Excess Molar Volumes and Surface Tensions of Xylene with Acetone or 2-Butanone at 298.15 K

Gangfeng Ouyang,* Yangyi Yang, Shushen Lu, Zhongqi Huang, and Beisheng Kang

School of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou 510275, China

Densities for binary mixtures of (acetone + *o*-xylene, + *m*-xylene, and + *p*-xylene and 2-butanone + *o*-xylene, + *m*-xylene, and + *p*-xylene) have been determined at 298.15 K, and excess molar volumes have been derived. Surface tensions of these binary mixtures have been measured at 298.15 K by the pendant drop method, and the values of the surface tension deviation for these mixtures were also calculated.

Introduction

In a previous paper the excess molar volumes and surface tensions at 298.15 K for the xylene + alkanol (2-propanol and 2-methyl-2-propanol) systems were reported.[1] In this paper, surface tensions and excess molar volumes at 298.15 K for xylene + alkanone, including acetone + *o*-xylene or *m*-xylene or *p*-xylene and 2-butanone + *o*-xylene or *m*-xylene or *p*-xylene, systems are reported.

Experimental Section

o-Xylene, *m*-xylene, and *p*-xylene (Shanghai Chem., China) were of high grade and were distilled under reduced pressure before use. Acetone and 2-butanone (Guangzhou Chem., China) were analytical grade and purified by distillation and then drying. The mass fraction purities of the substances were as follows: *o*-xylene (99.99%), *m*-xylene (99.56%), *p*-xylene (99.99%), acetone (99.99%), 2-butanone (99.99%), determined with a PE auto system XL gas chromatograph. All of the mixtures were prepared by mass using an Ohaus E12140 balance with an accuracy of ±0.1 mg. To avoid evaporation, alkanone must be added in the end, and then the sample bottle must be sealed with a stopper as soon as possible.

Densities of the pure liquids and their mixtures were measured with an Anton Paar DMA 4500 vibrating tube densimeter, thermostated at (298.15 ± 0.01) K. The densimeter precision was $\pm 5 \times 10^{-5}$ g·cm^{-3}. The surface tensions of the pure liquids and their mixtures were determined by the pendant drop method, using a Dataphysics OCA20 contact angle and surface tension measuring device. This instrument provides a CCD camera to take pictures and an electronic syringe unit to inject samples, so the surface tension of the sample can be determined very fast. The surface tension was given by[2]

$$\sigma = \frac{g\Delta\rho d_e^{\,2}}{H} \qquad (1)$$

where g is the gravitational acceleration, $\Delta\rho$ is the density difference between the droplet and the surroundings, d_e is the largest diameter of the drop, and H is a correction factor, which depends on the shape of the drop. The accuracy of the instrument is ±0.05 mN·m^{-1} (±0.1 K). The densities and surface tensions of the pure compounds are given in Table 1 and compared with the literature values.

* Corresponding author. E-mail: cesoygf@zsu.edu.cn.

Table 1. Physical Properties of the Pure Components at 298.15 K

	ρ/g·cm^{-3}		σ/mN·m^{-1}	
substance	exptl	lit.	exptl	lit.
o-xylene	0.875 92	0.875 63[a]	29.35	29.49[a]
m-xylene	0.859 78	0.859 86[a]	28.36	28.10[a]
p-xylene	0.856 85	0.856 62[a]	27.89	27.76[a]
acetone	0.784 39	0.784 40[b]	24.01	24.02[c]
2-butanone	0.799 62	0.799 93[b]	24.28	23.96[c]

[a] *TRC Databases for Chemistry and Engineering—Thermodynamic Tables*, Version 1998-2s; Thermodynamic Research Center, Texas A&M University System: College Station, TX, 1998. [b] Reference 5. [c] Reference 6.

