water, and the distribution coefficient, or ratio of acid mole fraction in the supercritical fluid phase to that in the aqueous phase. The selectivities observed are very high, being greater than several hundred for low acid mole fractions. As a consequence, substantially dehydrated propionic acid may be obtained from dilute solutions in a single extraction step. Distribution coefficients, by contrast, exhibit a relatively strong dependence on solvent properties. The more polar (i.e., water-soluble) solvents could potentially be useful for the selective extraction of propionic acid from aqueous solutions. Application of the water-immiscible solvents SF_6 and R116 to processing of aqueous solutions, however, would probably be limited to recovery of solutes less polar than propionic acid.

As observed previously (*13*, *17*), the modified Peng–Robinson model was successful in predicting the qualitative characteristics of the experimentally observed behavior for all the cases studied. The quantitative agreement between experimental results and model predictions derived from binary data is good in most cases, with the agreement being closest at low acid mole fractions, closest to the binary data from which the correlation parameters were derived.

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Isobaric Vapor–Liquid Equilibria for the Binary Systems Formed by Acetonitrile and Aromatic Hydrocarbons

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The isobaric vapor–liquid equilibria of the binary systems formed by acetonitrile + benzene, + toluene, + *m*-xylene, + *p*-xylene, or + ethylbenzene were measured at 28.0 and 101.3 kPa. The activity coefficients were correlated by using the NRTL equation.

Introduction

In the framework of an extensive study about the thermodynamic properties of the systems containing acetonitrile and aromatic hydrocarbons (*1*–*2*), isobaric vapor–liquid equilibria were measured at 28 and 101.3 kPa, for the five binary systems acetonitrile (1) + benzene (2), + toluene (2), + *m*-xylene (2), + *p*-xylene (2), or + ethylbenzene (2). Only partial information concerning these systems is reported in the literature: excess enthalpy data were measured for all the investigated systems (*1*) at 25 and 41.2 °C, and additional data are available for the systems containing benzene, toluene, and ethylbenzene at 25 °C (*3*) and for the systems containing toluene at 48.2 °C (*4*). Isothermal vapor–liquid equilibria are reported for the systems containing benzene (*5*–*8*) and toluene (*4*–*5*, *7*, *9*).

Table I. Refractive Indexes *n* and Normal Boiling Points of the Chemicals

chemical	*n*(D, 20 °C)		normal boiling points/°C	
	this work	lit.[a]	this work	lit.[b]
acetonitrile	1.3420	1.344 11	81.6	81.60
benzene	1.5011	1.501 12	80.1	80.100
toluene	1.4961	1.496 93	110.6	110.625
m-xylene	1.4973	1.497 22	139.0	139.103
p-xylene	1.4958	1.495 82	138.0	138.351
ethylbenzene	1.4959	1.495 88	136.0	136.186

[a] Riddick, J. A.; Bunger, W. B.; Sakano, T. K. In *Organic Solvents*, 4th ed.; Weissberger, A., Ed.; Techniques of Chemistry, Vol. II; John Wiley & Sons: New York, 1986. [b] Dreisbach, R. R. *Physical Properties of Chemical Compounds*; American Chemical Society: Washington, DC, 1955.

Some sets of isobaric vapor–liquid equilibria are available for the systems containing benzene (*5*, *10*–*12*) and toluene (*4*, *10*–*11*) and a single set at 101.3 kPa for the systems containing *p*-xylene, and ethylbenzene (*13*), while for the system acetonitrile *m*-xylene no vapor–liquid equilibrium data appear to be reported.

Table II. Vapor–Liquid Equilibrium Temperature *t*, Liquid Mole Fraction *x*, and Vapor Mole Fraction *y*, for the Acetonitrile (1) + Benzene (2) System

