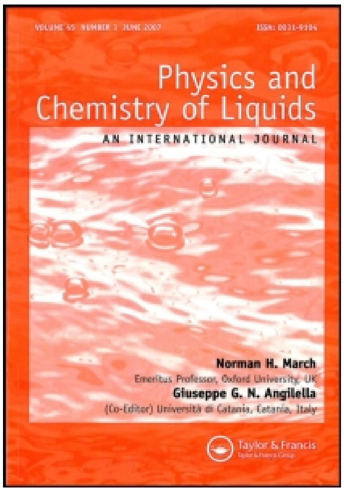

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Isobaric vapour–liquid equilibrium for the binary systems formed by a cyclic ether and bromocyclohexane at 40.0 and 101.3 kPa

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Experimental data of vapour–liquid equilibrium (VLE) for the binary systems tetrahydrofuran, or tetrahydropyran, or 2-methyl-tetrahydrofuran, or 2,5-dimethyl-tetrahydrofuran with bromocyclohexane have been measured in isobaric conditions at two pressures, 40.0 and 101.3 kPa. The equipment used was a dynamic recirculating still. The consistency of the measured VLE data has been tested with the Van Ness' point-to-point method. The activity coefficients have been correlated with the mole fraction through Wilson, NRTL and UNIQUAC equations.

Keywords: Experimental VLE; Cyclic ether; Bromocyclohexane

1. Introduction

The study of the vapour–liquid equilibrium (VLE) of organic liquid systems is part of a wider research program devoted to the determination of thermodynamic and transport properties of multicomponent mixtures involving oxygenated and halogenated organic substances [1–13].

The systematic studies in VLE bring together the practical and theoretical interest. On the one hand, they have many applications in chemical industry for the design and optimization of many units for distillation or separation processes. On the other hand, the most useful group contribution models (ASOG, UNIFAC) need an extensive database to determine the representative parameters of functional groups with specific interactions that could be used to develop reliable predictive models for the determination of the liquid phase activity coefficients.

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In this article, the attention has been focused towards the interaction between the oxygen atom from a cyclic ether (tetrahydrofuran, or tetrahydropyran, or 2-methyl-tetrahydrofuran, or 2,5-dimethyl-tetrahydrofuran) and the halogen one from bromocyclohexane. These results are compared with those obtained in previous works for the same cyclic ethers with chlorocyclohexane [6], or bromobenzene [7], and those for bromocyclohexane with isomeric butanols [2–5]. The thermodynamic consistency of the experimental data has been verified with the Van Ness method [14] modified by Fredenslund *et al*. [15]. The calculated activity coefficients have been correlated by fitting the binary interaction parameters of the different models (Wilson [16], NRTL [17] and UNIQUAC [18]).

Table 1. Densities at $T = 298.15\,\mathrm{K}$ and normal boiling points of the pure compounds and comparison with literature data.

	ρ (kg m^{-3})		T_b (K)	
Compound	Exp.	Lit.	Exp.	Lit.
Tetrahydrofuran	882.09	881.97[a]	339.12	339.115[d]
Tetrahydropyran	879.15	879.16[b]	361.17	361.15[e]
2-Methyl-tetrahydrofuran	849.90	848.82[c]	352.94	353.1[e]
2,5-Dimethyl-tetrahydrofuran	825.27	–	365.08	365.65[d]
Bromocyclohexane	1326.08	–	438.28	–

[a] Ref. [19]; [b] Ref. [20]; [c] Ref. [21]; [d] Ref. [22]; [e] Ref. [23].

Table 2. Experimental VLE data, T, x, y, and activity coefficients, γ_i, for the binary system tetrahydrofuran (1) + bromocyclohexane (2) at $P = 40.0$ and 101.3 kPa.

