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Vapor−Liquid Equilibria on Seven Binary Systems: Ethylene Oxide + 2-Methylpropane; Acetophenone + Phenol; *cis*-1,3-Dichloropropene + 1,2-Dichloropropane; 1,5-Hexadiene + Allyl Chloride; Isopropyl Acetate + Acetonitrile; Vinyl Chloride + Methyl Chloride; and 1,4-Butanediol + γ-Butyrolactone[†]

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Vapor−liquid equilibria are reported for the following seven binary systems: ethylene oxide + 2-methylpropane; acetophenone + phenol; *cis*-1,3-dichloropropene + 1,2-dichloropropane; 1,5-hexadiene + allyl chloride; isopropyl acetate + acetonitrile; vinyl chloride + methyl chloride; and 1,4-butanediol + γ-butyrolactone. The system pressure and temperature were measured at several charge compositions along two or three isotherms for the first six systems and along one isotherm for the seventh system. Equilibrium vapor- and liquid-phase compositions were derived from the *PTx* data using the Soave equation of state to represent the vapor phase and the Wilson or the Redlich−Kister activity coefficient model to represent the liquid phase. Additional vapor−liquid equilibrium studies were performed on the 1,4-butanediol + γ-butyrolactone system at six compositions by directly analyzing samples that were withdrawn from the equilibrium vapor and liquid phases.

Introduction

This work is part of an ongoing investigation of the phase equilibria for systems of industrial interest sponsored by Project 805 of the Design Institute for Physical Properties (DIPPR) of the American Institute of Chemical Engineers. This paper reports experimental measurements that have been made under Project 805/97 and Project 805/98 to obtain vapor−liquid equilibrium data on seven binary systems. These systems and their measurement conditions are as follows:

1. Ethylene oxide + 2-methylpropane at 25 °C and 75 °C.
2. Acetophenone + phenol at 100 °C and 160 °C.
3. *cis*-1,3-Dichloropropene + 1,2-dichloropropane at 60 °C and 80 °C.
4. 1,5-Hexadiene + allyl chloride at 60 °C and 100 °C.
5. Isopropyl acetate + acetonitrile at 60 °C, 120 °C, and 180 °C.
6. Vinyl chloride + methyl chloride at 0 °C and 40 °C.
7. 1,4-Butanediol + γ-butyrolactone at 110 °C.

Vapor−liquid equilibria (VLE) were determined for each of the binary systems from total pressure−temperature−composition (*PTx*) measurements. With accurate pressure measurements and equations to model the vapor and liquid phases, *PTx* data can yield reliable phase composition information. An equation of state was used to represent the nonidealities in the vapor phase, and an activity coefficient equation was used to represent the nonidealities in the liquid phase.

Additional vapor−liquid equilibrium studies were performed on the 1,4-butanediol + γ-butyrolactone system at six compositions by directly analyzing samples that were withdrawn from the equilibrium vapor and liquid phases. The results of these measurements were used in conjunction with the *PTx* data to determine the VLE behavior of this system.

Experimental Section

The apparatus and procedures used for the *PTx* measurements have been described earlier.[1] Temperatures were measured using ITS-90 with platinum resistance thermometers. These thermometers were calibrated using ice and steam points and referenced to a standard platinum resistance thermometer with a NIST traceable calibration. Temperatures were measured with a precision of ± 0.01 K and an uncertainty of less than ± 0.05 K.

The *PTx* measurements for both isotherms of systems 1, 4, and 6 and for the 120 °C and 180 °C isotherms of system 5 were performed using a stainless steel apparatus. Pressures were measured using a calibrated Paroscientific pressure transducer with an estimated uncertainty of ± 0.5 kPa.

PTx measurements were performed in a glass still apparatus for systems 2 and 7. Pressures measured using this apparatus have an estimated uncertainty of ± 0.03 kPa.

A glass cell apparatus with an attached mercury manometer was used to measure *PTx* data for both isotherms of system 3 and for the 60 °C isotherm of system 5. Pressures were measured with this apparatus with an estimated uncertainty of ± 0.05 kPa.

Txy measurements on system 7 were performed at approximate liquid mole fractions of (0.101, 0. 306, 0. 516, and 0.707) 1,4-butanediol using a glass still apparatus identical to the one used for the *PTx* measurements. Two additional *Txy* points were measured at liquid mole fractions of (0.411 and 0.609) 1,4-butanediol using a glass cell apparatus similar to the one used for the *PTx* measurements. The internal volume of

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[†] This contribution will be part of a special print edition containing papers reporting experimental results from the various projects of the Design Institute for Physical Properties of the American Institute of Chemical Engineers.

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Table 1. *PTx* Measurement Results on Ethylene Oxide (A) + 2-Methylpropane (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					t = 25 °C[a]							
1	100.00	100.00	100.00	174.71	174.71	1.000	4.700	0.969	0.960	1.0000	0.9925	8.988
1	94.65	95.04	72.67	231.87	232.48	1.006	3.770	0.959	0.946	1.0012	0.9949	7.208
1	89.14	89.70	59.91	273.45	272.75	1.022	3.086	0.952	0.936	1.0020	0.9966	5.826
1	81.53	82.11	50.76	308.20	308.36	1.062	2.442	0.945	0.927	1.0028	0.9981	4.452
1	67.56	67.94	42.26	343.70	343.66	1.182	1.762	0.939	0.919	1.0035	0.9996	2.895
1	59.47	59.72	38.98	356.18	355.77	1.281	1.528	0.937	0.916	1.0037	1.0001	2.321
2	52.20	52.38	36.32	364.46	363.99	1.390	1.377	0.936	0.914	1.0039	1.0005	1.928
1	46.14	46.22	34.10	369.77	369.53	1.500	1.279	0.935	0.913	1.0040	1.0007	1.661
2	44.90	45.06	33.67	371.01	370.44	1.523	1.263	0.935	0.913	1.0040	1.0008	1.616
2	38.14	38.26	31.02	375.21	375.07	1.671	1.181	0.934	0.911	1.0041	1.0010	1.378
2	25.75	25.76	25.09	379.21	379.48	2.030	1.078	0.934	0.910	1.0042	1.0012	1.036
2	11.20	11.11	14.38	371.97	373.39	2.659	1.014	0.935	0.912	1.0041	1.0009	0.744
2	4.30	4.24	6.51	361.91	362.84	3.075	1.002	0.937	0.914	1.0039	1.0004	0.635
2	0.00	0.00	0.00	352.39	352.39	3.386	1.000	0.939	0.917	1.0037	1.0000	0.576
					t = 75 °C[b]							
1	100.00	100.00	100.00	766.7	766.7	1.000	3.235	0.911	0.887	1.0000	0.9816	4.627
1	94.65	95.35	83.91	890.7	890.6	1.004	2.733	0.897	0.868	1.0024	0.9866	3.928
1	89.14	90.19	73.38	988.9	989.5	1.016	2.333	0.886	0.853	1.0043	0.9907	3.336
1	81.53	82.68	63.85	1089.3	1089.5	1.047	1.931	0.874	0.838	1.0063	0.9949	2.701
1	67.56	68.31	52.77	1205.5	1204.7	1.138	1.486	0.862	0.820	1.0085	0.9997	1.929
1	59.48	59.93	47.82	1248.3	1247.9	1.210	1.331	0.857	0.813	1.0094	1.0015	1.632
2	52.20	52.51	43.66	1276.7	1276.7	1.285	1.232	0.854	0.809	1.0099	1.0027	1.427
1	46.15	46.25	40.12	1295.3	1295.2	1.357	1.169	0.852	0.806	1.0103	1.0034	1.284
2	44.90	45.16	39.50	1297.3	1297.8	1.370	1.159	0.852	0.806	1.0104	1.0036	1.261
2	38.14	38.30	35.40	1309.7	1310.8	1.460	1.108	0.851	0.803	1.0106	1.0041	1.133
2	25.75	25.67	26.79	1314.5	1315.3	1.654	1.044	0.851	0.802	1.0107	1.0043	0.944
2	11.20	10.96	13.68	1279.5	1279.2	1.937	1.007	0.856	0.808	1.0100	1.0028	0.777
2	4.30	4.15	5.73	1241.7	1242.6	2.093	1.001	0.861	0.813	1.0093	1.0012	0.713
2	0.00	0.00	0.00	1212.7	1212.7	2.196	1.000	0.865	0.817	1.0087	1.0000	0.678