28 kPa			101.3 kPa		
x_1	y_1	t/°C	x_1	y_1	t/°C
0.000	0.000	43.4	0.000	0.000	80.1
0.013	0.035	42.9	0.039	0.090	78.4
0.027	0.058	42.3	0.071	0.142	77.5
0.028	0.065	42.0	0.085	0.158	77.1
0.060	0.120	41.3	0.131	0.213	76.1
0.070	0.138	40.9	0.133	0.211	76.1
0.112	0.200	40.2	0.170	0.263	75.3
0.180	0.270	39.3	0.213	0.283	74.8
0.238	0.322	38.6	0.288	0.357	74.1
0.276	0.355	38.3	0.337	0.377	73.9
0.328	0.390	38.0	0.373	0.412	73.7
0.377	0.420	37.8	0.392	0.418	73.7
0.430	0.448	37.7	0.459	0.462	73.6
0.465	0.470	37.6	0.616	0.563	73.8
0.562	0.528	37.7	0.660	0.590	74.0
0.630	0.572	38.0	0.732	0.634	74.6
0.648	0.582	38.1	0.782	0.677	75.2
0.688	0.603	38.3	0.805	0.704	75.7
0.700	0.610	38.4	0.852	0.747	76.4
0.752	0.635	38.8	0.877	0.780	77.1
0.788	0.670	39.2	0.942	0.871	79.0
0.827	0.710	39.3	0.952	0.898	79.5
0.862	0.740	40.3	0.973	0.935	80.3
0.867	0.742	40.4	0.983	0.961	80.7
0.882	0.763	40.7	1.000	1.000	81.6
0.902	0.793	41.2			
0.918	0.813	41.6			
0.932	0.843	42.1			
0.945	0.867	42.5			
0.956	0.890	42.8			
0.968	0.914	43.2			
0.978	0.935	43.6			
0.983	0.947	43.9			
0.999	0.990	44.5			
1.000	1.000	44.6			

Experimental Section

***Materials*.** All chemicals used in this work had a minimum stated purity from the manufacturer (Farmitalia Carlo Erba) as follows: acetonitrile, 99.8%; benzene, toluene, and ethylbenzene, 99.5%; *m*-xylene and *p*-xylene, 99%. No further purification was done. The actual refractive indices and normal boiling points of the chemicals are given in Table I.

***Apparatus*.** The measurements were carried out by using a modified Gillespie type recirculation still (*14*). The pressure P was maintained constant to within ±0.13 kPa by means of an electronic regulator connected to the condenser.

***Procedure*.** Equilibrium temperatures t were read by means of a digital thermometer with the probe placed into the well of the still: the accuracy of the temperature measurements was ±0.05 °C. The attainment of a constant temperature for at least 30 min was the sign that the steady state had been reached: in these conditions, samples of the liquid and of the vapor phases were withdrawn and analyzed.

The analyses were carried out by reading the refractive indexes of the condensed samples: a precision Abbe refractometer with the cell kept at 25 ± 0.05 °C was used. The standard refractive index vs mole fraction plot was prepared from known samples, and the estimated uncertainty in the composition measurements was ±0.001 mole fraction.

The reproducibility of the measurements was ±0.002 mole fraction for compositions and ±0.1 °C for temperatures.

Results and Discussion

The experimental data are reported in Tables II–VI. The systems acetonitrile + benzene and acetonitrile + toluene form azeotropes, while the other systems do not.

Table III. Vapor–Liquid Equilibrium Temperature *t*, Liquid Mole Fraction *x*, and Vapor Mole Fraction *y*, for the Acetonitrile (1) + Toluene (2) System

28 kPa			101.3 kPa		
x_1	y_1	t/°C	x_1	y_1	t/°C
0.000	0.000	70.8	0.000	0.000	110.6
0.040	0.153	67.2	0.024	0.090	108.0
0.050	0.195	66.3	0.027	0.115	107.1
0.063	0.240	65.5	0.037	0.145	106.2
0.078	0.293	63.8	0.050	0.183	105.0
0.095	0.343	62.4	0.060	0.215	103.8
0.102	0.358	61.6	0.063	0.240	102.4
0.110	0.382	60.7	0.080	0.275	101.6
0.120	0.420	59.6	0.083	0.287	100.7
0.135	0.428	58.8	0.103	0.353	99.3
0.155	0.460	57.6	0.120	0.378	97.5
0.168	0.495	56.8	0.133	0.387	97.0
0.193	0.513	55.7	0.156	0.434	95.2
0.222	0.557	54.8	0.163	0.454	94.6
0.232	0.569	54.2	0.214	0.526	92.0
0.262	0.605	52.8	0.228	0.532	91.3
0.288	0.627	52.1	0.297	0.607	88.4
0.327	0.650	51.2	0.377	0.649	86.2
0.429	0.705	49.0	0.415	0.677	85.3
0.581	0.768	47.0	0.495	0.717	83.9
0.725	0.820	45.9	0.534	0.733	83.4
0.778	0.837	45.2	0.607	0.767	82.5
0.812	0.855	45.0	0.708	0.795	81.6
0.860	0.877	44.7	0.847	0.865	80.9
0.900	0.908	44.5	0.883	0.887	80.7
0.917	0.919	44.4	0.910	0.908	80.7
0.930	0.927	44.5	0.912	0.909	80.8
0.942	0.938	44.5	0.930	0.924	80.9
0.961	0.953	44.5	0.952	0.943	81.0
0.981	0.975	44.6	1.000	1.000	81.6
0.992	0.984	44.6			
0.999	0.996	44.6			
1.000	1.000	44.6			