T (K)	x_1	y_1	γ_1	γ_2
$P = 40.0\,\mathrm{kPa}$				
398.16	0.0154	0.2151	1.200	0.983
385.40	0.0491	0.4904	1.138	0.997
376.03	0.0815	0.6446	1.126	0.995
366.27	0.1237	0.7582	1.118	1.016
358.04	0.1714	0.8377	1.113	0.994
345.27	0.2837	0.9207	1.072	0.960
336.51	0.3842	0.9521	1.078	1.001
330.99	0.4836	0.9688	1.046	1.011
324.60	0.6129	0.9818	1.043	1.081
319.72	0.7471	0.9904	1.029	1.124
316.36	0.8887	0.9965	0.987	1.115
313.79	0.9477	0.9986	1.022	1.092
$P = 101.3\,\mathrm{kPa}$				
433.57	0.0182	0.1555	0.946	0.983
430.08	0.0290	0.2266	0.918	0.994
425.54	0.0463	0.3315	0.910	0.984
409.79	0.1134	0.5954	0.894	0.988
394.30	0.2019	0.7765	0.901	0.968
384.77	0.2712	0.8538	0.912	0.946
374.59	0.3695	0.9180	0.918	0.873
366.57	0.4517	0.9443	0.948	0.916
356.78	0.5983	0.9721	0.960	0.917
347.67	0.7644	0.9878	0.993	0.998
343.95	0.8471	0.9950	1.010	0.741
341.08	0.9442	0.9985	0.994	0.692

Table 3. Experimental VLE data, T, x, y, and activity coefficients, γ_i, for the binary system tetrahydropyran (1) + bromocyclohexane (2) at $P = 40.0$ and 101.3 kPa.

T (K)	x_1	y_1	γ_1	γ_2
$P = 40.0$ kPa				
395.93	0.0471	0.2852	0.981	0.992
390.89	0.0788	0.4183	0.968	0.980
383.41	0.1301	0.5723	0.965	0.978
376.84	0.1841	0.6825	0.963	0.973
368.99	0.2581	0.7813	0.974	0.980
364.12	0.3211	0.8431	0.970	0.924
357.23	0.4098	0.8992	0.995	0.895
350.81	0.5206	0.9339	0.993	0.942
346.49	0.6116	0.9549	0.994	0.954
340.80	0.7510	0.9779	1.004	0.938
336.97	0.8705	0.9910	1.004	0.875
334.03	0.9684	0.9981	1.010	0.869
$P = 101.3$ kPa				
431.62	0.0414	0.2128	0.999	0.985
425.07	0.0859	0.3646	0.932	0.988
411.36	0.1970	0.6070	0.890	1.013
399.12	0.3198	0.7867	0.927	0.932
381.26	0.5473	0.9211	0.975	0.925
376.93	0.6263	0.9467	0.980	0.880
374.52	0.6788	0.9607	0.978	0.823
370.58	0.7525	0.9739	0.995	0.818
366.67	0.8414	0.9847	1.004	0.865
363.65	0.9293	0.9942	1.001	0.825
362.46	0.9624	0.9966	1.003	0.953
361.75	0.9828	0.9989	1.005	0.693

To the authors' knowledge, there is no experimental data (P, T, x_i, y_i) available in the literature for these mixtures.

2. Experimental section

The liquids used were: tetrahydrofuran (better than 99.8 mol%), tetrahydropyran, 2-methyl-tetrahydrofuran and 2,5-dimethyl-tetrahydrofuran (all better than 99.0 mol%), supplied by Aldrich, and bromocyclohexane (better than 99.0 mol%) provided by Fluka. All the liquids were subject to GC analysis and no other significant organic components were found. Therefore, they were directly employed without further purification. Measured densities and normal boiling points of the chemicals together with literature data [19–23] are gathered in table 1.

The experimental data have been obtained with a Labodest unit built by Fischer, and equipped with a Cottrell pump. This unit is an all-glass recirculating still, widely referenced in literature to carry out VLE measurements. The apparatus and procedure have been thoroughly described elsewhere [3]. The equilibrium temperatures were measured with a F25 thermometer from Automatic Systems Laboratories. The pressure was determined and controlled by means of a pressure transducer Druck PDCR 110/W (pressure indicator DPI 201). The accuracy in temperature and in pressure values is estimated to be ±0.01 K and ±0.1 kPa, respectively.

