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Liquid−Liquid Equilibrium of (Water + Pentane-2,4-dione + Ethyl Ethanoate) and (Water + Pentane-2,4-dione + Cyclohexane) at (298.15 and 313.15) K

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Liquid−liquid equilibrium (LLE) data of the solubility curves for ternary systems of water + pentane-2,4-dione + ethyl ethanoate and tie-line compositions for both of the ternary systems of water + pentane-2,4-dione + ethyl ethanoate and water + pentane-2,4-dione + cyclohexane were determined at (298.15 and 313.15) K and at a pressure of 101.3 kPa. Distribution coefficients were evaluated for the immiscible region. The reliability of the experimental tie-lines has been confirmed by using the Othmer−Tobias correlation. The experimental data were fitted using the nonrandom two-liquid (NRTL) and universal quasichemical activity coefficient (UNIQUAC) equations; parameters of these two models were regressed.

Introduction

Pentane-2,4-dione is an important reagent in analytical and coordination chemistry.[1] In the separation of pentane-2,4-dione using azeotrope distillation with water as an entrainer,[2] there is a small quantity of pentane-2,4-dione and acetic acid left in the wastewater. Direct emissions would cause significant pollution and loss of pentane-2,4-dione. As distillation can no longer efficiently separate pentane-2,4-dione of a low content from water, extraction is considered as a method to recycle it from water. In the scope of investigating more benign solvents as potential solvents for separations, we concentrated on ethyl ethanoate and cyclohexane, which have excellent properties for industrial applications. They are environmentally friendly and have a low cost, low toxicity, and chemical stability.

The aim of this work is to present the phase behavior of liquid−liquid equilibrium (LLE) for the ternary systems of water + pentane-2,4-dione + ethyl ethanoate and water + pentane-2,4-dione + cyclohexane at (298.15 or 313.15) K and a pressure of 101.3 kPa. The reliability of the experimental tie line data was confirmed by using the Othmer−Tobias correlation. The experimental data were fitted using the nonrandom two-liquid (NRTL) and universal quasichemical activity coefficient (UNIQUAC) equations and compared with the experimental data.

Experimental Section

Chemicals. Pentane-2,4-dione was supplied by Huzhou Xinaote Pharmaceutical & Chemical Co., Ltd. with a minimum mass fraction purity of 0.998. Cyclohexane was provided by Shanghai Lingfeng Chemical Reagent Co. Ltd., and had a minimum mass fraction purity of 0.998. Ethyl ethanoate was provided by Shanghai Chemical Reagent Co. Ltd. with a minimum mass fraction purity of 0.995. The purity of the chemicals was checked by a gas chromatograph (GC). All chemicals were used without further purification in this experiment. The densities of the pure liquids were measured at 298.15 K using an Anton Paar DMA 4100 densimeter. The temperature of the densimeter was maintained at 298.15 K with a precision of 0.01 K by means of a semiconductor Peltier element and measured by a calibrated platinum-resistance thermometer. The accuracies in density and refractive index measurements are ± 0.0001 $g \cdot cm^{-3}$ and ± 0.0002, respectively. The experimental values of these properties and the boiling points are given in Table 1 together with those given in the literature.

Apparatus and Procedure. The solubility curves were determined by the titration method[6] in a glass-made equilibrium cell with a water jacket to maintain isothermal conditions. The temperature in the cell was kept constant by circulating water

Table 1. Densities (ρ), Refractive Index (n_D), and Boiling Points of Pure Compounds Compared with Literature Data

	$\rho/(g \cdot cm^{-3})$ (298.15 K)		n_D (293.15 K)		T_b (K) (101.3 kPa)	
compound	exptl	lit.	exptl	lit.[3]	exptl	lit.[3]
pentane-2,4-dione	0.9717	0.9721[3]	1.4489	1.4494	413.60	413.55
cyclohexane	0.7734	0.7739[3]	1.4259	1.4264	353.90	353.87
ethyl ethanoate	0.8946	0.8946[4]	1.3701	1.3704	350.25	350.21
water	0.9968	0.9971[5]	1.3327	1.3325	373.30	373.26

