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Isothermal Vapor–Liquid Equilibrium Data for Ether + Glycol, Chloroalkene + Glycol, Epoxy Ether + Alkane, Epoxy Ether + Alkene, and Epoxy Ether + Chloroalkane Systems

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A Dvorak–Boublik equilibrium recirculation apparatus has been used to measure isothermal vapor–liquid equilibrium (VLE) data for 10 different binary systems: diisopropyl ether + 2-methoxyethanol, trichloroethylene + 2-methoxyethanol, 1,2-epoxybutane + *n*-hexane, 1,2-epoxyhexane + *n*-heptane, 1,2-epoxybutane + *n*-heptane, 1,2-epoxybutane + 1-hexene, 1,2-epoxybutane + 1-octene, 1,2-epoxybutane + 1-chlorobutane, 1,2-epoxybutane + 2-chlorobutane, and epichlorohydrin (1-chloro-2,3-epoxypropane) + 2-chlorobutane. For each system except the last one, two isothermal sets of VLE data at pressures ranging from 7 to 102 kPa have been measured. Computer programs, using a numerical routine based on the maximum likelihood principle, have been used to test the data for thermodynamic consistency and to calculate group interaction parameters (formerly not available) for the UNIFAC model.

Introduction

Vapor–liquid equilibrium (VLE) data were measured in order to estimate new group interaction parameters for the UNIFAC model, describing the interactions between the ether group (main group 13) and the glycol group (main group 47), the chlorine bound to an unsaturated carbon (main group 37) and the glycol group (main group 47), the alkane group (main group 1) and the epoxy ether group (main group 51), the alkene group (main group 2) and the epoxy ether group, and the chlorinated carbon group (main group 21) and the epoxy ether group. The group numbers in parentheses are those given in ref 8, except for the epoxy ether which is a new group. VLE data for the systems mentioned have not been published previously.

Experimental Section

Apparatus and Procedures. The VLE measurements were performed in an all-glass cell originally proposed by Dvorak and Boublik (*1*), and later modified by Boublikova and Lu (*2*). The apparatus has been used previously in the laboratory to produce accurate VLE data (*3–5*).

The cell provides for the recirculation of the liquid phase and the condensed vapor phase. The equilibrium temperature of the mixture was determined by a Systemteknik s 1220 digital thermometer equipped with a platinum resistance probe, with a resolution of 0.01 K. The thermomether was checked by measuring the ice point and the boiling point of distilled water.

The pressure was measured by a Crouzet Quartz Mano 2100 digital pressure gauge, with a resolution of 0.001 kPa and a calibration made by a "Service de Metrologie Habilite par le Bureau National de Metrologie" (attestation no. 74-02-1007) on October 26, 1989. Full agreement was found between this calibration and a calibration made at atmospheric pressure by a mercury U tube manometer and a cathetometer.

The compositions of the binary mixtures were determined by measuring either their refractive index or their density at 293.15 K and comparing the results with a calibration curve (refractive index vs composition or density vs composition).

Table 1. Source and Purity of the Compounds

substance	supplier	min purity, %
2-methoxyethanol	Merck	99.5
diisopropyl ether	Fluka	99.0
trichloroethylene	Merck	99.5
1,2-epoxybutane	Aldrich	99.0
1,2-epoxyhexane	Aldrich	99.0
epichlorohydrin	Aldrich	99.0
n-hexane	Merck	99.0
n-heptane	Merck	99.0
1-hexene	Aldrich	99.6
1-octene	Sigma	99.0
1-chlorobutane	Aldrich	99.5
2-chlorobutane	Aldrich	99.0

Table 2. Antoine Parameters, Equation 1, and Mean Deviations in Pressure

substance	A_i	B_i	C_i	σP/Pa
2-methoxyethanol	6.775 093 4	1654.319	222.844	8.0
diisopropyl ether	6.002 930 9	1141.731	217.654	54.7
trichloroethylene	6.100 307 8	1272.018	223.925	37.3
1,2-epoxybutane	6.259 151 9	1246.009	229.861	13.3
1,2-epoxyhexane	6.149 141 2	1372.835	212.888	46.7
epichlorohydrin	6.236 875 6	1368.299	207.710	82.7
n-hexane	5.980 837 9	1137.886	218.168	52.0
n-heptane	6.204 248 0	1367.651	227.542	32.0
1-hexene	6.494 082 0	1431.583	255.884	82.7
1-octene	5.883 763 1	1244.138	199.947	52.0
1-chlorobutane	6.082 035 4	1225.277	222.407	36.0
2-chlorobutane	5.825 701 0	1067.217	211.498	61.3

The refractive index was measured by an ABBEMAT digital automatic refractometer, with a resolution of 2×10^{-5} g/cm^3. The prism of the refractometer, the U tube of the density meter, and the samples were kept at the desired temperature by a HETO circulating thermostatic bath.