[a] Wilson equation parameters: $\Lambda_{AB} = 0.5810$; $\Lambda_{BA} = 0.3235$. [b] Wilson equation parameters: $\Lambda_{AB} = 0.8706$; $\Lambda_{BA} = 0.3518$.

Table 2. *PTx* Measurement Results on Acetophenone (A) + Phenol (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					t = 100 °C[a]							
1	100.00	100.00	100.00	3.573	3.573	1.000	0.328	0.998	0.999	1.0000	0.9999	0.506
1	95.62	95.62	97.60	3.508	3.496	0.999	0.348	0.998	0.999	1.0000	0.9999	0.536
1	89.56	89.55	93.59	3.412	3.391	0.992	0.378	0.998	0.999	1.0000	0.9999	0.587
1	79.36	79.36	84.63	3.232	3.234	0.965	0.438	0.998	0.999	1.0000	0.9999	0.698
1	69.24	69.23	72.52	3.118	3.126	0.917	0.508	0.998	0.999	1.0000	0.9999	0.853
1	58.88	58.88	57.03	3.098	3.106	0.842	0.590	0.998	0.999	1.0000	0.9999	1.079
2	50.91	50.92	43.98	3.172	3.178	0.769	0.659	0.998	0.999	1.0000	0.9999	1.321
1	49.11	49.11	41.03	3.222	3.207	0.750	0.676	0.998	0.999	1.0000	0.9999	1.387
2	40.74	40.74	28.08	3.408	3.409	0.658	0.752	0.998	0.999	1.0000	0.9999	1.761
2	31.41	31.42	16.27	3.774	3.765	0.545	0.835	0.998	0.999	1.0000	0.9999	2.359
2	20.95	20.97	7.26	4.305	4.307	0.417	0.918	0.997	0.998	1.0000	1.0000	3.387
2	10.29	10.30	2.21	4.904	4.940	0.296	0.978	0.997	0.998	1.0001	1.0000	5.090
2	4.82	4.83	0.79	5.229	5.255	0.240	0.995	0.997	0.998	1.0001	1.0000	6.373
2	0.00	0.00	0.00	5.506	5.506	0.196	1.000	0.997	0.998	1.0001	1.0000	7.840
					t = 160 °C[b]							
1	100.00	100.00	100.00	32.024	32.024	1.000	0.515	0.987	0.993	1.0000	0.9994	0.850
1	94.57	94.56	95.37	31.801	31.751	1.000	0.511	0.987	0.993	1.0000	0.9994	0.844
1	89.84	89.83	91.18	31.477	31.513	0.999	0.517	0.987	0.993	1.0000	0.9994	0.855
1	79.42	79.41	80.57	31.084	31.093	0.986	0.555	0.987	0.993	1.0000	0.9994	0.930
1	68.98	68.99	67.38	31.064	31.087	0.948	0.618	0.987	0.993	1.0000	0.9994	1.077
1	68.97	68.98	67.36	31.145	31.087	0.948	0.619	0.987	0.993	1.0000	0.9994	1.078
1	59.63	59.66	53.64	31.779	31.768	0.892	0.690	0.987	0.992	1.0000	0.9994	1.278
2	58.94	58.95	52.56	31.817	31.855	0.887	0.696	0.987	0.992	1.0000	0.9994	1.296
1	54.32	54.36	45.53	32.487	32.553	0.852	0.734	0.987	0.992	1.0000	0.9994	1.424
2	52.11	52.13	42.17	33.001	32.979	0.833	0.753	0.987	0.992	1.0000	0.9994	1.494
2	42.85	42.89	29.10	35.425	35.372	0.748	0.829	0.986	0.991	1.0001	0.9995	1.830
2	32.30	32.36	17.15	39.191	39.195	0.647	0.905	0.984	0.990	1.0003	0.9996	2.311
2	21.43	21.50	8.65	43.860	43.902	0.549	0.962	0.983	0.989	1.0004	0.9997	2.893
2	10.83	10.88	3.39	48.676	48.651	0.470	0.992	0.981	0.988	1.0006	0.9999	3.482
2	6.01	6.04	1.70	50.709	50.734	0.441	0.998	0.980	0.987	1.0007	0.9999	3.728
2	0.00	0.00	0.00	53.234	53.234	0.413	1.000	0.979	0.987	1.0008	1.0000	3.989

[a] Redlich−Kister parameters: A = −1.3588; B = 0.2571; C = −0.0120. [b] Redlich−Kister parameters: A = −0.9317; B = 0.1099; C = 0.1578.

the glass cell used for the *Txy* measurements was about 1200 cm^3. Temperatures were measured with a precision of ± 0.01 K and an uncertainty of less than ± 0.05 K.

The *Txy* measurements were made by charging the cell with the desired amount of each compound. After achieving equilibrium at the desired temperature, the system was degassed.

