

# Vapor–Liquid Equilibria of the Binary System 1-Pentanol + Anisole and the Quaternary System Benzene + Cyclohexane + 1-Pentanol + Anisole at 101.32 kPa

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Vapor–liquid equilibrium (VLE) at 101.32 kPa has been measured for the quaternary system benzene + cyclohexane + 1-pentanol + anisole in an isobaric equilibrium still with secondary recirculation of vapor and liquid phases covering a wide range of concentration. Accurate prediction of activity coefficients and the equilibrium compositions with the UNIFAC group contribution model were obtained with low standard deviations of vapor mole fraction and equilibrium temperatures. The consistency of the measured VLE data were tested with the McDermott and Ellis method.

## Introduction

Experimental data of phase equilibria for ternary or higher-order mixtures are scarce. These experiments are time consuming when the whole compositional range is investigated. This study is an extension of our earlier work that concerns vapor–liquid or liquid–liquid equilibria<sup>1–3</sup> (VLE or LLE), related to extractive distillation and liquid extraction processes. In the present work, phase equilibrium data for the separation of the benzene + cyclohexane azeotropic mixture, using a mixed extractive distillation solvent, are presented. The mixed solvent entrainer components are 1-pentanol + anisole. Binary mixtures of 1-pentanol with benzene have less positive deviation to ideality than the alcohol binary mixtures with cyclohexane. On the other hand, anisole + benzene mixtures have negative nonideal deviations, whereas anisole + cyclohexane mixtures exhibit positive deviations. Therefore, the combination of the two solvents may offer some potential for extractive distillation of alkane + aromatic mixtures. There is no literature data available for this system. VLE data of the quaternary mixture benzene + cyclohexane + 1-pentanol + anisole and the binary mixture 1-pentanol + anisole at a pressure of 101.32 kPa are reported. The multicomponent VLE conditions are also predicted with the UNIFAC group contribution thermodynamic model.<sup>4</sup> Comparison of predictions with the experimental measurements is presented.

## Experimental Section

**Materials.** The chemicals were supplied by Merck, except anisole, which was supplied by Aldrich. Further purification was achieved by ultrasonic degassing and molecular sieves drying (4Å, 1/16 in.). The purity of materials was checked by gas chromatography and found to be better than 99.9 mass % for benzene and cyclohexane, 99.0 mass % for 1-pentanol, and 99.7 mass % for anisole, and the maximum water contents of the pure liquids (Metrohm

**Table 1. Normal Boiling Temperatures  $T_b$  of the Pure Components**

component	$T_b$ /K	
	exp	lit <sup>5</sup>
benzene	353.16	353.250
cyclohexane	353.79	353.888
1-pentanol	410.78	410.95
anisole	426.77	426.75 <sup>6</sup>

737 Coulometer) were ( $3.0 \times 10^{-2}$ ,  $4.9 \times 10^{-3}$ ,  $2.3 \times 10^{-1}$ , and  $6.5 \times 10^{-2}$ ) mass % for benzene, cyclohexane, 1-pentanol, and anisole, respectively. Their purity was also checked by determining their normal boiling temperatures  $T_b$  (Table 1) prior to the measurements.

**Apparatus and Procedure.** VLE measurements were carried out in an all-glass vapor–liquid cell manufactured by Normag. In this recirculation cell, a volume of about 100 mL of the solution is heated to its boiling point by a 300-W heating blanket. The vapor–liquid mixture flows through a Cottrell pump tube that guarantees an intense vapor–liquid mixing and then enters a separation chamber whose construction prevents the entrainment of liquid droplets into the vapor phase. The separated vapor and liquid phases are condensed and returned to a boiler. The separation chamber and Cottrell pump are thermally isolated by vacuum. Besides, the vacuum chamber outside was kept to the boiling temperature. Temperature control is achieved by a thermostatic bath with a glass Pt-100 temperature sensor, with an accuracy of  $\pm 0.1$  K. Boiling temperatures of mixtures were measured with a Systemtechnik S1220 digital thermometer and a Pt-100 probe with a precision of  $\pm 10^{-2}$  K (temperature scale ITS-90). Pressure was kept constant at  $(101.32 \pm 5 \times 10^{-2})$  kPa by a controller device that controlled the flow of nitrogen to the apparatus in order to maintain the pressure difference with respect to the pressure in the laboratory. The pressure has been measured with a Paroscientific series 700 pressure transducer with an accuracy of  $\pm 0.05$  kPa. Each experiment was continued at least for 1 h after the boiling temperature had become stable. After equilibration, a small sample was taken from each phase with a syringe. The samples were analyzed by gas liquid chromatography using