Table 2. Experimental Binodal Curve Data in Mass Fraction for the Ternary Systems of Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3)

w_1	w_2	w_1	w_2	w_1	w_2
		298.15 K			
0.0302	0	0.0407	0.8833	0.8930	0.0669
0.0328	0.0928	0.0416	0.9258	0.8855	0.0818
0.0336	0.1861	0.0428	0.9572	0.8905	0.0601
0.0343	0.2802	0.8525	0.1475	0.9020	0.0484
0.0351	0.3692	0.8479	0.1366	0.9082	0.0360
0.0363	0.4972	0.8612	0.1314	0.9146	0.0234
0.0380	0.6632	0.8681	0.1174	0.9207	0.0114
0.0397	0.8060	0.8799	0.0932	0.9285	0
		313.15 K			
0.0388	0	0.0557	0.6926	0.8605	0.1172
0.0403	0.0450	0.0573	0.7405	0.8723	0.0980
0.0419	0.1354	0.0591	0.7887	0.8783	0.0886
0.0447	0.2720	0.0586	0.9414	0.8892	0.0713
0.0467	0.3637	0.8305	0.1695	0.8990	0.0556
0.0489	0.4569	0.8329	0.1621	0.9220	0.0194
0.0514	0.5506	0.8473	0.1386	0.9304	0.0063
0.0528	0.5977	0.8539	0.1277	0.9808	0

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Table 3. Experimental Tie-Line Data in Mass Fraction for the Ternary Systems of Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3) and Water (1) + Pentane-2,4-dione (2) + Cyclohexane (3)

aqueous phase		organic phase	
w_{11}	w_{21}	w_{13}	w_{23}
Water + Pentane-2,4-dione + Ethyl Ethanoate			
298.15 K			
0.9112	0.0217	0.0331	0.0969
0.9015	0.0322	0.0336	0.1840
0.8985	0.0464	0.0343	0.2910
0.8905	0.0601	0.0352	0.3657
0.8755	0.0818	0.0364	0.4891
0.8680	0.0916	0.0383	0.5586
0.8658	0.1098	0.0394	0.6480
0.8479	0.1366	0.0402	0.8007
0.8435	0.1479	0.0412	0.8805
313.15 K			
0.9342	0	0.0418	0
0.9221	0.0171	0.0435	0.0967
0.9149	0.0290	0.0445	0.1786
0.9052	0.0432	0.0459	0.2697
0.8804	0.0768	0.0475	0.4731
0.8546	0.1087	0.0489	0.5814
0.8535	0.1192	0.0504	0.6644
0.8488	0.1326	0.0521	0.7831
0.8274	0.1520	0.0548	0.8577
0.8305	0.1695	0.0586	0.9414
Water + Pentane-2,4-dione + Cyclohexane			
298.15 K			
0.9603	0.0397	0.0008	0.0557
0.9242	0.0758	0.0011	0.1753
0.9027	0.0973	0.0015	0.3293
0.8979	0.1021	0.0018	0.3399
0.8952	0.1048	0.0029	0.4318
0.8864	0.1136	0.0040	0.4802
0.8728	0.1272	0.0058	0.5696
0.8625	0.1375	0.0104	0.8201
0.8588	0.1412	0.0157	0.8485
313.15 K			
0.9893	0.0107	0.0015	0.0170
0.9585	0.0415	0.0018	0.0710
0.9196	0.0804	0.0020	0.1480
0.9015	0.0985	0.0028	0.2472
0.8858	0.1142	0.0060	0.3820
0.8695	0.1305	0.0240	0.5541
0.8625	0.1375	0.0322	0.6314
0.8568	0.1432	0.0362	0.7541
0.8427	0.1573	0.0451	0.8420
0.8305	0.1695	0.0586	0.9414

from a water bath (Super-Constant TEP Bath, Shanghai Precision Science Instrument Co., Ltd., China), which was equipped with a temperature controller capable of maintaining the temperature uncertainty within ± 0.1 K. A Teflon coated magnetic stirrer was used for the continual agitation of the mixtures. The major central part of the solubility curves was obtained by titrating heterogeneous mixtures with the solvent until the turbidity disappeared. The addition of a component was made with a micro syringe, the needle of which was pushed through the hermetic rubber stopper. The relative error in determinations of the solubility curves was within 1 %.

All mixtures were prepared by weighing with a Sartorius electronic balance with an accuracy of ± 0.0001 g. Mutual solubility values of binary systems were measured using the method based on the detection of the cloud point.[7,8] The transition point from the homogeneous to heterogeneous zones was determined visually. The reliability of the method depends on the precision of the micro buret with an accuracy of ± 0.01 cm^3 and is limited by the visual inspection of the transition. The accuracy of the visual inspection of the transition is achieved by waiting approximately 5 min in the transition point and observing the heterogeneity. All visual experiments were repeated at least three times to acquire high accuracy.