Table 3. *PTx* Measurement Results on *cis*-1,3-Dichloropropene (A) + 1,2-Dichloropropane (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					$t = 60$ °C[a]							
1	100.00	100.00	100.00	22.605	22.605	1.000	1.012	0.991	0.991	1.0000	0.9997	1.345
1	94.69	94.69	93.00	23.074	23.022	1.000	1.011	0.991	0.991	1.0000	0.9997	1.343
1	89.15	89.16	85.98	23.433	23.453	1.000	1.010	0.991	0.991	1.0000	0.9998	1.341
1	79.23	79.24	74.05	24.085	24.221	1.001	1.007	0.991	0.990	1.0001	0.9998	1.338
1	69.55	69.57	63.14	24.826	24.961	1.001	1.006	0.990	0.990	1.0001	0.9998	1.335
1	58.18	58.19	51.12	25.835	25.825	1.002	1.004	0.990	0.990	1.0001	0.9998	1.331
2	51.54	51.56	44.47	26.218	26.324	1.003	1.003	0.990	0.990	1.0001	0.9999	1.329
1	46.30	46.31	39.39	26.731	26.717	1.004	1.002	0.990	0.989	1.0001	0.9999	1.327
2	41.26	41.27	34.65	27.068	27.094	1.004	1.002	0.989	0.989	1.0002	0.9999	1.326
2	30.78	30.80	25.17	27.903	27.872	1.006	1.001	0.989	0.989	1.0002	0.9999	1.323
2	20.69	20.70	16.51	28.688	28.618	1.007	1.000	0.989	0.989	1.0002	0.9999	1.320
2	10.10	10.11	7.87	29.387	29.397	1.009	1.000	0.989	0.988	1.0002	1.0000	1.317
2	4.34	4.34	3.34	29.835	29.820	1.010	1.000	0.988	0.988	1.0002	1.0000	1.316
2	0.00	0.00	0.00	30.138	30.138	1.011	1.000	0.988	0.988	1.0003	1.0000	1.315
					$t = 80$ °C[b]							
1	100.00	100.00	100.00	47.292	47.292	1.000	1.011	0.984	0.984	1.0000	0.9995	1.299
1	94.30	94.31	92.75	48.105	48.107	1.000	1.010	0.984	0.984	1.0000	0.9995	1.297
1	88.83	88.84	86.01	48.912	48.886	1.000	1.009	0.984	0.983	1.0001	0.9996	1.295
1	79.36	79.39	74.87	50.232	50.223	1.001	1.007	0.983	0.983	1.0001	0.9996	1.292
1	69.13	69.16	63.49	51.765	51.654	1.001	1.005	0.983	0.982	1.0001	0.9997	1.289
1	58.95	58.97	52.77	53.089	53.067	1.002	1.003	0.982	0.982	1.0002	0.9997	1.287
2	52.54	52.56	46.30	54.036	53.951	1.002	1.003	0.982	0.982	1.0002	0.9997	1.285
1	49.03	49.05	42.85	54.441	54.433	1.003	1.002	0.982	0.982	1.0002	0.9998	1.284
1	44.73	44.75	38.70	54.933	55.023	1.003	1.002	0.982	0.981	1.0003	0.9998	1.283
2	41.72	41.74	35.85	55.565	55.433	1.004	1.002	0.981	0.981	1.0003	0.9998	1.282
2	31.59	31.62	26.55	56.878	56.810	1.005	1.001	0.981	0.981	1.0003	0.9998	1.280
2	22.20	22.23	18.29	58.185	58.081	1.006	1.000	0.981	0.980	1.0004	0.9999	1.277
2	11.29	11.31	9.09	59.451	59.553	1.008	1.000	0.980	0.980	1.0004	0.9999	1.275
2	6.13	6.14	4.89	60.259	60.246	1.009	1.000	0.980	0.980	1.0004	1.0000	1.274
2	0.00	0.00	0.00	61.068	61.068	1.010	1.000	0.980	0.979	1.0005	1.0000	1.272

[a] Wilson equation parameters: $\Lambda_{AB} = 1.102$; $\Lambda_{BA} = 0.892$. [b] Wilson equation parameters: $\Lambda_{AB} = 1.1010$; $\Lambda_{BA} = 0.8940$.

Table 4. *PTx* Measurement Results on 1,5-Hexadiene (A) + Allyl Chloride (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					$t = 60$ °C[a]							
1	100.00	100.00	100.00	103.15	103.15	1.000	1.170	0.963	0.975	1.0000	0.9981	1.832
1	94.02	94.06	89.74	108.11	108.39	1.000	1.158	0.961	0.974	1.0002	0.9982	1.811
1	87.23	87.30	79.38	113.90	114.14	1.002	1.143	0.959	0.972	1.0005	0.9984	1.786
1	77.31	77.39	66.23	122.45	122.14	1.006	1.123	0.957	0.970	1.0009	0.9987	1.745
1	68.35	68.43	55.99	128.93	128.92	1.012	1.104	0.954	0.968	1.0012	0.9989	1.704
1	57.84	57.91	45.47	136.38	136.31	1.024	1.082	0.952	0.966	1.0015	0.9991	1.650
2	50.93	50.98	39.25	141.41	140.82	1.035	1.068	0.950	0.965	1.0017	0.9993	1.610
1	47.17	47.22	36.05	142.93	143.16	1.043	1.060	0.950	0.964	1.0018	0.9993	1.587
2	41.23	41.29	31.23	146.31	146.66	1.057	1.049	0.948	0.963	1.0020	0.9994	1.549
2	30.83	30.89	23.27	152.17	152.28	1.091	1.031	0.947	0.962	1.0022	0.9996	1.474
2	21.13	21.18	16.16	157.06	156.91	1.136	1.016	0.945	0.961	1.0024	0.9998	1.395
2	10.39	10.42	8.24	161.48	161.30	1.209	1.004	0.944	0.959	1.0026	0.9999	1.295
2	5.34	5.35	4.35	162.92	163.05	1.255	1.001	0.944	0.959	1.0027	1.0000	1.243
2	0.00	0.00	0.00	164.65	164.65	1.315	1.000	0.943	0.959	1.0028	1.0000	1.185
					$t = 100$ °C[b]							
1	100.00	100.00	100.00	316.61	316.61	1.000	1.155	0.918	0.944	1.0000	0.9948	1.710
1	94.02	94.11	90.48	330.74	331.01	1.000	1.137	0.914	0.941	1.0006	0.9953	1.682
1	87.23	87.39	80.77	346.05	346.63	1.002	1.119	0.911	0.938	1.0013	0.9957	1.650
1	77.31	77.50	68.23	368.52	368.12	1.007	1.094	0.905	0.934	1.0022	0.9964	1.604
1	68.34	68.54	58.24	386.11	386.19	1.014	1.074	0.901	0.930	1.0030	0.9969	1.562
1	57.84	57.99	47.71	406.51	405.86	1.025	1.054	0.896	0.926	1.0039	0.9975	1.513
2	50.93	51.03	41.30	417.68	417.99	1.035	1.042	0.893	0.924	1.0044	0.9979	1.481
1	47.17	47.27	37.98	425.27	424.29	1.041	1.036	0.892	0.922	1.0047	0.9981	1.464
2	41.23	41.36	32.93	432.71	433.81	1.051	1.028	0.890	0.920	1.0051	0.9983	1.437
2	30.83	30.98	24.41	448.78	449.53	1.073	1.016	0.886	0.917	1.0058	0.9988	1.390
2	21.13	21.26	16.71	463.26	463.12	1.098	1.008	0.883	0.915	1.0064	0.9992	1.346
2	10.39	10.48	8.27	477.53	477.00	1.132	1.002	0.880	0.912	1.0070	0.9996	1.298
2	5.34	5.38	4.27	483.18	483.11	1.150	1.000	0.879	0.911	1.0072	0.9998	1.276
2	0.00	0.00	0.00	489.25	489.25	1.171	1.000	0.878	0.910	1.0075	1.0000	1.252

[a] Wilson equation parameters: $\Lambda_{AB} = 0.5168$; $\Lambda_{BA} = 1.3859$. [b] Wilson equation parameters: $\Lambda_{AB} = 0.8402$; $\Lambda_{BA} = 1.0162$.