The activity coefficients γ_i of the components in the liquid phase were calculated as

$$\gamma_i = y_i P / x_i P_{si} \tag{1}$$

where P_{si} is the vapor pressure, x_i the liquid mole fraction, and y_i the vapor mole fraction of component i. Because of the low experimental pressures, no correction for the vapor-phase nonideality was applied. The boiling points of the pure components were measured at 28 and 101.3 kPa (Tables II–VI) and were correlated on the basis of the Antoine equation:

$$\ln (P_{si}/\mathrm{kPa}) = A + B/(C + (t/°\mathrm{C})) \tag{2}$$

The values of B and C were taken from the literature (*15*), while A was adjusted to our experimental measurements.

The values of the parameters of the Antoine equation are summarized in Table VII.

The thermodynamic consistency of the data has been tested on the basis of the Gibbs–Duhem equation, by means of its integrated form for binary systems at isobaric conditions (*16*):

$$\int_0^1 \ln\left(\frac{\gamma_1}{\gamma_2}\right) \mathrm{d}x_1 = \int_{x_1=0}^{x_1=1} \frac{\Delta H}{RT^2}\,\mathrm{d}T \tag{3}$$

where ΔH is the molar excess enthalpy and T the Kelvin scale temperature.

For each set of isobaric data, $\ln (\gamma_1/\gamma_2)$ has been plotted vs x_1, and the deviation D between the areas A′ and B′, above and below the x_1 axis, respectively, has been evaluated as

$$D = 100\left|\frac{A' - B'}{A' + B'}\right| \tag{4}$$

According to the method suggested by Herington (*17*), the value

Table IV. Vapor–Liquid Equilibrium Temperature t, Liquid Mole Fraction x, and Vapor Mole Fraction y, for the Acetonitrile (1) + m-Xylene (2) System

28 kPa			101.3 kPa		
x_1	y_1	t/°C	x_1	y_1	t/°C
0.000	0.000	96.8	0.000	0.000	139.0
0.011	0.123	93.2	0.008	0.052	137.5
0.013	0.157	91.7	0.015	0.098	135.7
0.017	0.195	90.7	0.020	0.125	134.1
0.027	0.280	87.4	0.022	0.148	132.6
0.034	0.358	84.4	0.030	0.192	131.1
0.043	0.430	81.4	0.035	0.215	130.1
0.046	0.445	80.5	0.038	0.238	129.4
0.054	0.490	78.6	0.040	0.258	128.4
0.063	0.548	75.4	0.048	0.290	127.2
0.105	0.673	68.2	0.051	0.305	126.0
0.127	0.698	66.8	0.056	0.338	124.4
0.142	0.715	65.6	0.062	0.368	123.0
0.162	0.748	63.4	0.065	0.392	121.6
0.185	0.761	62.1	0.078	0.438	119.5
0.221	0.791	59.8	0.080	0.472	117.5
0.263	0.819	57.6	0.087	0.497	116.0
0.317	0.851	55.4	0.100	0.543	113.4
0.382	0.868	53.8	0.131	0.615	108.7
0.445	0.881	52.8	0.145	0.645	107.2
0.525	0.886	51.6	0.160	0.682	105.2
0.585	0.901	50.6	0.187	0.707	102.8
0.600	0.907	50.4	0.218	0.730	100.4
0.687	0.922	48.9	0.227	0.735	100.1
0.778	0.935	48.1	0.250	0.763	97.9
0.865	0.953	47.1	0.330	0.795	94.1
0.925	0.967	46.8	0.332	0.805	93.9
0.962	0.979	46.5	0.390	0.827	91.9
0.994	0.996	45.9	0.397	0.830	91.3
1.000	1.000	44.6	0.434	0.840	90.2
			0.445	0.847	89.9
			0.465	0.853	88.8
			0.480	0.858	88.7
			0.583	0.878	86.9
			0.635	0.888	86.3
			0.723	0.905	85.2
			0.766	0.915	84.5
			0.810	0.925	84.1
			0.850	0.935	83.5
			0.888	0.948	82.9
			0.930	0.962	82.5
			0.958	0.972	82.3
			1.000	1.000	81.6