Refractive Index and Density vs Composition. For each binary system, approximately 20 mixtures of known composition were prepared gravimetrically, using a Mettler AE 163 digital balance with a resolution of 10^{-5} g. The

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Table 3. VLE Data for Diisopropyl Ether (1) + 2-Methoxyethanol (2) at 331.02 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	7.612	0.3124	0.8771	51.275
0.0151	0.4049	13.248	0.4204	0.8924	55.624
0.0349	0.6113	19.003	0.5432	0.9091	59.045
0.0587	0.7157	25.396	0.6215	0.9171	61.090
0.0976	0.7794	32.045	0.7626	0.9353	64.670
0.1365	0.8221	38.064	0.8851	0.9578	68.015
0.1248	0.8121	36.590	1.0000	1.0000	72.370
0.2113	0.8560	45.275			

[a] Mean deviation in y_1 0.0037.

Table 4. VLE Data for Diisopropyl Ether (1) + 2-Methoxyethanol (2) at 341.01 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	12.143	0.3029	0.8611	71.010
0.0146	0.3694	19.008	0.4137	0.8756	77.147
0.0340	0.5695	27.082	0.5378	0.8916	82.280
0.0583	0.6761	35.322	0.6170	0.9026	85.194
0.0928	0.7431	44.005	0.7612	0.9273	90.468
0.1199	0.7773	50.120	0.8851	0.9534	95.232
0.1292	0.7872	51.894	1.0000	1.0000	100.946
0.2043	0.8343	62.370			

[a] Mean deviation in y_1 0.0028.

Table 5. VLE Data for Trichloroethylene (1) + 2-Methoxyethanol (2) at 341.01 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	12.143	0.4319	0.8139	43.168
0.0220	0.1769	14.363	0.5446	0.8483	47.052
0.0474	0.3311	17.345	0.6782	0.8809	50.460
0.1370	0.5867	25.942	0.7991	0.9083	52.880
0.2201	0.6942	32.167	0.8928	0.9347	54.265
0.3139	0.7604	37.776	1.0000	1.0000	55.090

[a] Mean deviation in y_1 0.0016.

Table 6. VLE Data for Trichloroethylene (1) + 2-Methoxyethanol (2) at 357.98 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	25.035	0.4319	0.7841	76.722
0.0227	0.1608	29.314	0.5578	0.8281	83.812
0.0608	0.3470	36.416	0.6779	0.8609	88.680
0.1373	0.5416	48.351	0.8000	0.8922	92.598
0.2181	0.6523	58.524	0.8939	0.9245	94.816
0.3265	0.7345	69.074	1.0000	1.0000	95.649

[a] Mean deviation in y_1 0.0025.

Table 7. VLE Data for 1,2-Epoxybutane (1) + *n*-Hexane (2) at 313.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	37.320	0.6091	0.6111	50.207
0.0732	0.1511	41.182	0.7079	0.6777	49.984
0.1614	0.2750	44.468	0.8170	0.7566	49.015
0.2288	0.3461	46.260	0.8744	0.8117	48.031
0.2827	0.3944	47.506	0.9525	0.9108	45.949
0.3615	0.4538	48.744	0.9780	0.9540	44.964
0.4304	0.5007	49.538	1.0000	1.0000	43.853
0.5258	0.5578	50.128			

[a] Mean deviation in y_1 0.0021.