The vapor line was further purged by withdrawing additional material through the vapor line into a weighed, evacuated sample vial. Three or more vapor samples were then withdrawn into weighed, evacuated sample vials. The system was allowed to

Table 5. *PTx* Measurement Results on Isopropyl Acetate (A) + Acetonitrile (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa measd	P/kPa calcd	γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
					$t = 60$ °C[a]							
1	100.00	100.00	100.00	37.733	37.733	1.000	1.662	0.983	0.988	1.0000	0.9998	2.156
1	94.05	94.07	88.59	40.125	40.178	1.002	1.578	0.982	0.987	1.0001	0.9998	2.043
1	88.43	88.46	79.81	42.087	42.173	1.006	1.506	0.981	0.987	1.0002	0.9999	1.940
1	79.24	79.28	68.26	45.100	44.868	1.020	1.401	0.980	0.986	1.0003	0.9999	1.779
1	70.23	70.26	59.18	46.879	46.936	1.043	1.312	0.979	0.985	1.0004	1.0000	1.630
1	58.68	58.70	49.50	48.893	48.911	1.087	1.217	0.978	0.984	1.0005	1.0000	1.450
1	50.47	50.49	43.40	49.877	49.926	1.131	1.161	0.978	0.984	1.0005	1.0000	1.330
1	40.01	40.02	36.01	50.856	50.809	1.204	1.102	0.978	0.984	1.0006	1.0000	1.185
2	35.77	35.78	33.03	50.945	51.040	1.241	1.082	0.977	0.984	1.0006	1.0000	1.129
1	31.92	31.93	30.28	51.369	51.185	1.278	1.066	0.977	0.984	1.0006	1.0000	1.080
2	30.57	30.57	29.29	51.164	51.221	1.292	1.061	0.977	0.984	1.0006	1.0000	1.063
2	20.38	20.38	21.42	51.277	51.215	1.418	1.028	0.977	0.984	1.0006	1.0000	0.939
2	10.62	10.61	12.54	50.595	50.655	1.578	1.008	0.978	0.984	1.0006	1.0000	0.828
2	4.68	4.68	6.04	49.995	49.957	1.700	1.002	0.978	0.984	1.0005	1.0000	0.764
2	0.00	0.00	0.00	49.155	49.155	1.813	1.000	0.979	0.984	1.0005	1.0000	0.715
					$t = 120$ °C[b]							
1	100.00	100.00	100.00	249.59	249.59	1.000	1.502	0.931	0.952	1.0000	0.9991	1.766
1	94.63	94.72	91.32	260.90	260.02	1.001	1.453	0.928	0.950	1.0004	0.9993	1.706
1	89.29	89.44	83.72	270.07	269.38	1.004	1.407	0.926	0.948	1.0008	0.9995	1.646
1	78.63	78.82	70.92	285.17	285.08	1.016	1.322	0.922	0.944	1.0015	0.9998	1.526
1	69.98	70.15	62.18	294.82	295.17	1.033	1.259	0.919	0.942	1.0019	1.0000	1.429
1	58.98	59.10	52.50	304.47	304.86	1.066	1.189	0.917	0.940	1.0023	1.0001	1.307
1	49.05	49.12	44.61	310.40	310.85	1.109	1.135	0.915	0.938	1.0026	1.0003	1.198
1	39.06	39.08	37.04	313.37	314.37	1.169	1.089	0.915	0.938	1.0027	1.0003	1.090
2	36.21	36.23	34.89	315.09	314.90	1.190	1.077	0.914	0.937	1.0027	1.0003	1.060
1	29.15	29.14	29.46	314.68	315.31	1.251	1.051	0.915	0.937	1.0027	1.0003	0.985
2	25.67	25.66	26.69	315.43	314.99	1.286	1.041	0.915	0.937	1.0027	1.0003	0.948
2	15.53	15.50	17.86	312.61	311.74	1.412	1.016	0.916	0.938	1.0026	1.0003	0.843
2	10.39	10.35	12.74	308.68	308.49	1.494	1.007	0.917	0.938	1.0025	1.0002	0.791
2	5.09	5.06	6.74	304.20	303.70	1.594	1.002	0.919	0.939	1.0023	1.0001	0.738
2	0.00	0.00	0.00	297.37	297.37	1.709	1.000	0.920	0.941	1.0020	1.0000	0.688
					$t = 180$ °C[c]							
1	100.00	100.00	100.00	939.9	939.9	1.000	1.332	0.835	0.885	1.0000	0.9971	1.504
1	94.63	94.85	92.62	972.5	970.6	1.001	1.304	0.829	0.880	1.0013	0.9976	1.469
1	89.29	89.65	85.81	1001.1	999.1	1.002	1.277	0.824	0.876	1.0025	0.9982	1.433
1	78.63	79.11	73.57	1049.7	1049.2	1.010	1.225	0.816	0.868	1.0045	0.9991	1.360
1	69.98	70.42	64.71	1082.1	1082.9	1.022	1.185	0.810	0.863	1.0059	0.9997	1.298
1	58.98	59.29	54.46	1114.7	1116.4	1.044	1.138	0.805	0.858	1.0073	1.0004	1.218
1	49.05	49.22	45.87	1136.2	1137.5	1.075	1.100	0.802	0.855	1.0082	1.0008	1.144
1	39.06	39.11	37.58	1147.2	1150.1	1.117	1.067	0.800	0.853	1.0087	1.0010	1.067
2	36.21	36.24	35.23	1151.2	1152.0	1.132	1.058	0.800	0.852	1.0088	1.0010	1.045
1	29.15	29.14	29.35	1153.0	1153.5	1.175	1.039	0.800	0.852	1.0089	1.0011	0.990
2	25.67	25.65	26.38	1152.5	1152.5	1.200	1.031	0.801	0.852	1.0088	1.0010	0.962
2	15.53	15.45	17.18	1142.7	1141.7	1.290	1.012	0.804	0.853	1.0084	1.0008	0.881
2	10.39	10.30	12.04	1133.1	1131.2	1.348	1.006	0.806	0.854	1.0080	1.0006	0.839
2	5.09	5.02	6.23	1117.3	1116.1	1.418	1.001	0.809	0.856	1.0073	1.0004	0.796
2	0.00	0.00	0.00	1096.9	1096.9	1.497	1.000	0.813	0.859	1.0065	1.0000	0.755

[a] Wilson equation parameters: $\Lambda_{AB} = 0.6244$; $\Lambda_{BA} = 0.8760$. [b] Wilson equation parameters: $\Lambda_{AB} = 0.5737$; $\Lambda_{BA} = 1.0198$. [c] Wilson equation parameters: $\Lambda_{AB} = 0.5772$; $\Lambda_{BA} = 1.1458$.

re-equilibrate to the run temperature between each of the vapor samples. The stirrer was then turned off, and the liquid line was purged. Three or more liquid samples were then withdrawn into weighed, evacuated sample vials.

The vapor and liquid samples were analyzed using gas chromatography to determine their compositions. A flame ionization detector was used to quantify the results. Each sample was injected three or more times onto the GC column in order to accurately determine the composition of each sample. The average of the analysis results from the three or more replicate samples was then used to determine the vapor and liquid compositions from each run. The standard deviations obtained from the three replicate vapor samples were typically less than ± 2 % of the reported composition of the minor component while the standard deviations obtained from the replicate liquid samples were always less than ± 0.5 % of the reported composition of the minor component.

Multiple calibration standards were prepared on a regular basis during the *Txy* measurements covering the composition ranges of interest. These standards were analyzed by GC on a daily basis and the resulting information was used to determine accurate GC response factors. The estimated overall accuracy of the relative volatilities obtained from these *Txy* measurements is conservatively estimated to be within ± 3 % of the reported values. The relative volatilities obtained from the measured *Txy* data using the glass cell apparatus and the glass still apparatus were consistent with one another.