of D has been compared with that of the quantity J, which is a semiempirical estimation of the right-hand side of eq 1 given by

$$J = 150|\Delta T_{\max}|/T_{\min} \tag{5}$$

where $\Delta T_{\max}$ is the maximum difference of boiling points in the total composition range and $T_{\min}$ is the lowest boiling temperature. The criterion assumed (*17*) for the thermodynamic consistency of a given set of data is $D - J \leq 10\%$. In the present case, the above-mentioned difference did not exceed 5% for the systems acetonitrile + benzene, acetonitrile + p-xylene, and acetonitrile + ethylbenzene and was close to 10% for the systems acetonitrile + toluene and acetonitrile + m-xylene. The γ_1 and γ_2 values were correlated by means of the NRTL equation (*18*):

$$\ln \gamma_1 = x_2^2\left[\tau_{21}\left(\frac{G_{21}}{x_1 + x_2G_{21}}\right)^2 + \frac{\tau_{12}G_{12}}{(x_2 + x_1G_{12})^2}\right] \tag{6}$$

$$\ln \gamma_2 = x_1^2\left[\tau_{12}\left(\frac{G_{12}}{x_2 + x_1G_{12}}\right)^2 + \frac{\tau_{21}G_{21}}{(x_1 + x_2G_{21})^2}\right] \tag{7}$$

where $\tau_{12} = (g_{12} - g_{22})/RT$, $\tau_{21} = (g_{12} - g_{11})/RT$, $G_{12} = \exp(-\alpha_{12}\tau_{12})$, $G_{21} = \exp(-\alpha_{21}\tau_{21})$, and $\alpha_{12} = \alpha_{21}$. To account

Table V. Vapor–Liquid Equilibrium Temperature t, Liquid Mole Fraction x, and Vapor Mole Fraction y, for the Acetonitrile (1) + p-Xylene (2) System

28 kPa			101.3 kPa		
x_1	y_1	t/°C	x_1	y_1	t/°C
0.000	0.000	95.8	0.000	0.000	138.0
0.008	0.083	93.7	0.010	0.046	136.1
0.017	0.175	90.7	0.015	0.090	135.1
0.025	0.258	87.5	0.020	0.125	133.7
0.026	0.278	86.7	0.022	0.141	132.0
0.038	0.360	83.1	0.027	0.173	130.8
0.053	0.445	79.1	0.033	0.202	129.4
0.063	0.497	76.7	0.045	0.270	127.0
0.075	0.555	73.5	0.060	0.355	123.1
0.100	0.620	69.5	0.063	0.403	121.1
0.128	0.685	65.7	0.078	0.460	117.4
0.158	0.725	63.1	0.094	0.495	116.0
0.207	0.770	59.2	0.107	0.555	112.4
0.220	0.783	58.4	0.128	0.595	109.8
0.240	0.795	57.5	0.147	0.643	106.8
0.255	0.805	56.4	0.165	0.670	104.7
0.318	0.830	54.4	0.175	0.690	103.3
0.458	0.855	51.4	0.200	0.720	100.9
0.588	0.890	49.0	0.238	0.745	98.5
0.678	0.915	48.0	0.281	0.780	95.7
0.738	0.924	47.4	0.375	0.818	92.1
0.795	0.935	46.8	0.498	0.855	88.7
0.830	0.943	46.4	0.607	0.880	86.7
0.904	0.958	45.8	0.694	0.897	85.5
1.000	1.000	44.6	0.787	0.918	84.1
			0.872	0.940	83.1
			0.957	0.974	81.8
			1.000	1.000	81.6