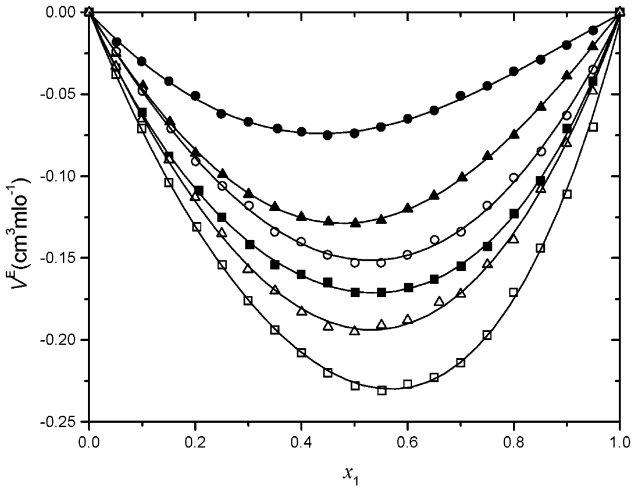

Figure 1. Excess molar volumes V^E for (x)acetone + (1 − x)*o*-xylene (■), + (1 − x)*m*-xylene (●), and + (1 − x)*p*-xylene (▲) and for (x)2-butanone + (1 − x)*o*-xylene (□), + (1 − x)*m*-xylene (○), and + (1 − x)*p*-xylene (△) at 298.15 K.

Results and Discussion

Excess molar volumes were determined from the density data by[3]

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Table 2. Experimental Excess Molar Volumes V^E at 298.15 K

x_1	V^E/cm³·mol⁻¹	x_1	V^E/cm³·mol⁻¹	x_1	V^E/cm³·mol⁻¹	x_1	V^E/cm³·mol⁻¹	x_1	V^E/cm³·mol⁻¹	x_1	V^E/cm³·mol⁻¹
	$(x)CH_3COCH_3 + (1-x)o\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)o\text{-}C_6H_4(CH_3)_2$				
0.0501	−0.034	0.3995	−0.160	0.7007	−0.155	0.0505	−0.038	0.4002	−0.208	0.6998	−0.214
0.1000	−0.061	0.4495	−0.165	0.7501	−0.143	0.0993	−0.071	0.4497	−0.220	0.7498	−0.197
0.1507	−0.088	0.5011	−0.171	0.8004	−0.123	0.1500	−0.104	0.5015	−0.228	0.7997	−0.171
0.2068	−0.109	0.5506	−0.171	0.8501	−0.103	0.2029	−0.131	0.5517	−0.231	0.8501	−0.144
0.2501	−0.125	0.6023	−0.168	0.9006	−0.071	0.2507	−0.154	0.5998	−0.227	0.9007	−0.111
0.3026	−0.142	0.6500	−0.163	0.9495	−0.042	0.2996	−0.176	0.6499	−0.223	0.9502	−0.070
0.3496	−0.154					0.3496	−0.194				
	$(x)CH_3COCH_3 + (1-x)m\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)m\text{-}C_6H_4(CH_3)_2$				
0.0520	−0.018	0.4006	−0.073	0.7000	−0.051	0.0510	−0.024	0.3995	−0.140	0.7008	−0.134
0.0991	−0.030	0.4493	−0.075	0.7504	−0.045	0.1005	−0.048	0.4495	−0.148	0.7504	−0.118
0.1503	−0.042	0.5000	−0.074	0.8000	−0.036	0.1547	−0.071	0.5008	−0.153	0.8001	−0.101
0.2003	−0.051	0.5498	−0.070	0.8507	−0.029	0.2009	−0.091	0.5502	−0.153	0.8519	−0.085
0.2488	−0.062	0.6005	−0.065	0.9002	−0.020	0.2509	−0.106	0.5995	−0.148	0.9002	−0.063
0.2998	−0.067	0.6500	−0.060	0.9498	−0.011	0.3013	−0.118	0.6512	−0.139	0.9495	−0.035
0.3550	−0.071					0.3499	−0.134				
	$(x)CH_3COCH_3 + (1-x)p\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)p\text{-}C_6H_4(CH_3)_2$				
0.0500	−0.025	0.4001	−0.125	0.7024	−0.101	0.0502	−0.033	0.4003	−0.183	0.7002	−0.172
0.1011	−0.045	0.4511	−0.128	0.7505	−0.088	0.1002	−0.065	0.4504	−0.192	0.7504	−0.154
0.1518	−0.067	0.5018	−0.129	0.8003	−0.075	0.1505	−0.090	0.4998	−0.195	0.7997	−0.139
0.2004	−0.086	0.5501	−0.127	0.8512	−0.058	0.1996	−0.113	0.5505	−0.191	0.8506	−0.108
0.2516	−0.099	0.6000	−0.120	0.9002	−0.039	0.2499	−0.135	0.5999	−0.188	0.8993	−0.080
0.3006	−0.111	0.6499	−0.112	0.9484	−0.021	0.2991	−0.157	0.6598	−0.177	0.9481	−0.048
0.3498	−0.119					0.3502	−0.170				