PTx Data Reduction Procedure

The results of the *PTx* measurements, which are total pressure as a function of charge composition at constant temperature, were reduced to equilibrium phase compositions and activity and fugacity coefficients. The Wilson[2] and three-parameter Redlich−Kister[3] activity coefficient models were used to represent the liquid-phase nonidealities. The three-parameter

Table 6. *PTx* Measurement Results on Vinyl Chloride (A) + Methyl Chloride (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					$t = 0$ °C[a]							
1	100.00	100.00	100.00	172.0	172.0	1.000	0.994	0.963	0.971	1.0000	0.9980	1.476
1	94.07	94.11	91.54	176.8	177.0	1.000	0.995	0.962	0.970	1.0001	0.9981	1.477
1	89.83	89.89	85.75	180.7	180.6	1.000	0.995	0.961	0.969	1.0003	0.9982	1.478
1	79.50	79.60	72.51	189.2	189.5	1.000	0.996	0.959	0.968	1.0005	0.9984	1.479
1	67.94	68.05	58.99	199.4	199.6	0.999	0.997	0.957	0.966	1.0008	0.9986	1.480
2	62.86	62.92	53.40	203.9	204.1	0.999	0.998	0.956	0.965	1.0009	0.9987	1.481
1	57.63	57.73	47.97	208.3	208.7	0.999	0.998	0.955	0.964	1.0011	0.9988	1.482
1	51.98	52.07	42.29	213.3	213.6	0.999	0.998	0.954	0.963	1.0012	0.9989	1.482
2	51.56	51.66	41.89	213.9	214.0	0.999	0.998	0.954	0.963	1.0012	0.9989	1.482
2	44.72	44.84	35.40	220.1	220.0	0.998	0.999	0.953	0.962	1.0014	0.9991	1.483
1	42.79	42.86	33.58	222.2	221.8	0.998	0.999	0.952	0.962	1.0015	0.9991	1.483
2	37.55	37.68	28.94	227.0	226.4	0.998	0.999	0.951	0.961	1.0016	0.9992	1.484
2	26.15	26.28	19.35	236.0	236.5	0.997	1.000	0.949	0.959	1.0019	0.9995	1.485
2	20.92	21.04	15.20	241.0	241.2	0.996	1.000	0.948	0.959	1.0020	0.9996	1.486
2	9.57	9.64	6.70	251.1	251.4	0.995	1.000	0.946	0.957	1.0023	0.9998	1.487
2	5.05	5.09	3.48	255.5	255.5	0.995	1.000	0.945	0.956	1.0024	0.9999	1.488
2	0.00	0.00	0.00	260.1	260.1	0.994	1.000	0.945	0.955	1.0026	1.0000	1.489
					$t = 40$ °C[b]							
1	100.00	100.00	100.00	601.5	601.5	1.000	0.999	0.910	0.931	1.0000	0.9941	1.386
1	94.07	94.17	92.10	617.8	616.8	1.000	0.999	0.907	0.929	1.0004	0.9944	1.386
1	89.83	89.99	86.64	628.7	627.9	1.000	0.999	0.906	0.927	1.0007	0.9947	1.386
1	79.50	79.75	73.98	655.2	655.0	1.000	0.999	0.902	0.924	1.0015	0.9953	1.385
1	67.93	68.22	60.79	685.5	685.7	1.000	0.999	0.897	0.920	1.0023	0.9959	1.384
2	62.87	63.01	55.18	700.1	699.6	1.000	1.000	0.895	0.918	1.0027	0.9962	1.384
1	57.63	57.89	49.84	712.6	713.3	1.000	1.000	0.893	0.916	1.0031	0.9965	1.383
1	51.98	52.21	44.13	727.7	728.6	1.000	1.000	0.891	0.915	1.0035	0.9969	1.383
2	51.56	51.81	43.74	728.7	729.7	1.000	1.000	0.891	0.914	1.0035	0.9969	1.383
2	44.72	45.02	37.20	747.9	748.0	1.000	1.000	0.889	0.912	1.0040	0.9973	1.382
1	42.79	42.96	35.27	753.6	753.6	1.000	1.000	0.888	0.912	1.0042	0.9974	1.382
2	37.55	37.88	30.62	767.2	767.3	1.000	1.000	0.886	0.910	1.0046	0.9977	1.382
2	26.15	26.49	20.69	796.5	798.3	0.999	1.000	0.882	0.906	1.0054	0.9984	1.381
2	20.92	21.23	16.33	812.0	812.6	0.999	1.000	0.880	0.904	1.0058	0.9987	1.381
2	9.57	9.76	7.27	843.2	844.1	0.999	1.000	0.875	0.901	1.0067	0.9994	1.380
2	5.05	5.16	3.79	856.0	856.7	0.999	1.000	0.874	0.899	1.0070	0.9997	1.379
2	0.00	0.00	0.00	870.9	870.9	0.999	1.000	0.872	0.898	1.0074	1.0000	1.379

[a] Wilson equation parameters: $\Lambda_{AB} = 1.0029$; $\Lambda_{BA} = 1.0029$. [b] Wilson equation parameters: $\Lambda_{AB} = 1.0006$; $\Lambda_{BA} = 1.0006$.

Table 7. *PTx* Measurement Results on 1,4-Butanediol (A) + γ-Butyrolactone (B)

run no.	$100z_A$	$100x_A$	$100y_A$	P/kPa		γ_A	γ_B	ϕ_A	ϕ_B	PF_A	PF_B	α_{BA}
				measd	calcd							
					$t = 110$ °C[a]							
1	100.00	100.00	100.00	0.664	0.664	1.000	2.611	1.000	1.000	1.0000	0.9999	20.211
1	92.94	92.96	42.44	1.452	1.461	1.004	2.322	0.999	0.999	1.0000	0.9999	17.899
1	88.09	88.11	31.05	1.917	1.909	1.012	2.152	0.999	0.999	1.0000	0.9999	16.457
1	77.34	77.37	20.06	2.694	2.682	1.046	1.842	0.998	0.999	1.0001	0.9999	13.629
1	66.00	66.03	14.90	3.265	3.267	1.108	1.590	0.998	0.999	1.0001	1.0000	11.104
1	56.99	57.01	12.39	3.610	3.619	1.183	1.433	0.998	0.998	1.0001	1.0000	9.376
2	55.51	55.53	12.05	3.658	3.671	1.198	1.410	0.998	0.998	1.0001	1.0000	9.111
2	49.83	49.84	10.87	3.833	3.852	1.263	1.330	0.998	0.998	1.0001	1.0000	8.150
1	45.41	45.42	10.04	3.993	3.981	1.323	1.275	0.998	0.998	1.0001	1.0000	7.455
2	41.98	42.00	9.44	4.068	4.074	1.377	1.236	0.998	0.998	1.0001	1.0000	6.943
1	40.73	40.75	9.23	4.110	4.107	1.398	1.222	0.998	0.998	1.0001	1.0000	6.763
2	34.16	34.17	8.13	4.268	4.274	1.529	1.159	0.998	0.998	1.0001	1.0000	5.863
2	20.21	20.22	5.69	4.632	4.612	1.949	1.059	0.997	0.998	1.0001	1.0000	4.204
2	10.91	10.91	3.62	4.892	4.847	2.414	1.018	0.997	0.998	1.0001	1.0000	3.264
2	5.49	5.49	2.05	5.048	4.993	2.803	1.005	0.997	0.998	1.0001	1.0000	2.773
2	0.00	0.00	0.00	5.150	5.150	3.340	1.000	0.997	0.998	1.0001	1.0000	2.316

[a] Wilson equation parameters: $\Lambda_{AB} = 0.4070$; $\Lambda_{BA} = 0.6931$.