Table VI. Vapor–Liquid Equilibrium Temperature t, Liquid Mole Fraction x, and Vapor Mole Fraction y, for the Acetonitrile (1) + Ethylbenzene (2) System

28 kPa			101.3 kPa		
x_1	y_1	t/°C	x_1	y_1	t/°C
0.000	0.000	93.9	0.000	0.000	136.0
0.005	0.064	91.6	0.006	0.102	132.5
0.020	0.221	86.6	0.015	0.162	129.9
0.028	0.313	83.4	0.035	0.245	126.9
0.040	0.372	80.2	0.040	0.326	123.2
0.058	0.473	75.5	0.062	0.390	119.6
0.079	0.555	71.6	0.090	0.466	115.7
0.108	0.638	67.4	0.095	0.512	113.0
0.134	0.713	63.7	0.118	0.550	109.3
0.203	0.765	59.4	0.133	0.613	107.2
0.285	0.803	55.8	0.160	0.658	104.3
0.315	0.820	54.7	0.182	0.690	101.5
0.340	0.832	53.8	0.235	0.713	100.0
0.407	0.853	52.2	0.271	0.745	97.1
0.441	0.865	51.6	0.282	0.758	95.6
0.485	0.874	51.0	0.302	0.772	94.3
0.517	0.883	50.3	0.335	0.780	92.9
0.528	0.888	49.6	0.364	0.801	91.6
0.580	0.895	49.1	0.400	0.813	90.3
0.645	0.908	48.0	0.464	0.835	89.1
0.675	0.912	47.6	0.518	0.852	88.2
0.748	0.927	46.8	0.566	0.863	87.1
0.818	0.939	46.3	0.882	0.942	82.8
0.845	0.945	46.0	0.957	0.971	81.9
0.892	0.957	45.5	0.984	0.988	81.6
0.978	0.982	45.2	1.000	1.000	81.6
1.000	1.000	44.6			

Table VII. Coefficients for Antoine Equation 2

	A	B	C
acetonitrile	14.8961	3413.099	250.523
benzene	13.8263	2755.642	219.161
toluene	13.9898	3090.783	219.187
m-xylene	14.1308	3366.992	215.110
p-xylene	14.0904	3346.646	215.310
ethylbenzene	14.0291	3291.661	213.767