Table 8. VLE Data for 1,2-Epoxybutane (1) + *n*-Hexane (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	77.404	0.5594	0.5812	101.684
0.0957	0.1782	86.107	0.6476	0.6406	101.889
0.1592	0.2628	90.385	0.7437	0.7081	101.085
0.2270	0.3376	94.255	0.8772	0.8256	97.977
0.2780	0.3844	96.358	0.9480	0.9116	94.748
0.3584	0.4480	98.513	0.9762	0.9540	93.398
0.4337	0.5029	100.434	1.0000	1.0000	91.299
0.5426	0.5739	101.611			

[a] Mean deviation in y_1 0.0033.

Table 9. VLE Data for 1,2-Epoxyhexane (1) + *n*-Heptane (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	21.037	0.5664	0.3550	22.654
0.0333	0.0267	20.924	0.6487	0.4164	21.406
0.0800	0.0602	20.681	0.7210	0.4814	20.105
0.1456	0.1027	27.107	0.7828	0.5464	18.896
0.2342	0.1567	26.285	0.8989	0.7203	16.187
0.3250	0.2094	25.428	0.9384	0.8077	15.154
0.4172	0.2615	24.527	0.9797	0.9240	13.797
0.4935	0.3079	23.607	1.0000	1.0000	13.138

[a] Mean deviation in y_1 0.0077.

Table 10. VLE Data for 1,2-Epoxyhexane (1) + *n*-Heptane (2) at 363.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	78.918	0.6335	0.4388	62.532
0.0523	0.0430	78.328	0.7039	0.5034	59.522
0.1456	0.1027	76.400	0.7786	0.5827	55.739
0.2466	0.1750	74.380	0.8441	0.6685	52.084
0.3159	0.2199	72.677	0.8970	0.7528	48.953
0.4209	0.2852	69.891	0.9365	0.8320	46.253
0.4983	0.3386	67.414	0.9762	0.9281	43.506
0.5697	0.3895	64.953	1.0000	1.0000	41.363

[a] Mean deviation in y_1 0.0081.

Table 11. VLE Data for 1,2-Epoxybutane (1) + *n*-Heptane (2) at 313.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	12.303	0.5891	0.8139	36.488
0.0366	0.2028	14.933	0.6950	0.8554	40.366
0.0967	0.4115	19.077	0.7915	0.8932	41.784
0.1557	0.5234	22.363	0.9386	0.9285	42.706
0.2499	0.6301	26.611	0.9775	0.9605	43.328
0.3450	0.7026	30.015	1.0000	1.0000	43.624
0.4665	0.7661	33.613			

[a] Mean deviation in y_1 0.0031.

Table 12. VLE Data for 1,2-Epoxybutane (1) + *n*-Heptane (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	28.077	0.5908	0.8034	75.787
0.0456	0.2028	34.118	0.6978	0.8483	80.300
0.1001	0.3783	41.006	0.7917	0.8878	83.850
0.1690	0.5018	48.085	0.8706	0.9245	86.527
0.2501	0.5983	55.347	0.9359	0.9585	88.773
0.3505	0.6782	62.629	0.9792	0.9850	90.195
0.4752	0.7498	69.985	1.0000	1.0000	90.718

[a] Mean deviation in y_1 0.0017.

composition of these samples covered the whole concentration range. To correlate the refractive index, an excess refractive index approach was used. The difference between the real and the ideal refractive index divided by the product of the mole fractions was fitted to third- or fourth-order polynomials. For the density a third- or fourth-order polynomial was used to fit the points obtained. The accuracy in determining the composition of the samples was more than ±0.0005 in molar fraction.

Materials. Table 1 lists the pure components used, their suppliers, an their minimum guaranteed purities. The compounds were all used without further purification except for 1-hexene which was purified from 98% to 99.6% by

Table 13. VLE Data for 1,2-Epoxybutane (1) + 1-Hexene (2) at 313.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	45.326	0.6567	0.6237	50.136
0.0476	0.0740	46.391	0.7445	0.7010	49.422
0.1112	0.1570	47.474	0.8238	0.7686	48.445
0.2156	0.2698	48.956	0.8929	0.8437	47.048
0.3383	0.3810	50.016	0.9508	0.9194	45.475
0.4541	0.4701	50.495	0.9833	0.9696	44.354
0.5702	0.5581	50.519	1.0000	1.0000	43.648

[a] Mean deviation in y_1 0.0056.