Table 4. Experimental VLE data, *T*, *x*, *y*, and activity coefficients, γ_i, for the binary system 2-methyl-tetrahydrofuran (1) + bromocyclohexane (2) at $P = 40.0$ and 101.3 kPa.

T (K)	x_1	y_1	γ_1	γ_2
$P = 40.0$ kPa				
399.47	0.0187	0.1474	0.971	1.029
397.18	0.0279	0.2326	1.080	1.004
389.67	0.0637	0.4053	0.977	1.026
381.00	0.1103	0.6047	1.036	0.960
374.13	0.1507	0.7045	1.051	0.958
365.17	0.2167	0.8027	1.058	0.967
355.49	0.3172	0.8975	1.064	0.845
346.03	0.4446	0.9417	1.062	0.880
339.28	0.5704	0.9627	1.052	0.983
334.40	0.6908	0.9790	1.041	0.965
329.96	0.8306	0.9897	1.022	1.070
328.14	0.8931	0.9937	1.019	1.134
$P = 101.3$ kPa				
432.24	0.0224	0.1767	1.282	0.995
427.54	0.0394	0.2802	1.256	0.998
421.01	0.0696	0.4216	1.208	0.984
416.06	0.0934	0.4994	1.172	1.001
405.86	0.1551	0.6451	1.120	1.020
398.47	0.2108	0.7342	1.099	1.022
388.98	0.3053	0.8354	1.070	0.972
381.50	0.3971	0.8978	1.057	0.893
375.78	0.4810	0.9254	1.037	0.924
369.17	0.5975	0.9546	1.023	0.922
364.71	0.6932	0.9711	1.013	0.910
359.18	0.8237	0.9850	1.009	1.020
354.23	0.9655	0.9972	1.007	1.187

The analysis of the composition of the equilibrium vapour and liquid phases was carried out through density measurements at 298.15 K, employing an Anton Paar DMA-58 vibrating tube densimeter. The precision of the density measurements is $\pm 5 \times 10^{-3}\,\mathrm{kg\,m^{-3}}$. The density-calibration curves for all systems studied were obtained previously [1]. The experimental error in both mole fractions is estimated to be ±0.0001.

The correct running of the different devices was periodically checked, and, if needed, rearranged, by measuring the normal boiling points and the densities for the pure liquids.

3. Results and discussion

Tables 2–5 collect the VLE data (T, x_1, y_1) for the two working pressures. The activity coefficients of the components in the liquid phase, γ_i, were calculated with the following equations:

$$\gamma_i = \frac{y_i P}{x_i p_i^o} \exp\left[\frac{\left(B_{ii} - V_i^0\right)\left(P - p_i^o\right) + \left(1 - y_i\right)^2 P \delta_{ij}}{RT}\right] \tag{1}$$

$$\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \tag{2}$$

Table 5. Experimental VLE data, T, x, y, and activity coefficients, γ_i, for the binary system 2,5-dimethyl-tetrahydrofuran (1) + bromocyclohexane (2) at $P = 40.0$ and 101.3 kPa.

T (K)	x	y	γ_i	γ_j
$P = 40.0$ kPa				
399.72	0.0233	0.1661	1.234	1.004
396.21	0.0381	0.2430	1.193	1.031
392.83	0.0594	0.3369	1.146	1.028
386.17	0.1003	0.4935	1.163	1.021
377.96	0.1622	0.6583	1.175	0.980
370.14	0.2326	0.7460	1.139	1.054
360.23	0.3573	0.8567	1.123	1.037
354.27	0.4457	0.8967	1.123	1.102
347.58	0.5964	0.9425	1.085	1.116
342.46	0.7385	0.9697	1.064	1.136
340.29	0.8389	0.9810	1.018	1.275
337.93	0.9179	0.9886	1.016	1.672
$P = 101.3$ kPa				
432.37	0.0337	0.1782	1.240	1.001
428.41	0.0537	0.2749	1.250	0.998
421.61	0.0945	0.4102	1.202	1.015
416.22	0.1333	0.5067	1.168	1.027
410.00	0.1812	0.6216	1.194	0.994
401.53	0.2519	0.7261	1.198	1.011
393.93	0.3331	0.8023	1.184	1.036
387.76	0.4247	0.8466	1.131	1.137
379.30	0.5807	0.9137	1.098	1.168
373.24	0.7112	0.9489	1.087	1.245
370.47	0.7897	0.9654	1.072	1.280
366.87	0.9415	0.9898	1.016	1.550
366.16	0.9743	0.9935	1.005	2.310