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**Table 2. Experimental Vapor–Liquid Equilibrium Data: Temperature  $T$ , Liquid Phase  $x_i$ , and Vapor Phase  $y_i$  Mole Fraction, Activity Coefficient  $\gamma_i$  for Benzene (1) + Cyclohexane (2) + 1-Pentanol (3) + Anisole (4) at 101.32 kPa**

$T/K$	$x_1$	$x_2$	$x_3$	$y_1$	$y_2$	$y_3$	$\gamma_1$	$\gamma_2$	$\gamma_3$	$\gamma_4$
352.97	0.152	0.786	0.044	0.224	0.750	0.023	1.468	0.976	5.931	2.017
353.01	0.248	0.670	0.059	0.246	0.728	0.023	0.987	1.110	4.414	1.576
353.10	0.106	0.856	0.026	0.199	0.777	0.022	1.863	0.925	9.537	2.007
353.23	0.269	0.580	0.103	0.314	0.652	0.029	1.154	1.141	3.150	1.246
353.24	0.083	0.880	0.023	0.175	0.801	0.021	2.084	0.924	10.217	2.565
353.55	0.392	0.451	0.113	0.443	0.520	0.032	1.107	1.160	3.115	1.339
354.10	0.454	0.375	0.124	0.507	0.457	0.031	1.075	1.206	2.673	1.224
354.55	0.852	0.042	0.067	0.925	0.044	0.027	1.032	1.024	4.211	1.153
355.08	0.381	0.400	0.158	0.458	0.498	0.037	1.124	1.198	2.380	1.266
356.16	0.356	0.359	0.204	0.422	0.518	0.048	1.074	1.346	2.261	1.563
356.72	0.765	0.029	0.180	0.856	0.058	0.082	0.997	1.836	4.245	1.578
357.14	0.150	0.622	0.065	0.192	0.756	0.029	1.126	1.102	4.085	1.432
357.15	0.677	0.093	0.163	0.792	0.148	0.042	1.029	1.443	2.356	2.710
357.38	0.357	0.416	0.167	0.444	0.484	0.058	1.087	1.048	3.136	2.338
357.45	0.421	0.189	0.313	0.621	0.323	0.049	1.286	1.536	1.410	0.907
357.71	0.109	0.558	0.280	0.172	0.765	0.055	1.365	1.223	1.745	1.496
358.25	0.120	0.601	0.160	0.226	0.691	0.058	1.604	1.010	3.133	2.034
358.59	0.085	0.691	0.032	0.113	0.840	0.014	1.121	1.058	3.730	1.644
358.82	0.116	0.492	0.329	0.189	0.743	0.059	1.365	1.306	1.507	1.352
359.10	0.139	0.598	0.139	0.251	0.665	0.055	1.500	0.954	3.280	2.186
359.37	0.588	0.116	0.122	0.752	0.196	0.034	1.054	1.439	2.283	0.953
359.45	0.100	0.440	0.432	0.187	0.706	0.072	1.538	1.363	1.356	11.520
359.50	0.537	0.071	0.318	0.784	0.148	0.060	1.199	1.769	1.533	0.990
359.64	0.416	0.229	0.255	0.544	0.379	0.060	1.069	1.399	1.899	1.550
360.25	0.154	0.456	0.257	0.271	0.629	0.074	1.414	1.146	2.253	1.743
360.79	0.643	0.046	0.064	0.825	0.114	0.029	1.015	2.028	3.463	1.125
361.05	0.477	0.127	0.257	0.665	0.238	0.079	1.095	1.523	2.312	1.114
361.53	0.430	0.165	0.220	0.640	0.297	0.045	1.153	1.443	1.507	0.821
361.63	0.022	0.448	0.520	0.050	0.854	0.093	1.756	1.524	1.307	2.534
362.05	0.263	0.328	0.210	0.364	0.577	0.036	1.056	1.390	1.232	0.958
362.13	0.753	0.079	0.110	0.818	0.118	0.032	0.827	1.178	2.083	4.539
362.39	0.407	0.166	0.304	0.574	0.336	0.068	1.066	1.585	1.578	1.459
362.46	0.289	0.243	0.221	0.432	0.479	0.055	1.127	1.540	1.751	1.121
362.92	0.055	0.569	0.027	0.107	0.797	0.016	1.447	1.080	4.087	1.838
364.08	0.657	0.037	0.034	0.861	0.082	0.017	0.944	1.656	3.265	1.119