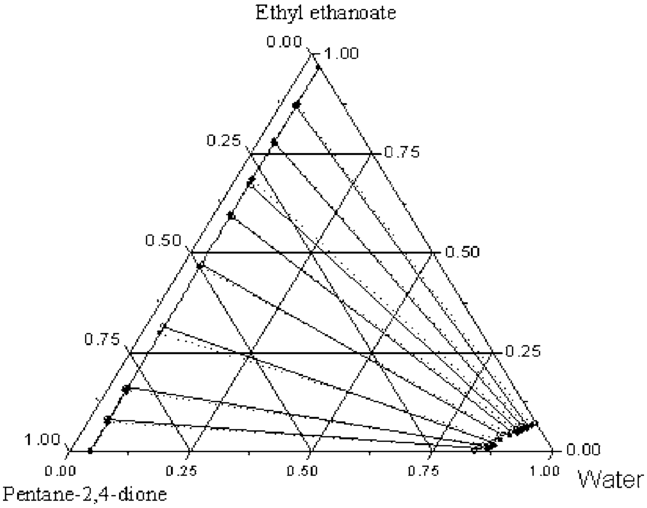

Figure 1. LLE of water + pentane-2,4-dione + ethyl ethanoate at T = 298.15 K: —, experimental solubility curve; ○, experimental tie-line data; ◆, NRTL.

The end-point determination of the tie-lines was based upon the independent analysis of the conjugate phases that were regarded as being in equilibrium. The equilibrium runs were performed in a glass cell of 50 cm^3 with a water jacket to maintain a constant temperature. The jackets were thermostatically controlled using a controller mounted on a water bath. The temperature was controlled at a set value with a deviation within ± 0.1 K.

Before the experiment, water, pentane-2,4-dione, and ethyl ethanoate or cyclohexane were introduced into the cell at known mass ratios. After being stirred for 1 h, the mixtures were kept still for more than 4 h to reach equilibrium. The compositions of liquid samples of the aqueous-rich layer and solvent-rich layer were analyzed by a GC (Varian CP-3800). A flame ionization detector was used together with a 30 m, 0.25 mm inner diameter capillary column CP-Wax 52 CB. The GC response peaks were treated with Varian Star #1 for Windows. High-purity hydrogen was used as the carrier gas at a constant flow rate of 50 cm^3·min^{-1}. The injector, detector, and column temperatures were kept at (443.15, 453.15, and 433.15) K, respectively. The GC was calibrated with mixtures of known compositions that were prepared gravimetrically by an electronic balance (uncertainty of ± 0.0001 g). The uncertainty of the measured mass fraction was ± 0.001.

Results and Discussion

The LLE measurements were made for the ternary system of water + pentane-2,4-dione + ethyl ethanoate and water + pentane-2,4-dione + cyclohexane at 298.15 K and 313.15 K and at a pressure of 101.3 kPa. The experimental binodal curves at each temperature were listed in Table 2, in which w_i refers to the mass fraction of i-th component. The experimental tie-line compositions of the equilibrium phases are shown in Table 3, where w_{i1} and w_{i3} refer to the mass fractions of the i-th component in the aqueous and solvent phase, respectively. The experimental and predicted equilibrium data of the ternary systems are plotted in Figure 1 to 4. It can be found that the system of water + pentane-2,4-dione + ethyl ethanoate exhibited type 3 phase behavior,[9,10] having two partially miscible

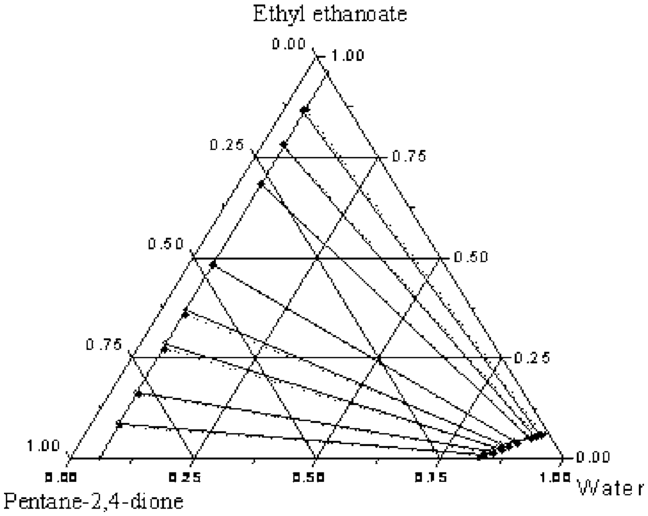

Figure 2. LLE of water + pentane-2,4-dione + ethyl ethanoate at T = 313.15 K: —, experimental solubility curve; ○, experimental tie-line data; ◆, NRTL.

pairs [(ethyl ethanoate + water) and (pentane-2,4-dione + water)] and one completely miscible pair (pentane-2,4-dione + ethyl ethanoate). In the system of water + pentane-2,4-dione + cyclohexane, there was one completely immiscible pair (cyclohexane + water).

