been correlated using the UNIQUAC equation for the activity coefficient.

Introduction

The industrial interest for aqueous mixtures of trioxane has been discussed in a previous paper (*1*). Despite the importance of the considered mixture, very few data are available (*2*) for solubilities.

We therefore investigated experimentally the solubility of trioxane in water from 20 to 55 °C.

Experimental Section

Trioxane was obtained from Aldrich Chemical Co. Its claimed purity was 99+%. Bidistilled water was used.

Mixtures of water and an excess of trioxane were equilibrated at several temperatures by stirring in a stoppered flask thermostated by circulating water. After 2 h, the sitrring was stopped, and after decanting, portions of solution were analyzed.

The analyses were carried out by gas chromatography (Perkin-Elmer 8310 with an LC-100 integrator), after calibration with gravimetrically prepared standard solutions. A thermoconducibility detector was used, together with a 6-ft, 1/8-in.-o.d. stainless steel separation column, packed with Hayesep T, 80–100 mesh. The injector, oven, and detector temperatures were set at 413, 453, and 473 K, respectively. The carrier gas was helium, with a flow rate of 25 cm^3/min. Reported values are means of data from 2–4 replications.

Results and Discussion

The measured solubilities are reported in Table I. The data exhibit strong deviations from ideal behavior. The experimental data were correlated, according to Prausnitz et al. (*3*), using the equation

$$\ln \gamma_2 x_2 = -\frac{\Delta s^f}{R}\left[\frac{T_m}{T} - 1\right] \qquad (1)$$

where

$$\Delta S^f = \frac{\Delta h^f}{T_m} \qquad (2)$$

and

$$\ln \gamma_2 = \ln \frac{\phi_2}{x_2} + 1 - \frac{\phi_2}{x_2} + 5q_2\left[\ln \frac{\theta_2}{\phi_2} + \frac{\phi_2}{\theta_2} - 1\right] - q_2 \ln(\theta_2 + \theta_1\tau_{12}) + q_2\theta_1\left[\frac{\tau_{12}}{\theta_2 + \theta_1\tau_{12}} - \frac{\tau_{21}}{\theta_1 + \theta_2\tau_{21}}\right] \qquad (3)$$

with

$$\tau_{12} = \exp(-a_{12}/T) \qquad (4)$$

$$\tau_{21} = \exp(-a_{21}/T) \qquad (5)$$

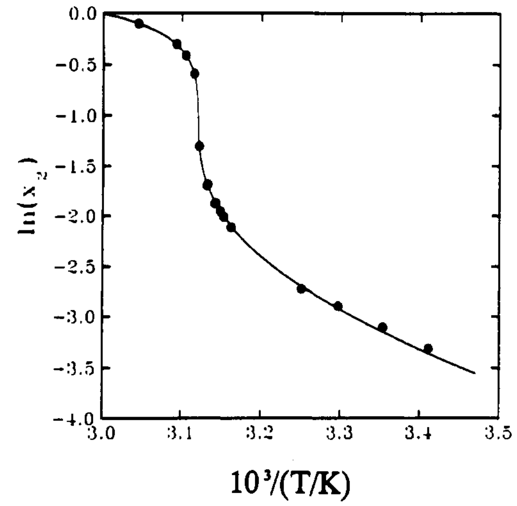

Figure 1. Solubility of trioxane in water: (—) calculated; (●) experimental points.

Table I. Solubility of Trioxane (x_2) in Water

t/°C	x_2	t/°C	x_2
20.00	0.0365	45.10	0.1531
25.00	0.0448	46.00	0.1862
30.10	0.0552	46.10	0.1833
34.45	0.0655	47.10	0.2721
43.00	0.1210	47.80	0.5545
44.00	0.1343	48.95	0.6641
44.40	0.1417	50.20	0.7401
45.00	0.1537	55.30	0.9056

and

$$\phi_i = \frac{r_i x_i}{r_1 x_1 + r_2 x_2} \qquad (6)$$

$$\theta_i = \frac{q_i x_i}{q_1 x_1 + q_2 x_2} \qquad (7)$$

The r and q UNIQUAC parameters ($r_1 = 0.92$, $q_1 = 1.40$, $r_2 = 2.76$, $q_2 = 2.34$) were taken from DECHEMA (*4*). The enthalpy of fusion, $\Delta h^f = 15\,105$ J/mol, and the melting point, $T_m = 333.44$ K, where taken from Van Bommel et al. (*5*). The obtained parameters are

$$a_{12}(K) = 16.41 - 0.2939T \qquad (8)$$

$$a_{21}(K) = 1422.40 - 3.0581T \qquad (9)$$

The average absolute deviation on x_2 was 0.0021. Figure 1 shows a comparison between calculated and experimental solubilities.

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