Table 6. Constants in Antoine's equation for vapour pressures of the pure compounds (temperature in °C, pressure in kPa).

Compound	A	B	C
Tetrahydrofuran[a]	6.12142	1203.11	226.355
Tetrahydropyran	5.85520	1131.93	205.83
2-Methyl-tetrahydrofuran[a]	5.95009	1175.51	217.80
2,5-Dimethyl-tetrahydrofuran[a]	5.69272	1099.53	205.72
Bromocyclohexane	6.12929	1568.13	214.459

[a] Ref. [22].

Table 7. Results of the thermodynamic consistency test, average deviation ΔP and Δy.

System	P (kPa)	ΔP (kPa)	Δy
Tetrahydrofuran + bromocyclohexane	40.0	0.5	0.0014
	101.3	1.7	0.0056
Tetrahydropyran + bromocyclohexane	40.0	0.3	0.0067
	101.3	1.3	0.0060
2-Methyl-tetrahydrofuran + bromocyclohexane	40.0	0.4	0.0081
	101.3	1.9	0.0086
2,5-Dimethyl-tetrahydrofuran + bromocyclohexane	40.0	0.5	0.0064
	101.3	0.9	0.0067

Table 8. Correlation parameters, average deviations, ΔT and Δy, and activity coefficients at infinite dilution, γ_i^∞.

Equation	A_{12} (J mol^{-1})	A_{21} (J mol^{-1})	ΔT (K)	Δy	γ_1^∞	γ_2^∞
Tetrahydrofuran (1) + bromocyclohexane (2) at 40.0 kPa						
Wilson	2158.1904	−1630.6739	0.36	0.0023	1.17	1.13
NRTL	−1056.7308	1680.8395	0.37	0.0023	1.17	1.13
UNIQUAC	−1004.8369	1289.4812	0.34	0.0022	1.17	1.15
Tetrahydrofuran (1) + bromocyclohexane (2) at 101.3 kPa						
Wilson	−1371.9636	2022.2109	0.50	0.0085	0.85	0.73
NRTL	3848.7786	−3328.5132	0.34	0.0068	0.87	0.73
UNIQUAC	2318.8913	−1906.6725	0.44	0.0031	0.93	0.65
Tetrahydropyran (1) + bromocyclohexane (2) at 40.0 kPa						
Wilson	−1458.8977	2200.8963	0.29	0.0073	0.93	0.90
NRTL	3560.1546	−2830.4668	0.24	0.0066	0.93	0.90
UNIQUAC	2656.0360	−1953.9850	0.28	0.0033	1.00	0.90
Tetrahydropyran (1) + bromocyclohexane (2) at 101.3 kPa						
Wilson	−2137.6294	3276.8510	0.29	0.0060	0.87	0.79
NRTL	4603.4564	−3679.3049	0.28	0.0058	0.87	0.79
UNIQUAC	3111.2430	−2277.3017	0.28	0.0040	0.94	0.79
2-Methyl-tetrahydrofuran (1) + bromocyclohexane (2) at 40.0 kPa						
Wilson	−2017.4796	5401.9915	0.26	0.0080	1.04	1.88
NRTL	6747.1233	−3641.9779	0.34	0.0079	1.02	1.61
UNIQUAC	−400.9690	359.1014	0.59	0.0095	1.04	1.05
2-Methyl-tetrahydrofuran (1) + bromocyclohexane (2) at 101.3 kPa						
Wilson	3873.4502	−2492.8251	0.42	0.0071	1.27	1.02
NRTL	−2342.8856	3563.0444	0.37	0.0076	1.22	1.05
UNIQUAC	−1578.1138	2101.0552	0.26	0.0062	1.24	1.04
2,5-Dimethyl-tetrahydrofuran (1) + bromocyclohexane (2) at 40.0 kPa						
Wilson	−1886.8096	5036.0850	0.41	0.0072	1.23	2.28
NRTL	5728.5209	−2815.4676	0.44	0.0070	1.20	1.99
UNIQUAC	3230.8903	−1955.1795	0.39	0.0099	1.29	1.96
2,5-Dimethyl-tetrahydrofuran (1) + bromocyclohexane (2) at 101.3 kPa						
Wilson	−1960.2626	5459.1576	0.28	0.0064	1.26	2.41
NRTL	6230.3050	−2935.8134	0.40	0.0073	1.24	2.14
UNIQUAC	3794.4070	−2200.7871	0.46	0.0097	1.33	2.29