Table 14. VLE Data for 1,2-Epoxybutane (1) + 1-Hexene (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	91.604	0.6522	0.6287	102.020
0.0480	0.0729	93.987	0.7459	0.7074	100.765
0.1152	0.1599	96.283	0.8273	0.7864	98.840
0.2163	0.2682	98.923	0.8962	0.8567	96.555
0.3266	0.3681	100.966	0.9469	0.9200	94.207
0.4357	0.4602	102.130	0.9844	0.9743	92.015
0.5478	0.5287	102.528	1.0000	1.0000	91.028

[a] Mean deviation in y_1 0.0054.

Table 15. VLE Data for 1,2-Epoxybutane (1) + 1-Octene (2) at 323.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	8.080	0.4213	0.8621	36.803
0.0187	0.1549	9.455	0.5164	0.8944	41.520
0.0540	0.3860	12.665	0.6107	0.9194	45.986
0.0658	0.4410	13.631	0.7856	0.9573	53.783
0.0993	0.5502	16.355	0.8506	0.9682	56.649
0.1338	0.6267	18.935	0.9123	0.9800	59.534
0.2293	0.7490	25.611	1.0000	1.0000	64.108
0.2952	0.7996	29.710			

[a] Mean deviation in y_1 0.0033.

Table 16. VLE Data for 1,2-Epoxybutane (1) + 1-Octene (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	12.486	0.4014	0.8414	50.668
0.0189	0.1496	14.501	0.4571	0.8764	57.646
0.0638	0.4080	19.877	0.4967	0.9077	64.195
0.0772	0.4571	21.351	0.5930	0.9573	75.961
0.1399	0.6123	27.983	0.7763	0.9656	80.040
0.2111	0.7112	34.922	0.8414	0.9827	84.531
0.3254	0.8024	44.883	1.0000	1.0000	90.888

[a] Mean deviation in y_1 0.0036.

Table 17. VLE Data for 1,2-Epoxybutane (1) + 1-Chlorobutane (2) at 313.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	25.799	0.5462	0.6656	35.874
0.0365	0.0609	26.501	0.6580	0.7598	37.785
0.0868	0.1398	27.457	0.7510	0.8305	39.421
0.1686	0.2569	28.995	0.8417	0.8919	41.003
0.2584	0.3716	30.671	0.9156	0.9399	42.222
0.3106	0.4317	31.684	0.9676	0.9780	43.122
0.4282	0.5566	33.785	1.0000	1.0000	43.642

[a] Mean deviation in y_1 0.0023.

Table 18. VLE Data for 1,2-Epoxybutane (1) + 1-Chlorobutane (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	55.238	0.5502	0.6628	75.310
0.0340	0.0556	56.516	0.6573	0.7496	79.092
0.0906	0.1408	58.585	0.7541	0.8290	82.428
0.1697	0.2521	61.538	0.8498	0.8861	85.704
0.2683	0.3751	65.147	0.9179	0.9453	88.011
0.3165	0.4297	66.988	0.9715	0.9774	89.913
0.4268	0.5465	70.955	1.0000	1.0000	90.888

[a] Mean deviation in y_1 0.0025.

Table 19. VLE Data for 1,2-Epoxybutane (1) + 2-Chlorobutane (2) at 313.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	38.150	0.5937	0.6228	41.825
0.0330	0.0429	38.396	0.6958	0.7179	42.411
0.0948	0.1128	38.799	0.7813	0.7990	42.804
0.1794	0.2074	39.414	0.8626	0.8730	43.122
0.2731	0.3049	39.981	0.9237	0.9302	43.333
0.3840	0.4270	40.682	0.9686	0.9716	43.555
0.4962	0.5298	41.363	1.0000	1.0000	43.653

[a] Mean deviation in y_1 0.0020.

Table 20. VLE Data for 1,2-Epoxybutane (1) + 2-Chlorobutane (2) at 333.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	78.355	0.6010	0.6322	86.697
0.0348	0.0459	79.066	0.6888	0.7148	87.818
0.0973	0.1173	79.979	0.7782	0.7941	88.740
0.1751	0.2004	81.265	0.8624	0.8748	89.674
0.2792	0.3139	82.650	0.9233	0.9242	90.255
0.3782	0.4154	83.931	0.9697	0.9738	90.935
0.4889	0.5242	85.386	1.0000	1.0000	90.035

[a] Mean deviation in y_1 0.0017.