It can also be found that ethyl ethanoate has a low solublility in water and vice versa. The solubility of water in the oil-rich phase can be obviously enhanced by the addition of pentane-2,4-dione. As the temperature increases, the solubility of water in the organic phase and pentane-2,4-dione in the aqueous phase increases, but the solubility of ethyl ethanoate in the aqueous phase decreases.

The experimental tie-line data at each temperature were correlated to test consistency by the method of Othmer and Tobias,[11] and the results are represented in Table 4. In this table, nearly linear correlations for every case are shown, which point out the consistency of the experimental data. The equation proposed by Othmer−Tobias was expressed for ternary mixtures as

$$\ln[(1 - w_{33})/w_{33}] = a + b \ln[(1 - w_{11})/w_{11}] \qquad (1)$$

where w_{11} is the mass fraction of water in the water-rich phase, w_{33} is the mass fraction of solvent in the solvent-rich phase,

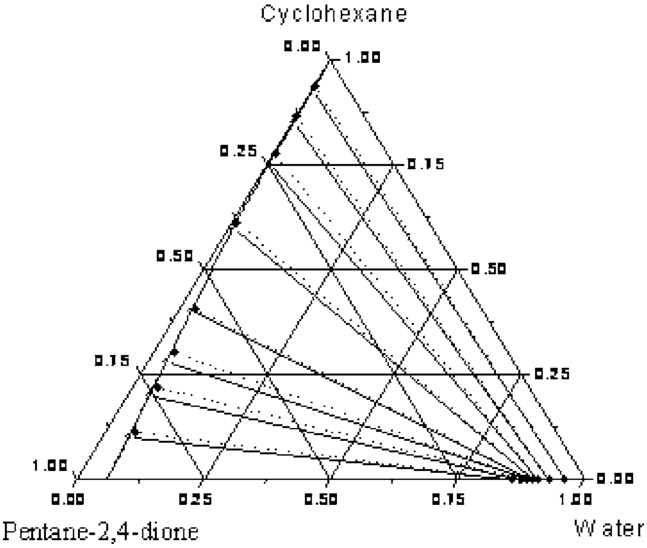

Figure 4. LLE of water + pentane-2,4-dione +cyclohexane at T = 313.15 K: ○, experimental tie-line data; ◆, NRTL.

Table 4. Fitting Parameters of the Othmer−Tobias Equation and Deviations for the Ternary Systems of Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3) and Water (1) + Pentane-2,4-dione (2) + Cyclohexane (3)

Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3)			
298.15 K	$a = -2.0114$	$b = 0.1630$	$R^2 = 0.9643$
313.15 K	$a = -2.3789$	$b = 0.3824$	$R^2 = 0.9371$
Water (1) + Pentane-2,4-dione (2) + Cyclohexane (3)			
298.15 K	$a = -2.0996$	$b = 0.1866$	$R^2 = 0.9302$
313.15 K	$a = -2.2406$	$b = 0.2578$	$R^2 = 0.9158$