These expressions take into account the non-ideality of the vapour phase. The different symbols mean the following: x_i and y_i are respectively the liquid and vapour-phase compositions in equilibrium, P is the total pressure, $p^{o;i}$ is the pure component vapour pressure calculated by using the Antoine equation, whose constants are listed in table 6, B_{ii} is the second virial coefficient of the pure gas, B_{ij} is the cross second virial coefficient estimated using the Amdur and Mason mixing rule [24], and $V^{o;i}$ is the molar volume of the saturated liquid phase determined by means of the Yen and Woods method [25].

The constants in the Antoine equation for tetrahydropyran and for bromocyclohexane have been calculated from the authors' vapour pressure measurements over the range 5.0–101.3 kPa employing the same device as for the binary systems. The others were taken from literature. The second virial coefficients were estimated using the Redlich and Kwong equation [26].

The thermodynamic consistency of the experimental data has been checked using the Van Ness point-to-point method [14] as described and modified by Fredenslund *et al.* [15]. A third order Legendre polynomial has been used for the excess Gibbs energies. According to this test, the data are considered consistent if the mean absolute deviation

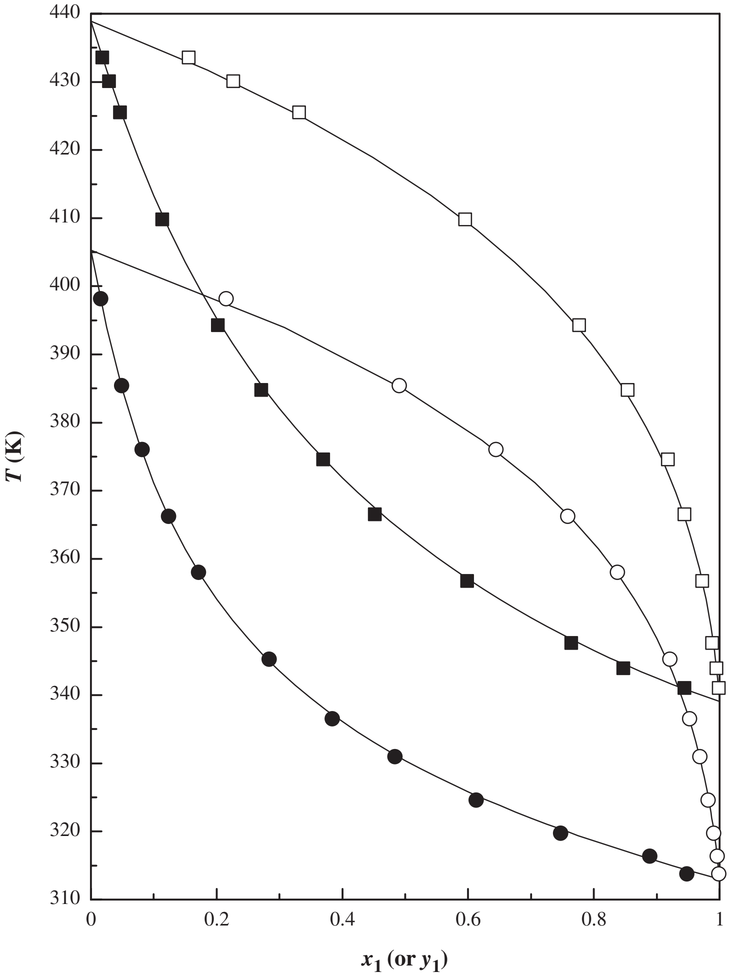