364.32	0.128	0.375	0.240	0.199	0.685	0.074	1.112	1.356	1.983	1.238
364.38	0.209	0.257	0.335	0.344	0.562	0.063	1.175	1.621	1.207	1.176
365.12	0.412	0.106	0.391	0.658	0.226	0.098	1.117	1.549	1.551	1.446
365.26	0.351	0.207	0.217	0.526	0.362	0.071	1.044	1.266	2.014	1.326
365.38	0.058	0.389	0.024	0.075	0.798	0.015	0.897	1.480	3.834	1.539
366.15	0.065	0.446	0.021	0.098	0.790	0.014	1.024	1.251	3.946	1.477
366.66	0.594	0.046	0.040	0.793	0.108	0.025	0.894	1.637	3.613	1.591
366.93	0.375	0.129	0.180	0.566	0.317	0.065	1.004	1.700	2.057	1.122
366.95	0.229	0.182	0.399	0.390	0.467	0.105	1.132	1.774	1.495	1.364
367.16	0.386	0.114	0.228	0.652	0.246	0.064	1.116	1.484	1.583	0.943
367.18	0.289	0.144	0.319	0.500	0.364	0.091	1.143	1.737	1.604	1.225
368.36	0.246	0.198	0.169	0.408	0.463	0.065	1.060	1.557	2.051	1.068
368.58	0.218	0.228	0.273	0.388	0.487	0.069	1.131	1.414	1.334	1.276
368.74	0.204	0.179	0.378	0.386	0.454	0.109	1.197	1.672	1.508	1.358
369.41	0.214	0.231	0.269	0.347	0.500	0.085	1.007	1.402	1.605	1.475
369.47	0.380	0.145	0.258	0.542	0.298	0.104	0.884	1.329	2.040	1.595
370.32	0.230	0.113	0.448	0.471	0.338	0.141	1.241	1.892	1.531	1.432
370.63	0.025	0.230	0.731	0.098	0.723	0.175	2.357	1.972	1.147	1.695
371.04	0.163	0.222	0.291	0.325	0.537	0.075	1.184	1.500	1.217	1.134
371.08	0.251	0.118	0.276	0.483	0.350	0.098	1.142	1.838	1.672	1.130
371.24	0.367	0.096	0.470	0.598	0.191	0.188	0.964	1.229	1.863	1.982
371.38	0.159	0.164	0.521	0.375	0.477	0.113	1.389	1.788	1.007	1.291
371.49	0.162	0.164	0.381	0.356	0.466	0.126	1.290	1.742	1.527	1.017
371.53	0.469	0.031	0.057	0.766	0.087	0.035	0.957	1.720	2.842	1.443
371.80	0.198	0.196	0.244	0.361	0.498	0.080	1.061	1.545	1.497	0.955
374.41	0.151	0.142	0.470	0.357	0.492	0.103	1.283	1.969	0.891	1.041
374.46	0.045	0.341	0.020	0.070	0.783	0.016	0.842	1.303	3.255	1.134
374.63	0.372	0.091	0.026	0.619	0.245	0.014	0.898	1.522	2.176	1.216
375.91	0.123	0.195	0.243	0.256	0.576	0.072	1.085	1.615	1.130	1.065
375.94	0.140	0.179	0.196	0.281	0.560	0.064	1.046	1.710	1.244	0.953
377.06	0.380	0.040	0.069	0.717	0.102	0.042	0.955	1.355	2.213	1.266
378.48	0.256	0.110	0.019	0.538	0.308	0.014	1.025	1.435	2.525	1.008
379.79	0.158	0.148	0.186	0.331	0.403	0.122	0.988	1.351	2.118	1.198
380.35	0.165	0.047	0.603	0.445	0.201	0.283	1.256	2.095	1.474	1.588
382.63	0.151	0.113	0.193	0.338	0.355	0.141	0.982	1.453	2.097	1.169
383.13	0.226	0.046	0.673	0.536	0.131	0.307	1.029	1.303	1.278	1.773
383.68	0.110	0.078	0.678	0.362	0.367	0.235	1.407	2.121	0.952	0.990
384.58	0.136	0.098	0.189	0.349	0.385	0.119	1.071	1.732	1.672	0.910
384.99	0.272	0.028	0.087	0.642	0.117	0.054	0.975	1.825	1.625	1.073
385.07	0.125	0.137	0.016	0.319	0.424	0.014	1.052	1.349	2.284	1.183