Table 21. VLE Data for 2-Chlorobutane (1) + Epichlorohydrin (2) at 338.15 K[a]

x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	16.498	0.2794	0.7412	48.923
0.0113	0.1130	18.354	0.3793	0.8010	56.407
0.0306	0.2517	21.410	0.4855	0.8424	63.150
0.0537	0.3677	24.848	0.5892	0.8760	69.171
0.0926	0.4972	30.110	0.7051	0.9087	75.432
0.1336	0.5841	34.963	0.8097	0.9394	81.256
0.2003	0.6736	41.927	1.0000	1.0000	92.511

[a] Mean deviation in y_1 0.0033.

distillation. The purity of 1-hexene was measured with a gas chromatograph GC 6000 from Carlo Erba Instruments.

Results and Discussion

The VLE measurements were carried out at as near to isothermal conditions as possible, but small differences between the selected temperature and the measured equilibrium temperature were observed in the first two systems.

For the thermodynamic treatment of the data, the pure component vapor pressures P^s_i at the equilibrium temperatures T were needed. On the basis of the measured data, the parameters for the Antoine vapor pressure equation were estimated for each component i:

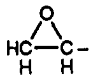
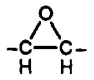
$$\log(P^s_i/\text{kPa}) = A_i - B_i/(T/°\text{C} + C_i) \qquad (1)$$

Good agreement was found between the experimental vapor pressures and the literature data (*6*). The estimated parameters A_i, B_i, and C_i are listed in Table 2.

Data for 10 different binary VLE systems were produced. Two isothermal sets of VLE data were produced for each system except the last one: system 1, diisopropyl ether + 2-methoxyethanol at 331.02 and 341.01 K; system 2, trichloroethylene + 2-methoxyethanol at 341.01 and 357.98 K; system 3, 1,2-epoxybutane + *n*-hexane at 313.15 and 333.15 K; system 4, 1,2-epoxyhexane + *n*-heptane at 333.15 and 353.15 K; system 5, 1,2-epoxybutane + *n*-heptane at 313.15 and 333.15 K; system 6, 1,2-epoxybutane + 1-hexene at 313.15 and 333.15 K; system 7, 1,2-epoxybutane + 1-octene at 323.15 and 333.15

Table 22. New UNIFAC Group Interaction Parameters[a]

main group	1	2	13	21	37	47	51
1, CH_2	0.0	pa	pa	pa	pa	pa	408.3
2, C=C	pa	0.0	pa	pa	pa	pa	219.9
13, CH_2O	pa	pa	0.0	pa	pa	−135.3	na
21, CCl	pa	pa	pa	0.0	pa	na	−127.9
37, ClC=C	pa	pa	pa	pa	0.0	531.2	na
47, OCCOH	pa	pa	493.1	na	−142.0	0.0	na
51, epoxy	21.49	−2.799	na	291.1	na	na	0.0

epoxy group		
R_k	1.3652	1.1378
Q_k	1.008	0.696

[a] pa = previously available. na = not available.

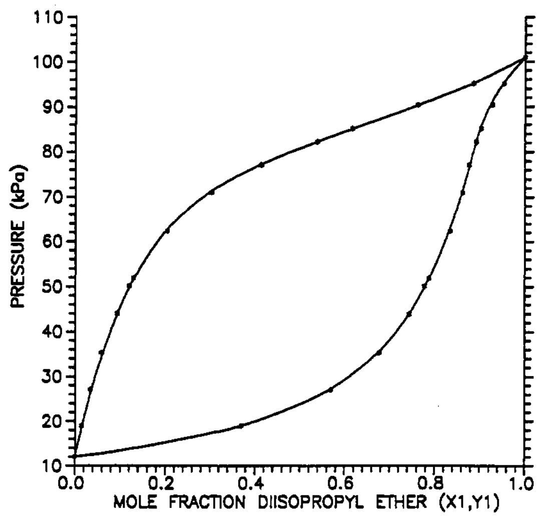


Figure 1. Binary system diisopropyl ether (1) + 2-methoxyethanol (2) at 341.01 K.