Figure 1. Temperature plotted against mole fraction in the (T, x_1, y_1) diagram for tetrahydrofuran (1) + bromocyclohexane (2): (●, ○) experimental data at 40.0 kPa; (■, □) experimental data at 101.3 kPa; (——) Wilson equation.

between calculated and measured y (Δy) is lower than 0.01. All the systems satisfy this condition as can be confirmed in table 7.

The activity coefficients have been correlated with Wilson [16], NRTL [17] and UNIQUAC [18] equations. In the NRTL equation, the mixture nonrandomness parameter α_{ij} was fixed at 0.3 (as recommended by Renon and Prausnitz [17]). For all the equations cited earlier, the estimation of parameters has been carried out by minimization with the Simplex method [27] of an objective function F. For a binary system this function can be expressed in terms of experimental and calculated γ_i values as:

$$F = \sum_{i=1}^{i=N} \left[\left(\frac{\gamma_1^{\mathrm{exp}} - \gamma_1^{\mathrm{cal}}}{\gamma_1^{\mathrm{exp}}} \right)^2 + \left(\frac{\gamma_2^{\mathrm{exp}} - \gamma_2^{\mathrm{cal}}}{\gamma_2^{\mathrm{exp}}} \right)^2 \right]_i \tag{3}$$

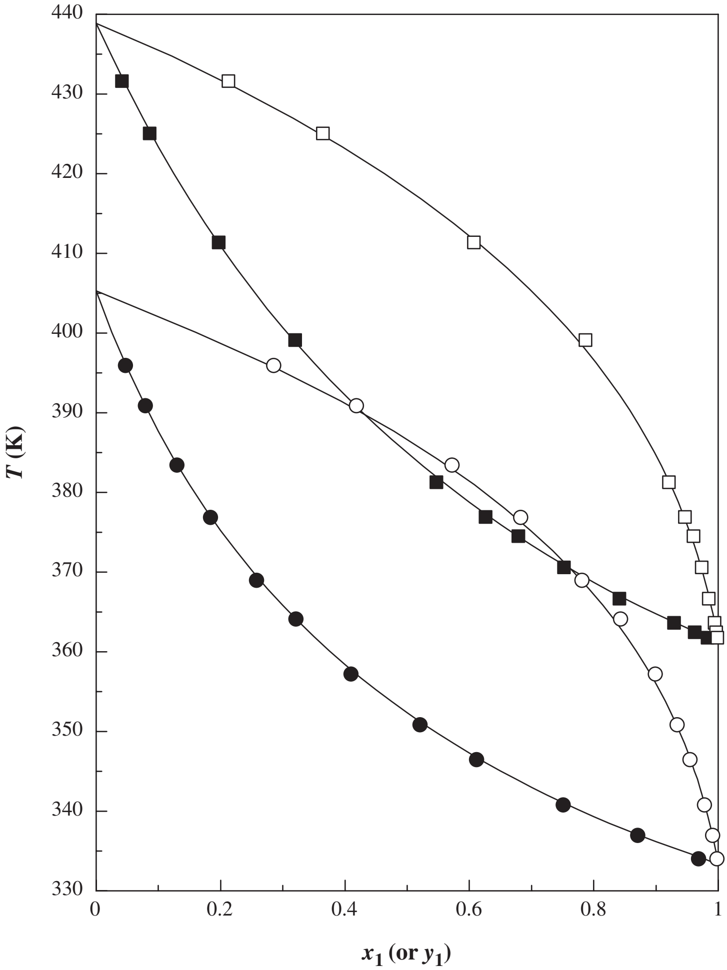

Figure 2. Temperature plotted against mole fraction in the (T, x_1, y_1) diagram for tetrahydropyran (1) + bromocyclohexane (2): (●, ○) experimental data at 40.0 kPa; (■, □) experimental data at 101.3 kPa; (——) Wilson equation.

where γ_i are the corresponding activity coefficients and N is the number of experimental data [28].