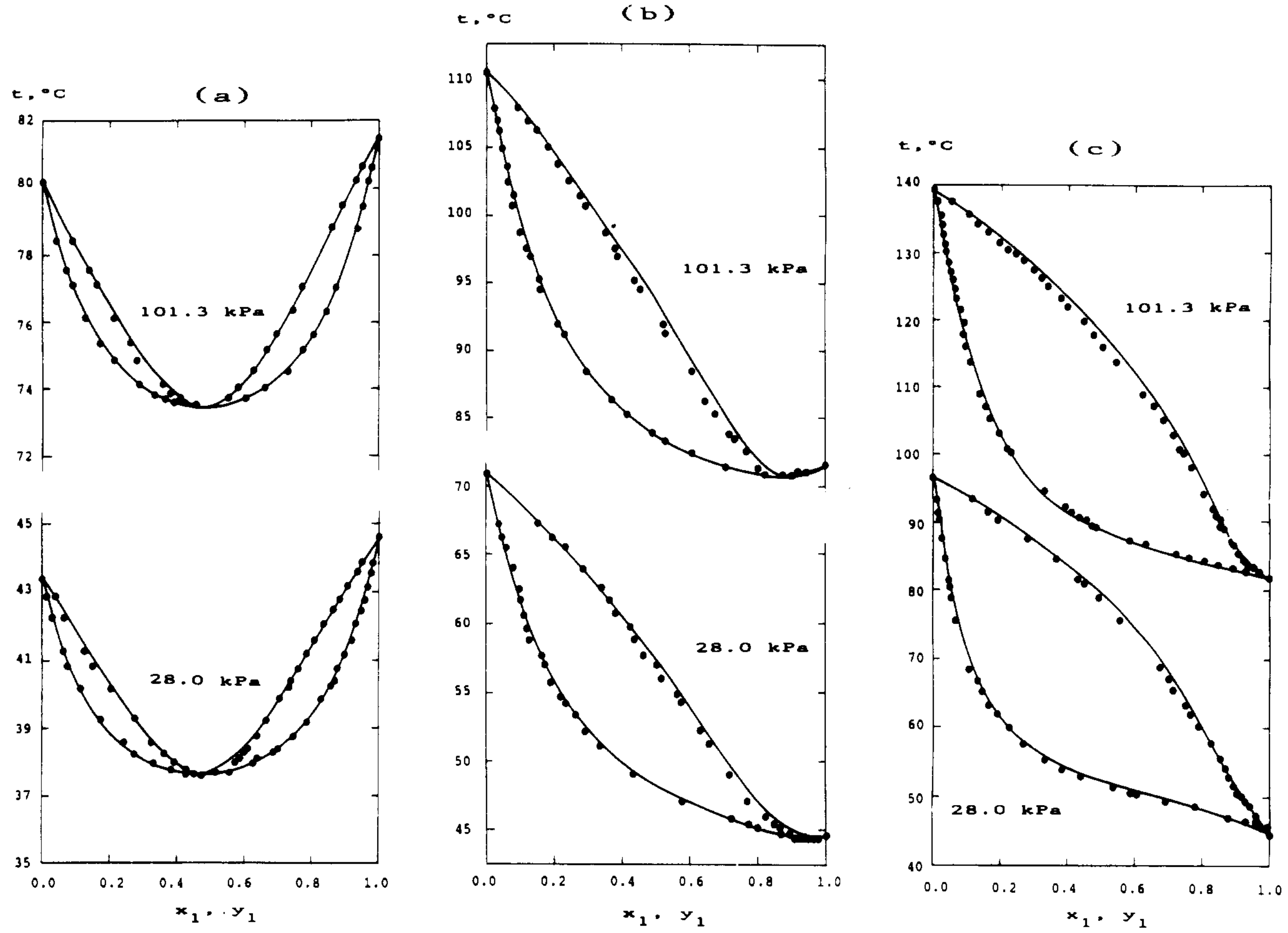

Figure 1. Binary vapor-liquid equilibria for the acetonitrile (1)-solvent (2) systems for solvents (a) benzene, (b) toluene, and (c) *m*-xylene: (●) experimental measurements; (—) calculated curve.

for the large range of temperatures investigated, the parameters $g_{12} - g_{22}$ and $g_{12} - g_{11}$ were assumed to depend on the temperature, according to the following relationships (*19*):

$$g_{12} - g_{22} = a_{12} + b_{12}((T/\mathrm{K}) - 273.15) \quad (8)$$

$$g_{12} - g_{11} = a_{21} + b_{21}((T/\mathrm{K}) - 273.15) \quad (9)$$

The parameter α_{12} was assumed to be independent of the temperature and was set equal to 0.3 (*18*), for all the examined binary systems.

The values of the parameters a_{12}, b_{12}, a_{21}, and b_{21} were determined for each system by submitting to a unique regression analysis the equilibrium data measured at 28.0 and 101.3 kPa. The calculation procedure (*20*) was based on the minimization of the objective function:

$$S = \sum_{k=1}^{N} \{[F_{y_1}(y_{1k,\mathrm{exp}} - y_{1k,\mathrm{calc}})]^2 + [(t_{k,\mathrm{exp}}/°\mathrm{C}) - (t_{k,\mathrm{calc}}/°\mathrm{C})]^2\} \quad (10)$$

The parameter F_{y_1} was introduced to balance the effects of deviations on y_1 and t: its values for the five binary systems are reported in Table VIII.

The values of the NRTL parameters obtained from the minimization are reported in Table IX.

The mean deviations between calculated and experimental data are reported in Table VIII for the five binary systems. For the systems acetonitrile + toluene, acetonitrile + *p*-xylene, and acetonitrile + ethylbenzene, their values are comparable with those reported by the literature (*5*), while, for the system acetonitrile + benzene, the deviations obtained here are much lower than those relevant to previous measurements.