Table 3. Least-Squares Parameters and Standard Deviations s

	A_0	A_1	A_2	A_3	A_4	s/cm³·mol⁻¹
o-xylene + acetone	−0.6807	0.0855	−0.1422	−0.0025	0.0459	0.0015
m-xylene + acetone	−0.2933	−0.0920	0.0806	0.0313	−0.0984	0.0009
p-xylene + acetone	−0.5140	−0.0558	0.0469	0.0152	0.0158	0.0010
o-xylene + 2-butanone	−0.9118	0.1887	−0.0011	0.1351	−0.2807	0.0026
m-xylene + 2-butanone	−0.6068	0.0564	0.0643	0.0661	−0.1154	0.0018
p-xylene + 2-butanone	−0.7749	0.0706	0.0215	0.0914	−0.0991	0.0022

Table 4. Surface Tensions σ at 298.15 K

x_1	σ/mN·m⁻¹	$\delta\sigma$	x_1	σ/mN·m⁻¹	$\delta\sigma$	x_1	σ/mN·m⁻¹	$\delta\sigma$	x_1	σ/mN·m⁻¹	$\delta\sigma$
	$(x)CH_3COCH_3 + (1-x)o\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)o\text{-}C_6H_4(CH_3)_2$				
0.0995	29.13	0.31	0.6017	26.99	0.85	0.1001	29.00	0.16	0.6018	26.65	0.35
0.2016	28.84	0.57	0.6991	26.34	0.72	0.2028	28.58	0.26	0.7012	26.11	0.32
0.3047	28.45	0.73	0.7998	25.65	0.57	0.3001	28.17	0.34	0.8006	25.55	0.26
0.4030	28.07	0.87	0.9002	24.86	0.32	0.4017	27.68	0.37	0.8994	24.96	0.17
0.4999	27.58	0.90				0.5006	27.19	0.38			
	$(x)CH_3COCH_3 + (1-x)m\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)m\text{-}C_6H_4(CH_3)_2$				
0.1027	28.16	0.25	0.6024	26.41	0.67	0.1044	27.99	0.06	0.6009	26.11	0.20
0.1996	27.95	0.46	0.7002	25.86	0.55	0.2015	27.66	0.12	0.6999	25.68	0.18
0.3049	27.67	0.64	0.8010	25.27	0.39	0.3028	27.29	0.17	0.7999	25.24	0.14
0.4029	27.31	0.70	0.9014	24.66	0.22	0.4011	26.93	0.21	0.9000	24.76	0.07
0.4993	26.91	0.72				0.5013	26.53	0.22			
	$(x)CH_3COCH_3 + (1-x)p\text{-}C_6H_4(CH_3)_2$						$(x)CH_3COCH_2CH_3 + (1-x)p\text{-}C_6H_4(CH_3)_2$				
0.1027	27.69	0.20	0.6006	25.98	0.42	0.0999	27.58	0.05	0.6006	25.91	0.19
0.2022	27.41	0.31	0.7005	25.51	0.34	0.2007	27.27	0.11	0.7009	25.51	0.15
0.3029	27.11	0.40	0.8002	25.03	0.25	0.3001	26.95	0.14	0.8009	25.12	0.12
0.3993	26.78	0.44	0.9007	24.51	0.12	0.402	26.62	0.18	0.8999	24.71	0.07
0.5009	26.41	0.46				0.5001	26.28	0.20			

$$V^E/\text{cm}^3\cdot\text{mol}^{-1} = \frac{x_1M_1 + x_2M_2}{\rho} - x_1\frac{M_1}{\rho_1} - x_2\frac{M_2}{\rho_2} \quad (2)$$

where M_i are the molar masses of components i, ρ and ρ_i are the densities of the mixture and components i, and x_i are the molar fractions of components i.