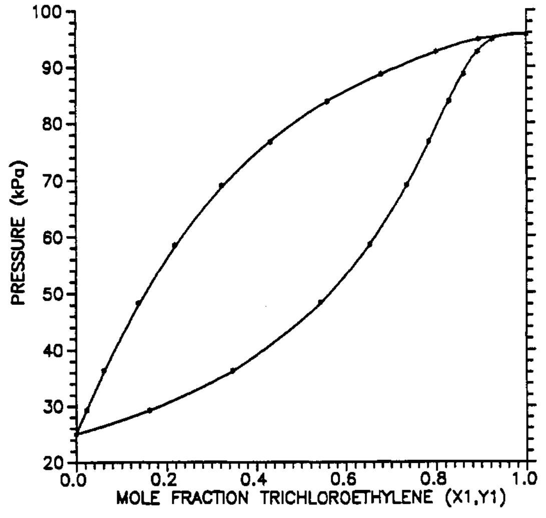


Figure 2. Binary system trichloroethylene (1) + 2-methoxyethanol (2) at 357.98 K.

K; system 8, 1,2-epoxybutane + 1-chlorobutane at 313.15 and 333.15 K; system 9, 1,2-epoxybutane + 2-chlorobutane at 313.15 and 333.15 K; system 10, epichlorohydrin + 2-chlorobutane at 338.15 K. The results are shown in Tables 3–21. Systems 3 and 6 form an azeotrope. In system 3 it is approximately at 0.5 mole fraction epoxybutane, and in system 6 it is approximately at 0.6 mole fraction epoxybutane.

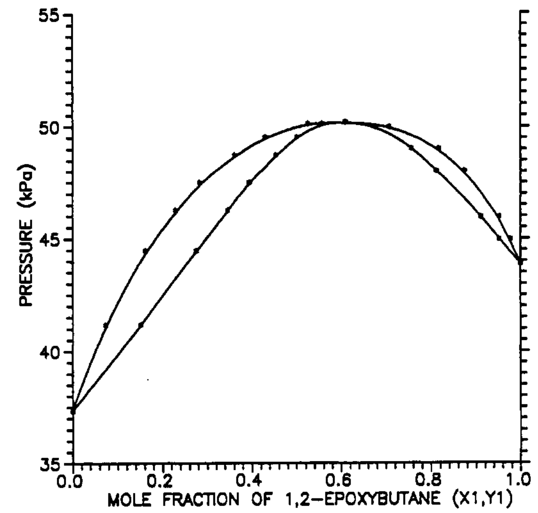


Figure 3. Binary system 1,2-epoxybutane (1) + *n*-hexane (2) at 313.15 K.

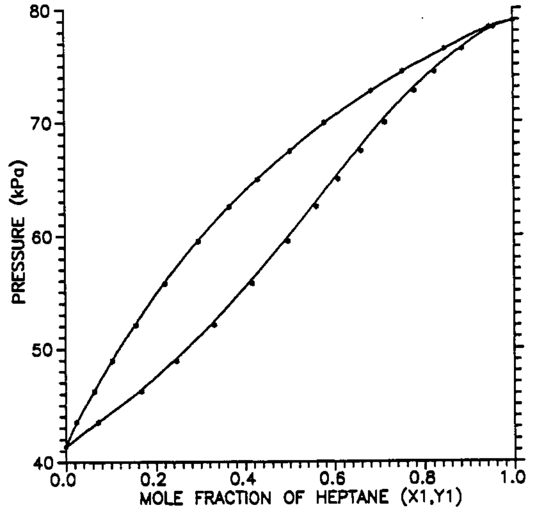


Figure 4. Binary system *n*-heptane (1) + 1,2-epoxyhexane (2) at 363.15 K.

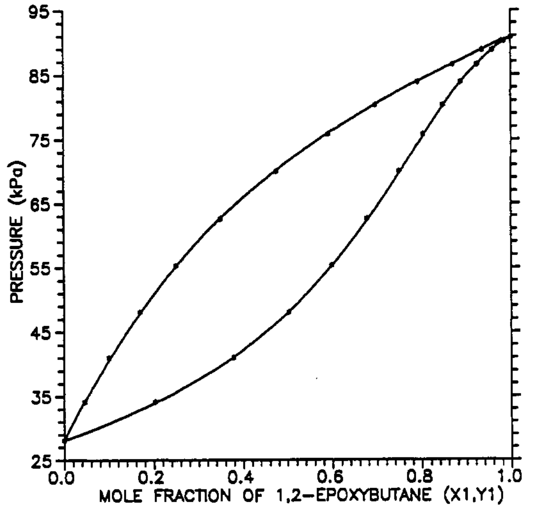


Figure 5. Binary system 1,2-epoxybutane (1) + *n*-heptane (2) at 333.15 K.