The adjustable parameters A_{12} and A_{21} (see definitions in Gmehling *et al.* [29]) together with the average deviations ΔT and Δy as well as the activity coefficients at infinite dilution are presented in table 8. The average deviations in temperature are between 0.24 and 0.59 K, and the average deviations of the vapour composition are less than 0.0099. It can be asserted that the three equations show a good performance in correlating the activity coefficients, the results being similar for the same mixture at a given pressure.

The experimental VLE data are graphically represented in figures 1–4. The solid lines in these diagrams were obtained from the Wilson equation that has been arbitrarily chosen for this purpose. As it can be seen in these diagrams, the systems do not show azeotropic behaviour, a point that is confirmed by the calculations.

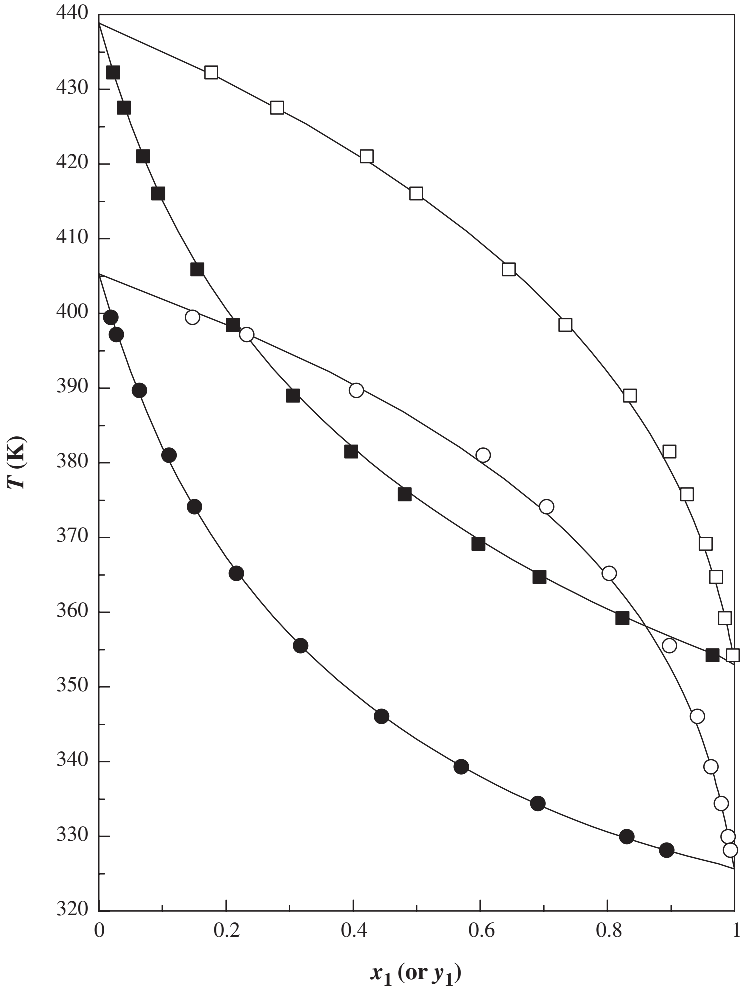

Figure 3. Temperature plotted against mole fraction in the (T, x_1, y_1) diagram for 2-methyl-tetrahydrofuran (1) + bromocyclohexane (2): (●, ○) experimental data at 40.0 kPa; (■, □) experimental data at 101.3 kPa; (——) Wilson equation.

The four systems here studied at the two working pressures present values for the activity coefficients of the components close to one. The deviations are hardly noticeable in all cases, the activity coefficients being less than one for the mixtures with tetrahydrofuran or tetrahydropyran and greater than unity for the systems containing the branched tetrahydrofuran. Such a behaviour, close to the ideality, can be interpreted as a result of the compensation of opposite effects in the mixing process, including energetic (weakening of dipole–dipole interactions in pure liquids and the establishment of halogen–oxygen interactions) and structural factors.

