Vapor−Liquid Equilibrium of Durene in Methanol or Ethanol

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The vapor−liquid equilibrium behavior of durene in methanol or ethanol was measured at atmospheric pressure (98 kPa) in the dilute composition range of durene with a recirculation still. Equilibrium compositions were determined with an ultraviolet spectrometer. The reliability of the compositions seems to be $\pm 1 \times 10^{-6}$ mole fraction of durene. The accuracies of temperature and pressure are ±0.01 K and ±0.01 kPa, respectively. The volatilities $K_i = y_i/x_i$ of durene at infinite dilution were determined to be 0.173 and 0.162 in methanol and ethanol, respectively.

Introduction

In the previous studies of Kodama et al.,[1,2] vapor−liquid equilibrium measurements were made for mixtures containing ferrocene[1] or 1,4-dihydroxybenzene[2] in methanol or ethanol at atmospheric pressure. A complex such as ferrocene is used as a catalyst in polymer synthesis. 1,4-Dihydroxybenzene is practically used such as a polymerization inhibitor and assistant developer.

In the present study, the vapor−liquid equilibrium behavior of 1,2,4,5-tetramethylbenzene (durene) in methanol or ethanol was measured at atmospheric pressure in the dilute composition range of durene. Durene is practically used as a thermal resistance plasticizer of polymers.

Experimental Section

Chemicals. Durene was supplied by Wako Pure Chemical Industries, Ltd. with a guaranteed purity of at least 98.0 mol %. Special-grade reagents of methanol and ethanol were supplied by Wako Pure Chemical Industries, Ltd. and were used without further purification. The physical properties of methanol and ethanol used in this work are listed in Table 1. The purities of methanol and ethanol seem to be more than 99.9 mol % by gas chromatographic area analysis.

Apparatus and Procedures. The experimental apparatus and procedures are almost the same as those described previously.[1−3] The recirculation still is entirely constructed from borosilicate glass. The amount of solution required is about 45 cm^3 per determination. The experimental atmospheric pressure was measured with a Fortin barometer with an accuracy of ±0.01 kPa. The equilibrium temperature was measured with a Hewlett-Packard 2804A quartz thermometer, calibrated at the triple point of water in a reference cell, with an accuracy of ±0.01 K. The equilibrium vapor and liquid compositions were determined with a Jasco V-560DS ultraviolet spectrophotometer at 277 nm. The reliability of liquid and vapor compositions seems to be $\pm 1 \times 10^{-6}$ mole fraction of durene. Linear relations were experimentally observed between the absorbance and composition in the dilute range of durene.

Table 1. Normal Boiling Points T_b and Densities ρ of the Alcohols Used

	T_b/K		ρ(298.15 K)/(kg·m^{-3})	
material	exptl	lit[a]	exptl	lit[b]
methanol	337.67	337.651	786.5	786.64
ethanol	351.46	351.475	785.1	785.09

[a] Reference 4. [b] Reference 5.

Table 2. Experimental Vapor−Liquid Equilibrium Data, Liquid-Phase (x_1) and Vapor-Phase (y_1) Mole Fractions, Volatility K_1, Equilibrium Temperature T, and Atmospheric Pressure P

x_1	y_1	$K_1(= y_1/x_1)$	T/K	P/kPa
		Durene (1) + Methanol (2)		
0.001955	0.000345	0.176	336.89	98.31
0.003911	0.000708	0.181	336.92	98.36
0.006144	0.001036	0.169	337.00	98.33
0.008112	0.001370	0.169	337.01	98.13
		Durene (1) + Ethanol (2)		
0.002283	0.000378	0.166	350.69	98.39
0.004470	0.000741	0.166	350.71	98.34
0.006396	0.001014	0.159	350.71	98.21
0.008492	0.001347	0.159	350.72	98.08

Results

Table 2 gives the vapor−liquid equilibrium measurements obtained at atmospheric pressure in the dilute composition range of durene in methanol or ethanol. The volatility K_1 of durene is the ratio of vapor composition to liquid composition of durene. Figure 1 shows the equilibrium vapor and liquid composition diagram at atmospheric pressure in the dilute composition range of durene, giving linear relations for both systems. The linearity is true only within the range of the present experimental values. An extrapolation of linear relations cannot be recommended. Volatilities of durene at infinite dilution were determined to be 0.173 and 0.162 in methanol and ethanol, respectively.

The boiling point of methanol is lower than that of ethanol. The vapor pressure of durene in methanol is therefore lower than that in ethanol. However, a higher volatility in methanol than in ethanol was observed. The reason seems to be that the infinite dilution activity

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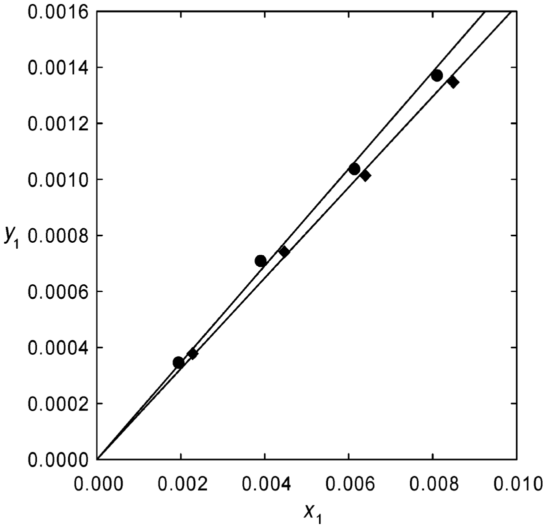

Figure 1. Experimental vapor−liquid equilibrium composition diagram at atmospheric pressure: ●, durene (1) + methanol (2); ◆, durene (1) + ethanol (2).

coefficient of durene in methanol is much higher than in ethanol. The activity coefficients of durene were evaluated to be 9.72 and 5.11 in methanol and ethanol, respectively, by applying Trouton's rule and the Clausius−Clapeyron equation for the calculation of the vapor pressure of durene with the normal boiling point of durene as 470 K.[6]

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