The data reported in Tables 3–21 were subjected to a thermodynamic consistency test according to Barker's method as described by Fredenslund (7), Chapter 5.2. At the bottoms of each of Tables 3–21 we report the average deviations between the experimental vapor-phase mole fractions and those computed by the consistency test program. All of the reported data are seen to be thermodynamically consistent.

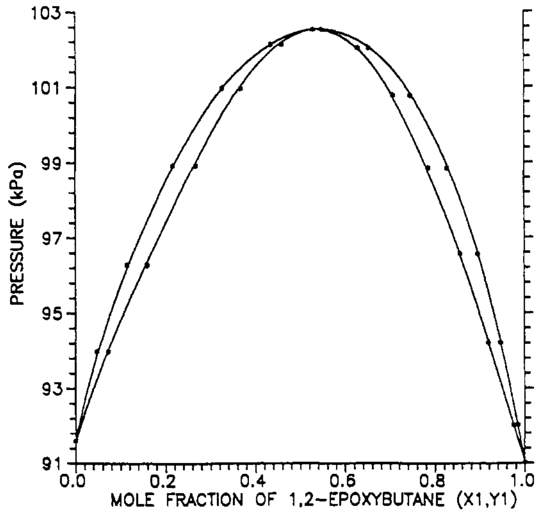


Figure 6. Binary system 1,2-epoxybutane (1) + 1-hexene (2) at 333.15 K.

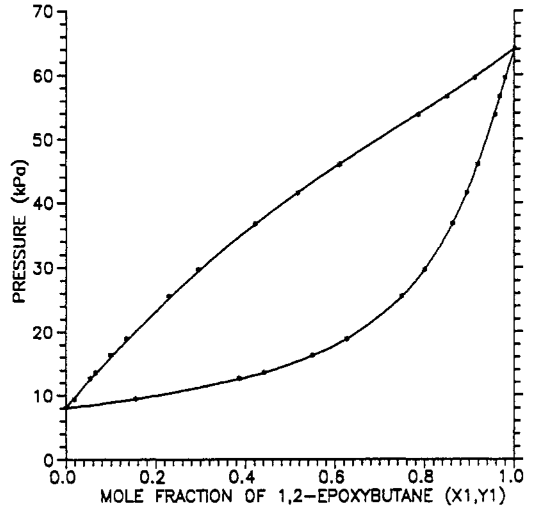


Figure 7. Binary system 1,2-epoxybutane (1) + 1-octene (2) at 323.15 K.

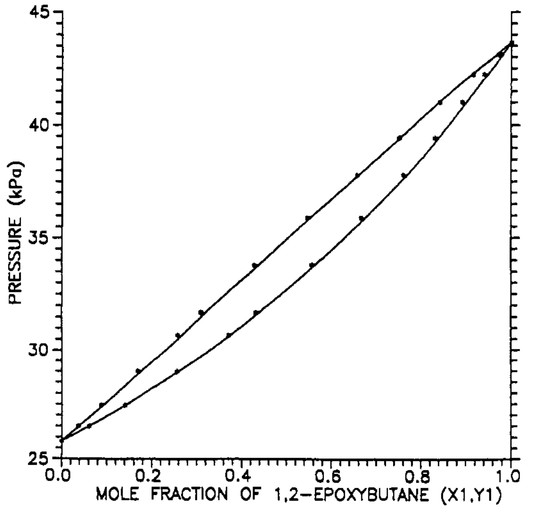


Figure 8. Binary system 1,2-epoxybutane (1) + 1-chlorobutane (2) at 313.15 K.