**Table 2. (Continued)**

<i>T</i> /K	$x_1$	$x_2$	$x_3$	$y_1$	$y_2$	$y_3$	$\gamma_1$	$\gamma_2$	$\gamma_3$	$\gamma_4$
385.80	0.026	0.199	0.026	0.063	0.626	0.026	0.980	1.346	2.532	1.306
386.73	0.181	0.029	0.755	0.471	0.095	0.410	1.033	1.375	1.315	2.272
387.02	0.083	0.060	0.662	0.309	0.294	0.314	1.465	2.040	1.137	1.398
388.25	0.120	0.074	0.193	0.319	0.301	0.167	1.013	1.644	1.983	1.095
390.80	0.022	0.092	0.782	0.094	0.434	0.412	1.535	1.797	1.089	1.671
390.81	0.107	0.062	0.194	0.313	0.287	0.158	1.048	1.761	1.690	1.099
391.38	0.078	0.022	0.876	0.368	0.151	0.464	1.673	2.581	1.070	2.009
393.63	0.096	0.059	0.169	0.292	0.262	0.171	1.018	1.582	1.886	1.072
395.44	0.102	0.061	0.188	0.311	0.270	0.166	0.978	1.513	1.539	0.969
396.00	0.046	0.011	0.922	0.313	0.097	0.576	2.164	2.985	1.061	1.628
399.34	0.072	0.040	0.157	0.248	0.198	0.200	1.009	1.550	1.924	1.063
403.26	0.060	0.029	0.128	0.233	0.174	0.176	1.040	1.723	1.807	1.035
403.27	0.020	0.009	0.899	0.153	0.088	0.691	2.062	2.819	1.005	1.837
407.16	0.049	0.028	0.105	0.195	0.161	0.150	0.977	1.518	1.641	1.043
409.77	0.002	0.002	0.989	0.013	0.017	0.963	1.523	2.139	1.019	1.603
410.62	0.044	0.029	0.082	0.167	0.129	0.147	0.864	1.092	1.832	1.028
412.73	0.028	0.018	0.052	0.140	0.130	0.110	1.087	1.696	2.016	1.008
413.03	0.034	0.025	0.026	0.162	0.155	0.053	1.029	1.446	1.926	1.001
416.98	0.021	0.015	0.017	0.115	0.116	0.038	1.087	1.664	1.858	1.002
418.32	0.019	0.013	0.016	0.094	0.089	0.036	0.955	1.434	1.792	1.026
420.98	0.013	0.006	0.010	0.081	0.057	0.023	1.138	1.887	1.685	1.004
423.64	0.008	0.003	0.003	0.046	0.021	0.009	0.995	1.319	2.024	1.012