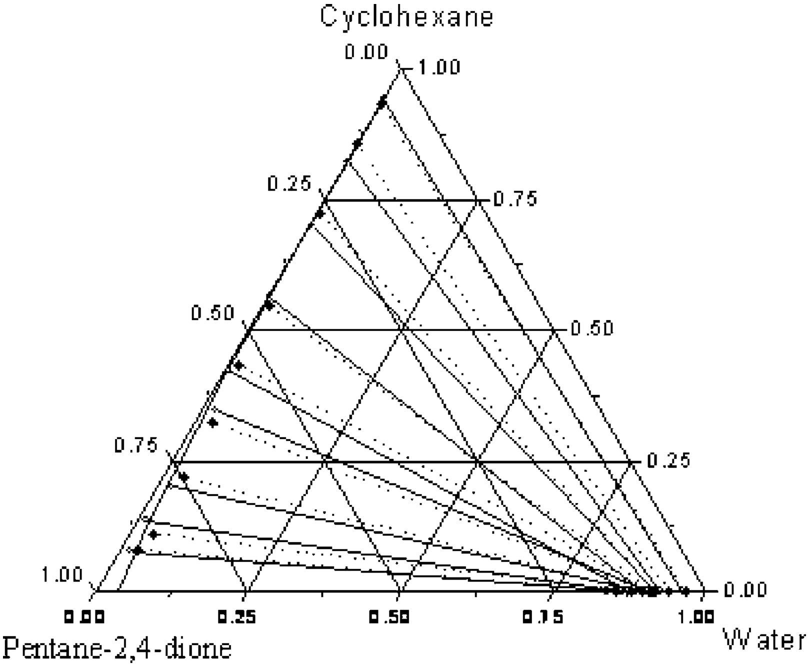

Figure 3. LLE of water + pentane-2,4-dione + cyclohexane at T = 298.15 K: ○, experimental tie-line data; ◆, NRTL.

Table 5. UNIQUAC Structural Parameters

compound	van der Waals volume, *r*	van der Waals area, *q*
water	0.92	1.4
pentane-2,4-dione	4.019	3.516
ethyl ethanoate	3.479	3.116
cyclohexane	4.046	3.24

and *a* and *b* are the constant and slope of the equation, respectively.

The NRTL[12] model and the UNIQUAC[13] model were fitted to experimental tie-line data. The interaction parameter for the NRTL and UNIQUAC models, b_{ij}, was regressed using the commercial simulator (Aspen Plus). The binary parameters, b_{ij}, are $(g_{ij} - g_{ii})/R$ (K) and $(u_{ij} - u_{ii})/R$ (K) for the NRTL and UNIQUAC models, respectively, where R is the universal gas constant and g_{ij} and u_{ij} are the energy parameters. The nonrandomness parameter, α_{ij}, for the NRTL model was fixed to be 0.3 for nonassociated liquids and 0.2 for immiscible liquids. The volume parameter and surface area parameter of the UNIQUAC model are presented in Table 5.

The regressed NRTL binary parameters and UNIQUAC binary parameters of both ternary systems are listed in Tables 6 and 7 with the root-mean-square deviation (rmsd) values. The rmsd value is a measure of the agreement between the experimental data and the calculated values and is defined as follows:

$$\text{rmsd} = \left(\sum_{k}^{M}\sum_{j}^{2}\sum_{i}^{3}(x_{ijk}^{\text{exp}} - x_{ijk}^{\text{calc}})^2/6M\right)^{1/2} \tag{2}$$

where M is the number of tie lines, x_{exp} is the experimental mole fraction, x_{cal} is the calculated mole fraction, and the subscript i indexes the components, j the phases, and k the tie lines.

The effectiveness of pentane-2,4-dione extraction by ethyl ethanoate is given by its separation factor, which is an indication of the ability of this solvent to separate pentane-2,4-dione from water. The separation factor is calculated according to the following equations:

$$S = D_2/D_1 \tag{3}$$

$$D_i = W_{i3}/W_{i1} \tag{4}$$

where W_{i3} and W_{i1} are the mass fractions of component i in solvent-rich and water-rich phases, and D_1 and D_2 are the distribution coefficients of water and pentane-2,4-dione, respectively.

Separation factors were found to be far more than 1 for the systems we studied, which means that the extraction of pentane-2,4-dione by ethyl ethanoate and cyclohexane is feasible.

The distribution coefficients and separation factors at each temperature for the systems of water + pentane-2,4-dione + ethyl ethanoate and water + pentane-2,4-dione + ethyl ethanoate are given in Tables 8 and 9, respectively. The distribution coefficients D_2 versus W_{21} were plotted in Figure 5, and the separation factors S versus W_{21} were plotted in Figures 6 and 7, respectively. It can be found that the separation factors were bigger at low temperature, which means a higher recovery yield of pentane-2,4-dione from water in extraction with ethyl ethanoate and cyclohexane at low temperatures.

Conclusions

The liquid−liquid phase equilibrium data for the systems water + pentane-2,4-dione + ethyl ethanoate and water + pentane-2,4-dione + cyclohexane were obtained at (298.15 and 313.15) K and at a pressure of 101.3 kPa. Pentane-2,4-dione can be separated from water using solvents such as ethyl ethanoate and cyclohexane. The tie-line correlation was fitted using the UNIQUAC and NRTL models, and the parameters for both models were calculated. The calculations based on both UNIQUAC and NRTL equations give a good representation of the tie-line data for the system studied, and better results were achieved with the NRTL model.