Table VIII. Values of the Weighting Factor F_{y_1}, Equation 10, and of Mean Deviations Δt and Δy_1 between Calculated and Experimental Data for Acetonitrile + Solvent Systems[a]

solvent	F_{y_1}	Δt/°C	Δy_1
benzene	15	0.073	0.708
toluene	30	0.525	1.332
m-xylene	60	0.556	1.067
p-xylene	60	0.708	1.383
ethylbenzene	60	0.613	1.179

[a] $\Delta t = [\sum_{k=1}^{N} |(t_{k,\mathrm{exp}} - t_{k,\mathrm{calc}})|]/N$. $\Delta y_1 = 100[\sum_{k=1}^{N} |(y_{1k,\mathrm{exp}} - y_{1k,\mathrm{calc}})|]/N$.

Table IX. NRTL Parameters, Equations 8 and 9, for the Acetonitrile (1) + Solvent (2) Systems

solvent	α_{12}	a_{12}/(cal mol^{-1})	a_{21}/(cal mol^{-1})	b_{12}/(cal mol^{-1})	b_{21}/(cal mol^{-1})
benzene	0.3	143.62	548.74	3.290	−3.305
toluene	0.3	378.41	36.83	9.491	−2.421
m-xylene	0.3	−566.06	1140.48	16.615	−11.468
p-xylene	0.3	−208.13	798.70	14.872	−8.981
ethylbenzene	0.3	363.69	632.87	3.408	−4.182

The comparison between experimental and predicted vapor–liquid equilibria appears to be satisfactory, as shown in Figure 1, for the systems acetonitrile + benzene, acetonitrile + toluene, and acetonitrile + *m*-xylene. The plots for the systems acetonitrile + *p*-xylene and acetonitrile + ethylbenzene are similar to those for the system acetonitrile + *m*-xylene.

In order to quantitatively compare the present data with those reported by the literature, the latter were correlated by

Table X. Values of Mean Deviations Δt and Δy_1 between Calculated and Literature Data for Acetonitrile + Solvent Systems[a]

solvent	$\Delta t/°C$	Δy_1
benzene (*10*)	0.115	0.564
benzene (*11*)	0.289	0.863
toluene (*4*)	1.964	3.370
toluene (*10*)	1.044	1.626
toluene (*11*)	0.938	3.243
p-xylene (*13*)	0.643	2.752
ethylbenzene (*13*)	0.327	2.133

[a] $\Delta t = [\sum_{k=1}^{N} |(t_{k,\mathrm{exp}} - t_{k,\mathrm{calc}})|]/N$. $\Delta y_1 = 100[\sum_{k=1}^{N} |(y_{1k,\mathrm{exp}} - y_{1k,\mathrm{calc}})|]/N$.

using the NRTL parameters determined here: the mean deviations between calculated and literature data are shown in Table X. The comparison is limited to the binary systems acetonitrile + benzene (*10*–*11*), acetonitrile + toluene (*4*, *10*–*11*), acetonitrile + *p*-xylene, and acetonitrile + ethylbenzene (*13*) at 101.3 kPa and shows a good agreement (see Table VIII) for the systems containing benzene, *p*-xylene, and ethylbenzene and for two (*10*–*11*) of the three sets of literature data available for the systems containing toluene, while greater deviations can be observed for the third one (*4*).

Glossary

A, B, C	parameters of the Antoine equation, eq 2, kPa
a_{12}	parameter, eq 8, cal mol^{-1}
a_{21}	parameter, eq 9, cal mol^{-1}
b_{12}	parameter, eq 8, cal mol^{-1}
b_{21}	parameter, eq 9, cal mol^{-1}
F_{y_1}	weighting factor for vapor-phase composition deviations of component 1, eq 10
g_{ij}	energy of interaction between an i–j pair of molecules, cal mol^{-1}
N	total number of vapor-liquid equilibrium data of each binary system
P	total pressure of the system, kPa
P_{si}	vapor pressure of pure component i, kPa
R	gas constant, cal mol^{-1} K^{-1}
t	temperature, °C
T	temperature, K
x_i	liquid-phase mole fraction of component i
y_i	vapor-phase mole fraction of component i
α_{12}	parameter of NRTL equation, eqs 6 and 7
γ_i	activity coefficient of component i
ΔH	molar enthalpy of mixing, cal mol^{-1}
τ_{12}	parameter of NRTL equation, eqs 6 and 7
τ_{21}	parameter of NRTL equation, eqs 6 and 7

Subscripts

calc	calculated
exp	experimental
i	component indexes (1, acetonitrile; 2, aromatic hydrocarbon)

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