**Table 3. Experimental Vapor–Liquid Equilibrium Data for 1-Pentanol (1) + Anisole (2) at 101.32 kPa**

<i>T</i> /K	$x_1$	$y_1$	$\gamma_1$	$\gamma_2$	<i>T</i> /K	$x_1$	$y_1$	$\gamma_1$	$\gamma_2$
422.80	0.057	0.153	1.843	0.993	410.87	0.588	0.667	1.146	1.252
419.69	0.125	0.276	1.688	0.995	410.62	0.622	0.689	1.127	1.286
418.69	0.146	0.310	1.663	1.001	410.53	0.644	0.701	1.112	1.314
417.55	0.175	0.351	1.621	1.002	410.44	0.669	0.717	1.098	1.340
416.70	0.213	0.395	1.547	1.006	410.33	0.688	0.729	1.090	1.367
414.80	0.283	0.470	1.476	1.022	410.17	0.720	0.748	1.075	1.420
413.71	0.349	0.521	1.377	1.048	410.12	0.730	0.758	1.074	1.423
413.00	0.393	0.554	1.326	1.071	410.14	0.755	0.776	1.062	1.451
412.42	0.435	0.575	1.268	1.115	410.06	0.781	0.792	1.051	1.510
412.13	0.459	0.588	1.241	1.137	410.08	0.796	0.803	1.045	1.535
411.76	0.488	0.609	1.224	1.153	410.06	0.830	0.828	1.035	1.605
411.45	0.515	0.626	1.204	1.176	410.07	0.868	0.858	1.025	1.705
411.21	0.543	0.642	1.181	1.201	410.17	0.904	0.892	1.019	1.783
411.07	0.568	0.652	1.152	1.241	410.31	0.941	0.930	1.016	1.874

**Table 4. Physical Properties of the Pure Components: Critical Pressure  $P_c$ , Mean Gyration Radius  $RD$ , Dipole Moment  $\mu$ , Association Parameter  $ETA$ , Critical Temperature  $T_c$ , Critical Compressibility Factor  $Z_c$ , and Antoine Constants  $A$ ,  $B$ , and  $C$** 

compound	$P_c^{11}$ /kPa	$RD^{11} \times 10^{10}$ /m	$\mu^{11} \times 10^{30}$ /C·m	$ETA^{12}$	$T_c^{11}$ /K	$Z_c^{11}$	Antoine constants <sup>13</sup>			range <i>T</i> /K
							$A$	$B$	$C$	
benzene	4898.051	3.0040	0.00	0.00	562.16	0.271	6.32580	1415.800	-25.122	353–523
cyclohexane	4075.292	3.2420	0.00	0.00	553.54	0.273	6.24778	1418.380	-19.379	354–501
1-pentanol	3879.734	3.6790	5.67	2.20	586.15	0.260	6.30736	1287.625	-111.820	347–429
anisole	4174.590	3.719	4.54	0.00	641.65	0.264	6.11015 <sup>14</sup>	1446.845 <sup>14</sup>	-73.9870 <sup>14</sup>	314–427

a Varian Star 3400 CX chromatograph equipped with a flame-ionization detector and an integrator (Hewlett-Packard 3392A). A 4-m stainless steel column filled with 10% Carbowax 1540 chromosorb W/HP 80/100 was used. The optimum operating conditions were the following: injection temperature, 170 °C; oven temperature, 110 °C (5.5 min) to 165 °C (3 min) with a heating rate of 30 °C·min<sup>-1</sup>; detector temperature, 250 °C; carrier gas, nitrogen with a flow rate of 16.64 mL·min<sup>-1</sup>. The peak areas were converted to mole fractions using weight factors determined by the gas chromatographic analysis of mixtures of known composition. The estimated uncertainty for mole fractions was determined as  $\pm 7 \times 10^{-3}$ .

## Results and Discussion

The thermodynamic consistency of the measured vapor–liquid equilibria data (binary and quaternary mixtures) has been tested with the McDermott and Ellis method<sup>7</sup> to reject

possible inconsistent equilibrium points. According to this test, two experimental points a and b are thermodynamically consistent when

$$D < D_{\max} \quad (1)$$

where  $D_{\max}$  is the maximum deviation and  $D$  is the local deviation, which is expressed as

$$D = \sum_{i=1}^{nc} [(x_{ia} + x_{ib}) |\ln \gamma_{ib} - \ln \gamma_{ia}|] \quad (2)$$

In this equation,  $x_{ia}$ ,  $\gamma_{ia}$ ,  $x_{ib}$ , and  $\gamma_{ib}$  are the mole fractions and the activity coefficients of component  $i$  in the points a and b, respectively, and  $nc$  is the number of components. McDermott and Ellis proposed a value of 0.01 for  $D_{\max}$  if the uncertainty in the mole fraction of the liquid and vapor compositions is between  $\pm 0.001$ . The maximum local deviation is not a constant, and Wisniak and Tamir<sup>8</sup>