Redlich−Kister expansion did a good job of correlating the strong negative deviation from ideality that was found in the acetophenone + phenol system (system 2). The Wilson equation was used for the other six systems. The Soave−Redlich−Kwong equation of state[4] was used to represent the vapor phase in the data reduction procedure. All Soave binary interaction parameters were assumed to be zero. The procedure used to reduce the *PTx* data has been described earlier[1] and is similar to the method proposed by Barker.[5]

Results and Discussion

The results of the vapor−liquid equilibrium measurements are described below. The *PTx* data are presented in Tables 1 through 7. These tables give the run number, the charge compositions (z_A) on a mole basis, the calculated liquid (x_A) and vapor (y_A) compositions on a mole basis, the measured and correlated pressures, the activity (γ_A and γ_B) and fugacity coefficients (φ_A and φ_B), the Poynting corrections (PF_A and

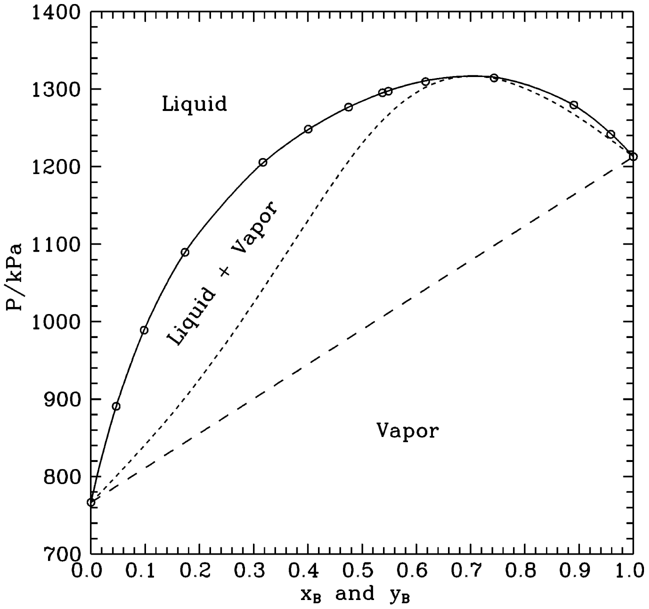

Figure 1. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for ethylene oxide (A) + 2-methylpropane (B) at 75 °C.

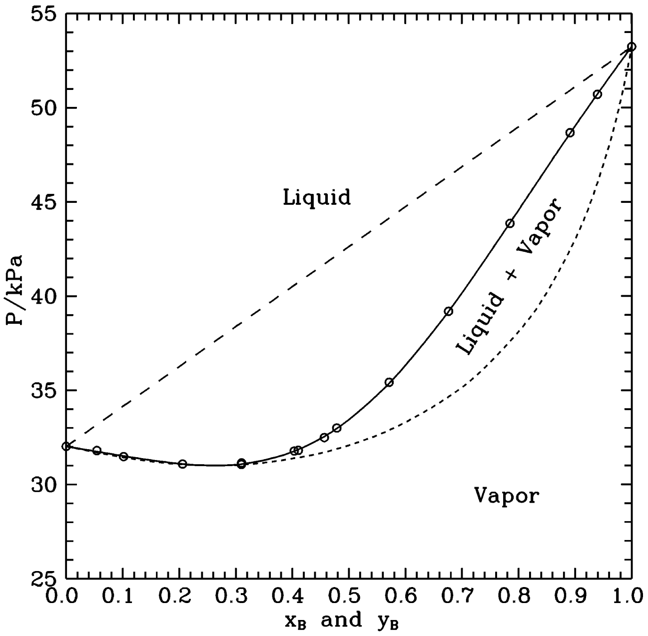

Figure 2. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for acetophenone (A) + phenol (B) at 160 °C.

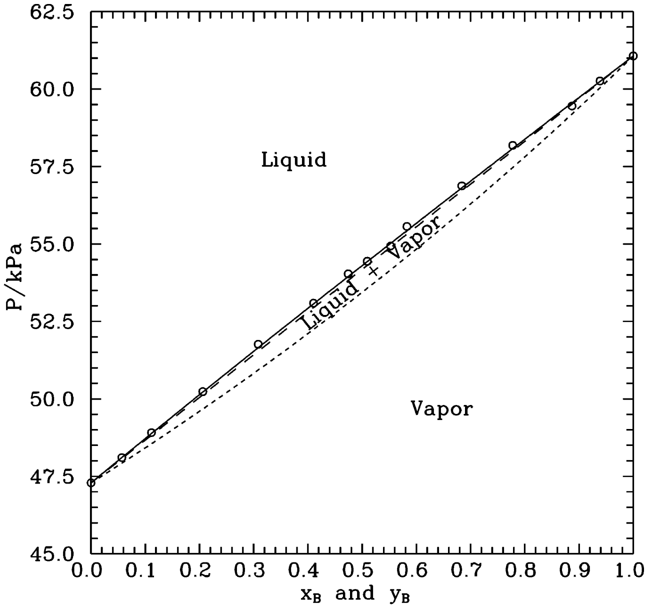

Figure 3. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for *cis*-1,3-dichloropropene (A) + 1,2-dichloropropane (B) at 80 °C.

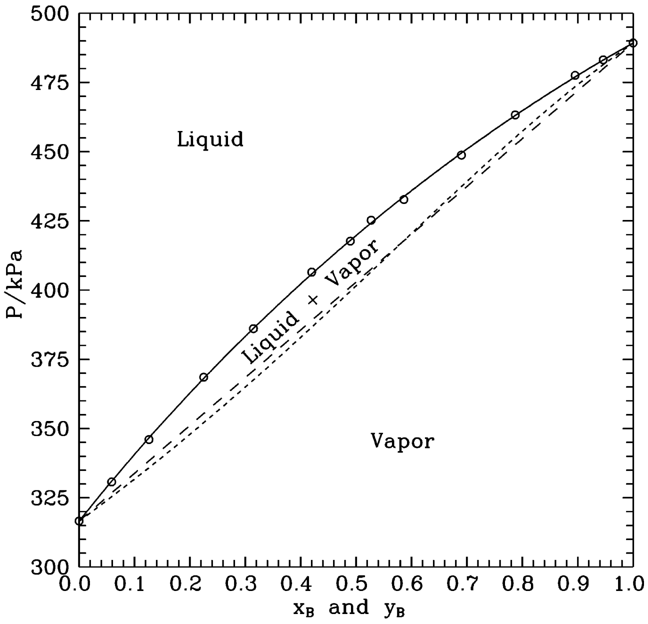

Figure 4. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for 1,5-hexadiene (A) + allyl chloride (B) at 100 °C.

PF_B), and the relative volatilities (α_{BA}). The relative volatility was determined from

$$\alpha_{BA} = \frac{y_B/x_B}{y_A/x_A} \tag{1}$$

The activity coefficient parameters used in the correlation are given at the bottom of each table. Figures 1−7 show total pressure as a function of liquid and vapor composition to illustrate the *PTx* data of each binary system at one of the measured temperatures.

The *Txy* data that were measured on the 1,4-butanediol + γ-butyrolactone system (system 7) are presented in Table 8. This table reports the correlated pressure, the measured liquid composition, and the measured and correlated vapor composition for each measured point. The measured and correlated relative volatility of γ-butyrolactone over 1,4-butanediol is also shown. The correlated values were obtained from the *PTx* correlation using the Wilson parameters shown in the footnote of Table 7. A plot of the measured and correlated relative volatility versus liquid composition is included to illustrate the data in Figure 8.