Experimental excess molar volumes V^E for six binary mixtures (acetone + *o*, *m*, and *p*-xylene and 2-butanone + *o*, *m*, and *p*-xylene) at 298.15 K are listed in Table 2 and graphically presented in Figure 1. The experimental results were fitted by the method of least squares with all points weighted equally to the smoothing equation[4]

$$V^E/\text{cm}^3\cdot\text{mol}^{-1} = x(1-x)\sum_{i=0}^{k}A_i(1-2x)^i \quad (3)$$

The continuous lines in Figure 1 represent values calculated from the smoothing equation. The parameters A_0, A_1, A_2, A_3, and A_4 and the standard deviation s are given in Table 3.

Figure 1 shows that the excess molar volumes V^E are negative for mixtures of *o*, *m*, and *p*-xylene with acetone

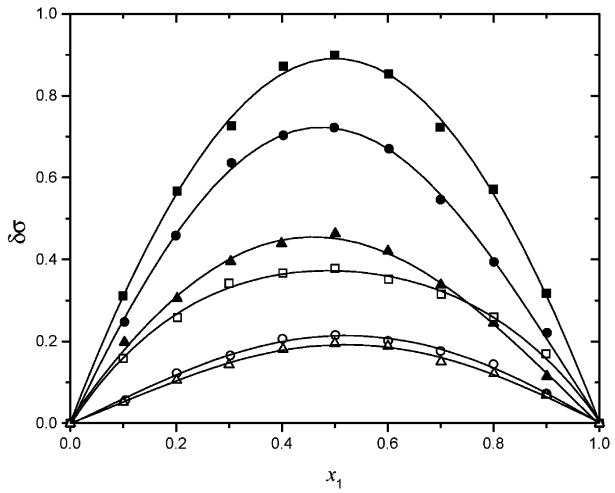

Figure 2. Surface tension deviation $\delta\sigma$ for (x)acetone + (1 − x)-*o*-xylene (■), + (1 − x)*m*-xylene (●), and + (1 − x)*p*-xylene (▲) and for (x)2-butanone + (1 − x)*o*-xylene (□), + (1 − x)*m*-xylene (○), and + (1 − x)*p*-xylene (△) at 298.15 K.

or 2-butanone. The V^E values at $x = 0.5$ for (*o*, *m*, and *p*-xylene + acetone or 2-butanone) follow the order *m*-xylene > *p*-xylene > *o*-xylene.

Table 4 lists the surface tensions and surface tension deviations for {(x)acetone + *o*, *m*, and *p*-xylene and (x)2-butanone + *o*, *m*, and *p*-xylene} at 298.15 K. The surface tension deviations $\delta\sigma$ are defined by[3]

$$\delta\sigma = \sigma - x_1\sigma_1 - x_2\sigma_2 \tag{4}$$

Figure 2 shows that the surface tension deviations $\delta\sigma$ are positive for mixtures of *o*, *m*, and *p*-xylene with acetone or 2-butanone. The maximum values of $\delta\sigma$ for acetone + xylene and 2-butanone + xylene follow the order *o*-xylene > *m*-xylene > *p*-xylene.

The excess molar volumes V^E are negative and the surface tension deviations $\delta\sigma$ are positive for mixtures of *o*, *m*, and *p*-xylene with acetone or 2-butanone, showing that there are quite strong interactions between xylene molecules and alkanone molecules. It seems that the lone-pair electrons on the oxygen atom of the acetone or 2-butanone charge transfer with *o*, *m*, and *p*-xylene.

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