**Table 5. Solvation Parameters<sup>12</sup>**

benzene–cyclohexane	0.00
benzene–1-pentanol	0.00
benzene–anisole	0.30
cyclohexane–1-pentanol	0.00
cyclohexane–anisole	0.00
1-pentanol–anisole	0.50

propose the following expression for this magnitude

$$D_{\max} = \sum_{i=1}^{nc} (x_{ia} + x_{ib}) \left( \frac{1}{x_{ia}} + \frac{1}{x_{ib}} + \frac{1}{y_{ia}} + \frac{1}{y_{ib}} \right) \Delta x + 2 \sum_{i=1}^{nc} |\ln \gamma_{ib} - \ln \gamma_{ia}| \Delta x + \sum_{i=1}^{nc} (x_{ia} + x_{ib}) \frac{\Delta P}{P} + \sum_{i=1}^{nc} (x_{ia} + x_{ib}) B_i \left( \frac{1}{(t_a + C_i)^2} + \frac{1}{(t_b + C_i)^2} \right) \Delta t \quad (3)$$

In eq 3,  $B_i$  and  $C_i$  are the Antoine constants and  $\Delta x$ ,  $\Delta P$ , and  $\Delta t$  are the uncertainties of mole fraction, pressure, and temperature, respectively. Only four out of all experimental data points did not meet the consistency criteria and thus were rejected.

The experimental VLE data for the quaternary mixture cyclohexane + benzene + 1-pentanol + anisole are given in Table 2 and the values for the binary 1-pentanol + anisole are given in Table 3. The values of the activity coefficients ( $\gamma_i$ ) were computed as follows

$$\gamma_i = \{\phi_i y_i P_i^S\} / \{\phi_i^S x_i P_i^S \exp[v_i^L(P - P_i^S)/RT]\} \quad (4)$$

where the liquid molar volume,  $v_i^L$ , was calculated by the Yen and Woods<sup>9</sup> equation and the fugacity coefficients,  $\phi_i$  and  $\phi_i^S$ , were obtained using a value of the second virial coefficient computed by the Hayden and O'Connell<sup>10</sup> method to characterize the vapor-phase deviation from ideal behavior.  $P_i^S$  is the vapor pressure that was calculated from the Antoine equation

$$\log P_i^S/\text{kPa} = A - B/(TK + C) \quad (5)$$

The properties of the pure components required to calculate  $\gamma_i$  are listed in Table 4. The necessary solvation parameters are shown in Table 5. The quaternary system does not exhibit azeotropic behavior. There are two binary azeotropes corresponding to the benzene + cyclohexane mixture<sup>15</sup> (unstable node, minimum azeotrope) and the 1-pentanol + anisole mixture. The vapor–liquid equilibrium data for this binary mixture are given in Table 3. At 101.32 kPa, the estimated azeotrope boiling temperature was 410.05 K and the estimated azeotrope mole fraction composition of 1-pentanol was 0.823.

**Activity Coefficients Prediction Model.** Prediction of VLE for the binary and quaternary systems studied at 101.32 kPa has been carried out by the UNIFAC group contribution method.<sup>5</sup> The group interaction parameters were those published by Hansen et al.<sup>16</sup> However, the interaction parameters reported by Yañez Torres et al.<sup>14</sup> were used for the aromatic ether group instead of those of the conventional paraffinic ether group. The results are compared with the experimental values, and the root-mean-square deviations for the temperature  $\sigma(T)$  and the composition of the vapor phase  $\sigma(y_i)$  are  $\sigma(T/K) = 2.11$ ,  $\sigma(y_1) = 0.033$ ,  $\sigma(y_2) = 0.031$ ,  $\sigma(y_3) = 0.029$ , and  $\sigma(y_4) = 0.018$

**Table 6. UNIFAC Parameters Used for the Vapor–Liquid Equilibria Predictions**

Pure group parameters <sup>16</sup>				
main group	subgroup	$R_k$	$Q_k$	
CH2	CH3	0.9011	0.848	
	CH2	0.6744	0.540	
ACH	ACH	0.5313	0.400	
	AC	0.3652	0.120	
OH		1.0000	1.200	
ACOCH2 <sup>14</sup>	ACOCH3 <sup>14</sup>	1.5102 <sup>14</sup>	1.208 <sup>14</sup>	
UNIFAC <sup>16</sup> binary interaction parameters				
	CH2	ACH	OH	ACOCH2 <sup>14</sup>
CH2		61.13	986.5	181.7 <sup>14</sup>
ACH	-11.12		636.1	35.48 <sup>14</sup>
OH	156.4	89.6		246.3 <sup>14</sup>
ACOCH2 <sup>14</sup>	33.31 <sup>14</sup>	74.76 <sup>14</sup>	251.5 <sup>14</sup>	

for the quaternary system and  $\sigma(T/K) = 1.09$  and  $\sigma(y_1) = 0.018$  for the binary system. The small differences between experimental and predicted values indicate good accuracy of the prediction for both studied systems. The parameters used for UNIFAC predictions are reported in Table 6.