1. Ethylene Oxide + 2-Methylpropane. Results of the *PTx* measurements on ethylene oxide + 2-methylpropane at 25 °C and 75 °C are given in Table 1. The Wilson activity coefficient equation was used to reduce the data. The system pressure as a function of liquid and vapor composition at 75 °C is plotted in Figure 1 to illustrate the data. This system exhibits significant

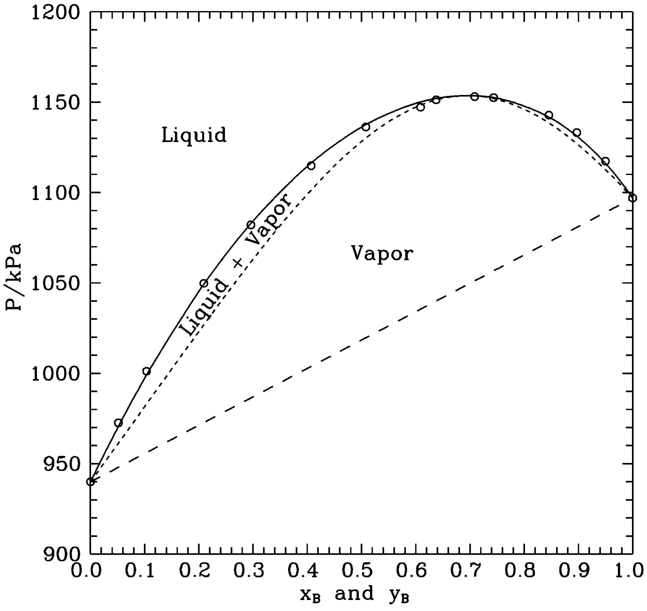

Figure 5. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for isopropyl acetate (A) + acetonitrile (B) at 180 °C.

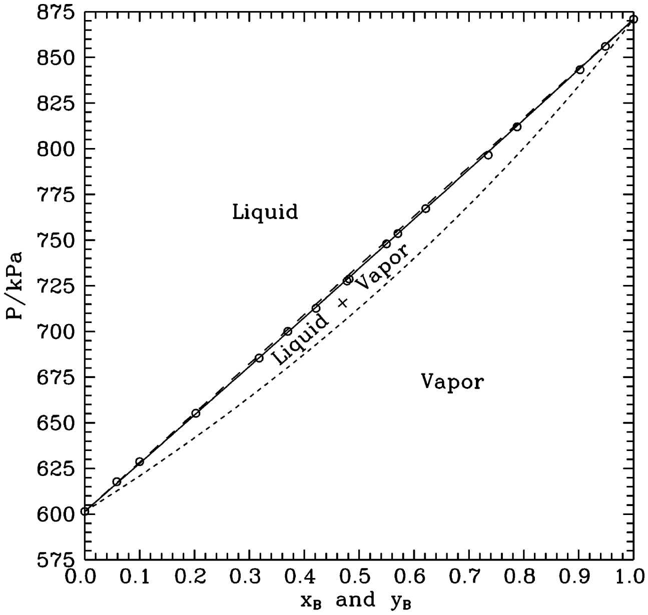

Figure 6. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for vinyl chloride (A) + methyl chloride (B) at 40 °C.

positive deviation from Raoult's law, and the data indicate that a minimum-boiling azeotrope exists at each of the two temperatures. The expression $P = \sum(P_i^\circ x_i)$ defines Raoult's law, where P is the total system pressure, P_i° is the vapor pressure of component i, and x_i is the liquid mole fraction of component i.

2. Acetophenone + Phenol. *PTx* measurements on acetophenone + phenol were performed at 100 °C and 160 °C. The three-parameter Redlich−Kister activity coefficient model was used to correlate the measured data. Results of the measurements are given in Table 2, and the results at 160 °C are plotted in Figure 2. This system shows significant negative deviation from ideality with a maximum-boiling azeotrope at each of the two temperatures.

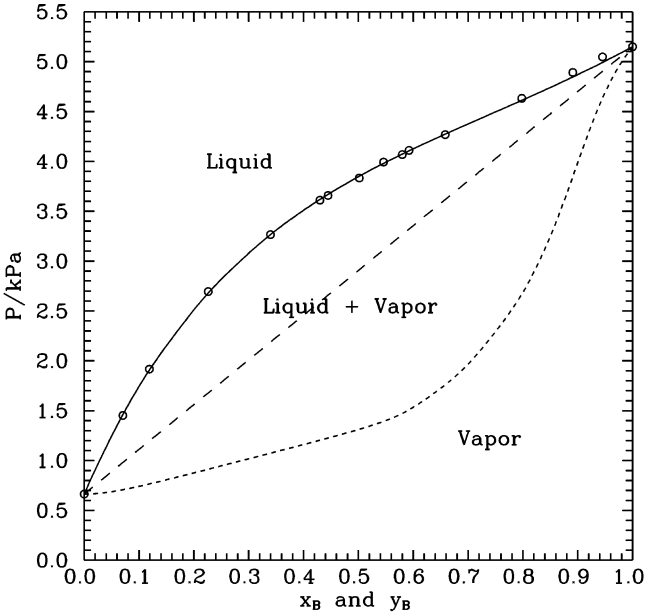

Figure 7. ○, measured *PTx* data; —, *P*−*x* correlation; - - -, *P*−*y* correlation; − −, Raoult's law for 1,4-butanediol (A) + γ-butyrolactone (B) at 110 °C.

Table 8. *Txy* Measurement Results on 1,4-Butanediol (A) + γ-Butyrolactone (B)[a]

P/kPa correlated	$100x_A$ measured	$100y_A$ measured	$100y_A$ correlated	α_{BA} measured	α_{BA} correlated
		t = 110 °C			
3.050	70.67	16.59	16.62	12.12	12.09
3.476	60.91	13.28	13.37	10.18	10.10
3.799	51.57	11.06	11.21	8.56	8.43
4.098	41.08	9.43	9.29	6.70	6.81
4.361	30.61	7.73	7.54	5.27	5.41
4.869	10.08	3.53	3.40	3.06	3.19

[a] The correlated values were obtained at the measured liquid compositions using the model described in the *PTx* Data Reduction Procedure section using the Wilson equation parameters shown in the footnotes of Table 7.

3. *cis*-1,3-Dichloropropene + 1,2-Dichloropropane. Results of measurements on *cis*-1,3-dichloropropene + 1,2-dichloropropane at 60 °C and 80 °C are reported in Table 3. The data were reduced using the Wilson activity coefficient equation. This system exhibits nearly ideal behavior with activity coefficients that are only slightly greater than unity. The results of the 80 °C measurements are plotted in Figure 3. Measurements were attempted at 100 °C, but the *cis*-1,3-dichloropropene was not sufficiently stable at this temperature to obtain accurate *PTx* data.

4. 1,5-Hexadiene + Allyl Chloride. *PTx* measurements were performed at 60 °C and 100 °C on 1,5-hexadiene + allyl chloride. The Wilson activity coefficient model was used to reduce the data. Results of the measurements are given in Table 4 and the 100 °C data are plotted in Figure 4. This system exhibits slight positive deviation from ideality.