It is interesting to compare the values here obtained with those corresponding to the same cyclic ethers with chlorocyclohexane [6] and bromobenzene [7]. In both cases, the γ_i values are closer to the ideality than that of the systems here studied. As expected, the interaction between chlorine and oxygen atoms in the first one, or the

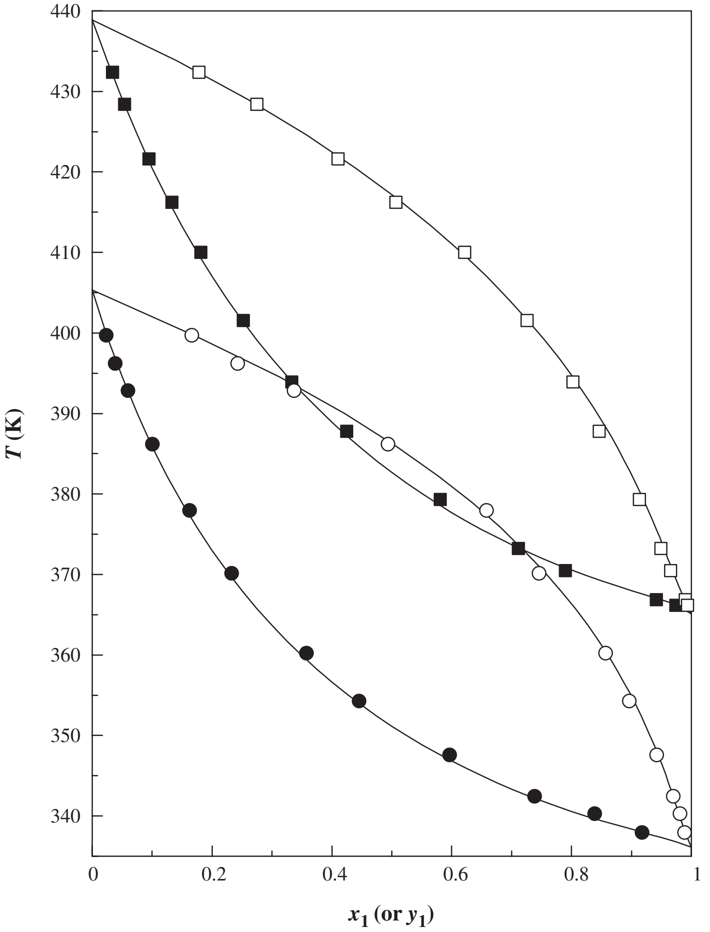

Figure 4. Temperature plotted against mole fraction in the (T, x_1, y_1) diagram for 2,5-dimethyl-tetrahydrofuran (1) + bromocyclohexane (2): (●, ○) experimental data at 40.0 kPa; (■, □) experimental data at 101.3 kPa; (——) Wilson equation.

π-bromine in the latter, are stronger than those for the present work and lead to a behaviour closer to ideality. In the same context, the branched cyclic ethers present more noticeable deviations from ideality when the halogen atom is bromine instead of chlorine, due to a higher steric hindrance in the structural accommodation.

On the other hand, the substitution of cyclic ethers by the isomers of butanol [2–5] leads to more marked deviations from ideality, attributable to the breaking of the hydrogen-bonding self-associated structure of alkanols.

4. Conclusions

A dynamic recirculating still has been employed to measure the experimental VLE data at 40.0 and 101.3 kPa for the binary systems tetrahydrofuran, or tetrahydropyran, or 2-methyl-tetrahydrofuran, or 2,5-dimethyl-tetrahydrofuran with bromocyclohexane.

The experimental data proved to be thermodynamically consistent.

The activity coefficients have been satisfactorily correlated with the Wilson, NRTL and UNIQUAC equations. The observed behaviour is close to ideality, although less marked than that corresponding to systems containing chlorocyclohexane or bromobenzene instead of bromocyclohexane.

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