### Literature Cited

- Iglesias, M.; Orge, B.; Marino, G.; Tojo, J. Vapor-Liquid Equilibria for the Ternary System Acetone + Methanol + Water at 101.325 kPa. *J. Chem. Eng. Data* **1999**, *44*, 661–665.
- Orge, B.; Marino, G.; Iglesias, M.; Tojo, J. Phase Equilibria of the Ternary System Benzene + Cyclohexane + 1-Pentanol at  $P = 101.3$  kPa. *J. Chem. Eng. Data* **2001**, *46*, 410–413.
- Iglesias, M.; Marino, G.; Orge, B.; Piñeiro, M. M.; Tojo, J. Liquid–Liquid Equilibria, and Thermodynamic Properties of the System Methyl Acetate + Methanol + Water at 298.15 K. *Phys. Chem. Liq.* **1999**, *37*, 193–213.
- Fredenslund, A.; Gmehling, J.; Rasmussen, P. *Vapor-Liquid Equilibria Using UNIFAC*; Elsevier: Amsterdam, 1977.
- TRC Thermodynamic Tables*; Thermodynamic Research Center, Texas A&M University: College Station, TX, 1994.
- Riddick, J. A.; Bunger, W. B.; Sakano, T. K. *Organic Solvents, Physical Properties and Methods of Purification*, 4th ed.; Wiley-Interscience: New York, 1986.
- McDermott, C.; Ellis, S. R. M. A Multicomponent Consistency Test. *Chem. Eng. Sci.* **1965**, *20*, 293–296.
- Wisniak, J.; Tamir, A. Vapor-Liquid Equilibria in the Ternary Systems Water–Formic Acid–Acetic Acid and Water–Acetic Acid–Propionic Acid. *J. Chem. Eng. Data* **1977**, *22*, 253–260.
- Yen, L. C.; Woods, S. S. A Generalized Equation for Computer Calculation of Liquid Densities. *AIChE J.* **1966**, *12*, 95–99.
- Hayden, J. G.; O'Connell, J. P. A Generalized Method for Predicting Second Virial Coefficients. *Ind. Eng. Chem. Process Des. Dev.* **1975**, *14*, 209–213.
- Daubert, T. E.; Danner, R. P. *Physical and Thermodynamic Properties of Pure Chemicals. Data Compilation*; Taylor and Francis: Washington, 1989.
- Prausnitz, J.; Anderson, T.; Greens, E.; Eckert, C.; Hsieh, R.; O'Connell, J. *Computer Calculations for Multicomponent Vapor-Liquid and Liquid-Liquid Equilibria*; Prentice Hall: New Jersey, 1980.
- Vapor-Liquid Equilibrium Data Collection: Chemistry Data Series*; Gmehling, J., Onken, U., Eds.; DECHEMA: Frankfurt/Main, Germany, 1977–1999.
- Yañez Torres, M. A.; Botini, S. B.; Brignole, E. A.; Samhuesa, V.; Reich, R. Vapor-Liquid Equilibria for Binary Mixtures with Anisole. *Fluid Phase Equilib.* **1992**, *8*, 85–98.
- Hiaki, T.; Tochigi, K.; Kojima, K. Measurement of Vapor-Liquid Equilibria and Determination of Azeotropic Point. *Fluid Phase Equilib.* **1986**, *26*, 83–102.
- Hansen, H. K.; Rasmussen, P.; Fredenslund, A.; Schiller, M.; Gmehling, J. Vapor-Liquid Equilibria by UNIFAC Group Contribution. 5. Revision and Extension. *Ind. Eng. Chem. Res.* **1991**, *30*, 2352–2355.