5. Isopropyl Acetate + Acetonitrile. *PTx* measurements on isopropyl acetate + acetonitrile were performed at 60 °C, 120 °C, and 180 °C. The Wilson activity coefficient model was used to correlate the measured data. Results of the measurements are reported in Table 5, and the 180 °C data are plotted in Figure 5. This system shows positive deviation from ideality with a minimum-boiling azeotrope at each of the three temperatures.

6. Vinyl Chloride + Methyl Chloride. The results of the *PTx* measurements on vinyl chloride + methyl chloride at 0

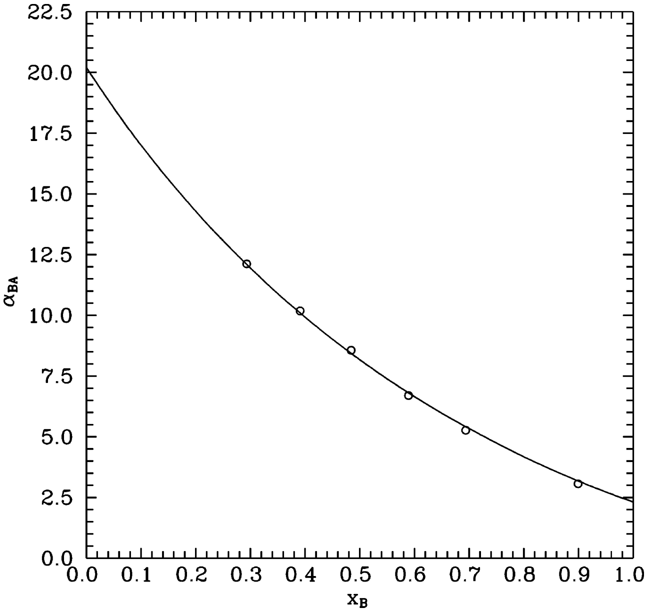

Figure 8. Relative volatility of γ-butyrolactone (B) over 1,4-butanediol (A) at 110 °C obtained from ○, measured *Txy* data; —, *P*−*x* correlation.

Table 9. Constants Used in Data Reduction Procedure[a]

compound	MW	T_C/K	P_C/kPa	Z_C	ω
ethylene oxide	44.053	469.15	7190	0.259	0.1974
2-methylpropane	58.123	407.8	3640	0.278	0.1835
acetophenone	120.151	709.6	4010	0.262	0.3830
phenol	94.113	694.25	6130	0.243	0.4435
cis-1,3-dichloropropene	110.970	594.4	4704	0.264	0.2307
1,2-dichloropropane	112.986	572	4240	0.259	0.2564
1,5-hexadiene	82.145	508	3350	0.269	0.2259
allyl chloride	76.525	514.15	4710	0.258	0.1478
isopropyl acetate	102.133	532	3290	0.250	0.3678
acetonitrile	41.053	545.5	4830	0.184	0.3379
vinyl chloride	62.499	432	5670	0.283	0.1001
methyl chloride	50.488	416.25	6680	0.276	0.1531
1,4-butanediol	90.122	667	4880	0.261	1.1770
γ-butyrolactone	86.090	739	5940	0.256	0.3690

[a] Constants are measured and/or estimated values reported in ref 6.

Table 10. Measured and Literature Vapor Pressures.

compound	t/°C	*P*/kPa measured	*P*/kPa literature[a]	% dev[b]
ethylene oxide	25	174.7	175.2	-0.27
	75	766.7	772.4	-0.74
2-methylpropane	25	352.4	351.2	0.33
	75	1212.7	1209.5	0.26
acetophenone	100	3.573	3.595	-0.61
	160	32.024	31.955	0.22
phenol	100	5.506	5.474	0.58
	160	53.234	53.308	-0.14
cis-1,3-dichloropropene	60	22.61	22.83	-0.96
	80	47.29	47.21	0.17
1,2-dichloropropane	60	30.14	30.51	-1.23
	80	61.07	61.44	-0.61
1,5-hexadiene	60	103.2	103.5	-0.34
	100	316.6	312.0	1.49
allyl chloride	60	164.7	161.3	2.07
	100	489.3	460.0[c]	6.37
isopropyl acetate	60	37.73	37.26	1.28
	120	249.6	252.1	-1.01
	180	939.9	958.32	-1.92
acetonitrile	60	49.16	49.57	-0.90
	120	297.4	297.1	0.09
	180	1096.9	1096.3	0.05
vinyl chloride	0	172.0	175.1	-1.77
	40	601.5	604.7	-0.53
methyl chloride	0	260.1	259.3	0.31
	40	870.9	866.0	0.57
1,4-butanediol	110	0.664	0.674	-1.48
γ-butyrolactone	110	5.150	5.209	-1.13

[a] Literature data calculated from correlations in ref 6. [b] Percent deviation: 100 × (measured − literature)/literature. [c] The DIPPR 801 correlation[6] for allyl chloride is based on experimental vapor pressure data that were measured up to a temperature of 55 °C. At higher temperatures, this correlation is an extrapolation of the measured vapor pressure curve up to a measured critical temperature (241 °C) and a predicted critical pressure (4710 kPa).

Table 11. Source and Purity of Chemicals

compound	CAS Registry No.	supplier	purity, mass % Wiltec analysis	purity, mass % supplier analysis
ethylene oxide	75-21-8	Aldrich		99.5+
2-methylpropane	75-28-5	Aldrich	99.4	99.4
acetophenone	98-86-2	Aldrich	99.6	99.7
phenol	108-95-2	Aldrich	99.91	99.97
cis-1,3-dichloropropene	10061-01-5	DowElanco	97.5	98.23
1,2-dichloropropane	78-87-5	Aldrich	99.6	99.6
1,5-hexadiene	592-42-7	Aldrich	99.0	99.3
allyl chloride	107-05-1	Aldrich	98.8	98.7
isopropyl acetate	108-21-4	Aldrich	99.9	99.9
acetonitrile	75-05-8	Aldrich	99.97	99.95
vinyl chloride	75-01-4	Aldrich		99.5+
methyl chloride	74-87-3	Aldrich		99.9
1,4-butanediol	110-63-4	Aldrich	99.7	99.8
γ-butyrolactone	96-48-0	Aldrich	99.8	99.5

°C and 40 °C are given in Table 6. The Wilson activity coefficient equation with symmetrical parameters was used to reduce the measured data. The system pressure as a function of liquid and vapor composition at 40 °C is plotted in Figure 6. This system exhibits nearly ideal behavior.

7. 1,4-Butanediol + γ-Butyrolactone. Results of the *PTx* measurements on 1,4-butanediol + γ-butyrolactone at 110 °C are listed in Table 7 and plotted in Figure 7. The Wilson activity coefficient equation was used to reduce the data. *Txy* data are shown in Table 8 together with a comparison between the measured *Txy* data and the correlation of the measured *PTx* data. Relative volatilities obtained from the *Txy* data agree well with corresponding values obtained from the *PTx* correlation. Figure 8 is a plot of the relative volatility of γ-butyrolactone over 1,4-butanediol versus liquid composition. The *PTx* correlation is shown as a smooth curve while the measured *Txy* points are shown as open circles. This system exhibits moderate positive deviation from ideality.

Ancillary Data. Table 9 gives the physical constants for each compound used in the data reduction procedures. Table 10 compares the measured pure component vapor pressures to correlations reported in the DIPPR 801 database.[6] Table 11 lists the source and purity of the chemicals used in this study. The chemicals were thoroughly degassed before being used whenever possible. Table 11 also lists the Chemical Abstracts Service Registry number for each chemical.

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