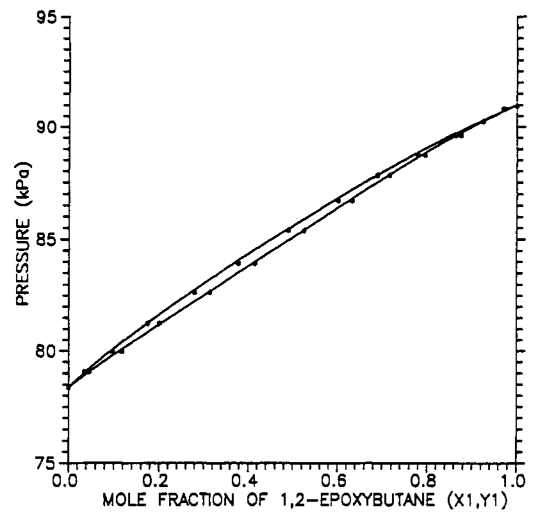


Figure 9. Binary system 1,2-epoxybutane (1) + 2-chlorobutane (2) at 333.15 K.

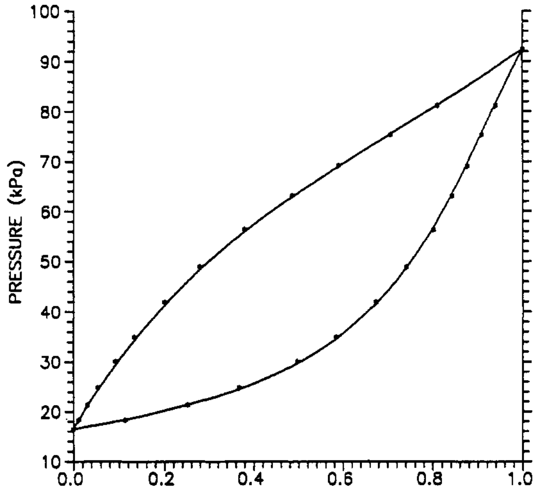


Figure 10. Binary system 2-chlorobutane (1) + epichlorohydrin (2) at 338.15 K.

UNIFAC Group Interaction Parameter Estimation. The multiresponse maximum likelihood principle (*9*) was used to estimate the UNIFAC model parameters. Nonideality of the vapor phase was taken into account using the virial equation of state with second virial coefficients obtained by the method of Hayden and O'Connell (*7*).

The UNIFAC group interaction parameters obtained are listed in Table 22. In Figures 1–10 is shown how the UNIFAC model correlates with the experimental data for one isotherm of each system. The second isotherm correlates very similarly.

Conclusions

Ten binary systems, for which no VLE data were found previously in the literature, were studied in order to obtain isothermal sets of VLE data. Using these data, it was possible to estimate group interaction parameters for the UNIFAC model, formerly not available. The UNIFAC model correlates the experimental data very well, as can be seen in Figures 1–10.

List of Symbols

P	pressure
T	temperature
x	composition of the liquid phase (mole fraction)
y	composition of the vapor phase (mole fraction)

Subscripts

i	component i

Superscripts

s	saturated

Literature Cited

(1) Dvorak, K.; Boublik, T. *Collect. Czech. Chem. Commun.* **1963**, *28*, 1249.
(2) Boublikova, L.; Lu, B. C.-Y. *J. Appl. Chem.* **1969**, *19*, 89.
(3) Macedo, M. E.; Rasmussen, P.; Fredenslund, Aa. *AIChE Symp. Ser.* **1985**, *244* (81), 102.
(4) Radnai, G.; Bottini, S.; Rasmussen, P.; Fredenslund, Aa. *AIChE Symp. Ser.* **1985**, *244* (81), 102.
(5) Radnai, G.; Rasmussen, P.; Fredenslund, Aa. *AIChE Symp. Ser.* **1987**, *256* (83), 70.
(6) Boublik, T.; Fried, V.; Hala, E. *The Vapour Pressure for Pure Substances*; Elsevier: Amsterdam, 1973.
(7) Fredenslund, Aa.; Gmehling, J.; Rasmussen, P. *Vapor-Liquid Equilibria Using UNIFAC*; Elsevier: Amsterdam, 1977.
(8) Hansen, H. K.; Rasmussen, P.; Fredenslund, Aa.; Schiller, M.; Gmehling, J. *Ind. Eng. Chem. Res.* **1991**, *30*, 2352.
(9) Kemeny, S.; Manczinger, J.; Skjold-Jørgensen, S.; Toth, K. *AIChE J.* **1982**, *28*, 20.

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