Table 6. Parameters of the UNIQUAC and NRTL Models for the Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3) System at (298.15 and 313.15) K and Their rmsd Values

T/K	model	b_{ij}/K and α_{ij}			rmsd
298.15	UNIQUAC	$b_{12} = 39.895$	$b_{13} = 698.75$	$b_{23} = 84.1850$	0.0085
		$b_{21} = -528.042$	$b_{31} = 389.19$	$b_{32} = -144.387$	
	NRTL	$b_{12} = 959.00$	$b_{13} = 1125.15$	$b_{23} = -365.845$	0.0065
		$b_{21} = 121.988$	$b_{31} = -207.07$	$b_{32} = 789.749$	
		0.2	0.2	0.3	
313.15	UNIQUAC	$b_{12} = 33.7375$	$b_{13} = -121.80$	$b_{23} = -670.234$	0.0074
		$b_{21} = -577.443$	$b_{31} = -326.78$	$b_{32} = 252.235$	
	NRTL	$b_{12} = 1111.58$	$b_{13} = 1290.14$	$b_{23} = 891.510$	0.0063
		$b_{21} = 37.484$	$b_{31} = -70.588$	$b_{32} = -315.406$	
		0.2	0.2	0.3	

Table 7. Parameters of the UNIQUAC and NRTL Models for the Water (1) + Pentane-2,4-dione (2) + Cyclohexane (3) Systems at (298.15 and 313.15) K and Their rmsd Values

T/K	model	b_{ij}/K and α_{ij}			rmsd
298.15	UNIQUAC	$b_{12} = -12.0305$	$b_{13} = -521.875$	$b_{23} = 54.8647$	0.015
		$b_{21} = -308.556$	$b_{31} = -1378.99$	$b_{32} = -221.860$	
	NRTL	$b_{12} = 1023.241$	$b_{13} = -1143.91$	$b_{23} = -138.422$	0.010
		$b_{21} = 98.5698$	$b_{31} = 4928.68$	$b_{32} = 637.475$	
		0.2	0.2	0.3	
313.15	UNIQUAC	$b_{12} = 39.8434$	$b_{13} = -85.9408$	$b_{23} = -163.856$	0.021
		$b_{21} = -494.613$	$b_{31} = -1034.16$	$b_{32} = -24.5068$	
	NRTL	$b_{12} = 1061.89$	$b_{13} = 3851.745$	$b_{23} = 762.93$	0.014
		$b_{21} = 101.890$	$b_{31} = 1366.33$	$b_{32} = -868.90$	
		0.2	0.2	0.3	

Table 8. Distribution Coefficients of Water (1) and Pentane-2,4-dione (2) and Separation Factors (*S*) for the Water (1) + Pentane-2,4-dione (2) + Ethyl Ethanoate (3) System

T/K	D_1	D_2	S
298.15	0.0363	4.4654	122.93
	0.0372	5.7142	153.32
	0.0381	6.2715	164.29
	0.0395	6.0848	153.94
	0.0415	5.9792	143.81
	0.0441	6.0982	138.21
	0.0455	5.9016	129.69
	0.0474	5.8610	123.63
	0.0488	5.9533	121.88
	0.0471	5.6549	119.87
	0.0486	6.1586	126.62
	0.0507	6.2430	123.12
	0.0539	6.1601	114.18
	0.0572	5.3486	93.476
	0.0590	5.5738	94.390
	0.0613	5.9057	96.215
	0.0662	5.6427	85.197

Table 9. Distribution Coefficients of Water (1) and Pentane-2,4-dione (2) and Separation Factors (*S*) for the Water (1) + Pentane-2,4-dione (2) + Cyclohexane (3) System

T/K	D_1	D_2	S
298.15	0.0008	1.4030	1684.2
	0.0012	2.3127	1943.1
	0.0016	3.3843	2036.7
	0.0020	3.3290	1660.7
	0.0032	4.1202	1271.9
	0.0045	4.2271	936.73
	0.0066	4.4779	673.86
	0.0120	5.9643	494.64
	0.0183	6.0092	328.71
313.15	0.0015	1.5887	1047.9
	0.0018	1.7108	911.02
	0.0022	1.8407	846.40
	0.0049	2.5096	502.77
	0.0067	3.3450	493.83
	0.0276	4.2459	153.83
	0.0373	4.5920	123.25
	0.0422	5.2660	124.64
	0.0535	5.3528	100.02
	0.0705	5.5539	78.713

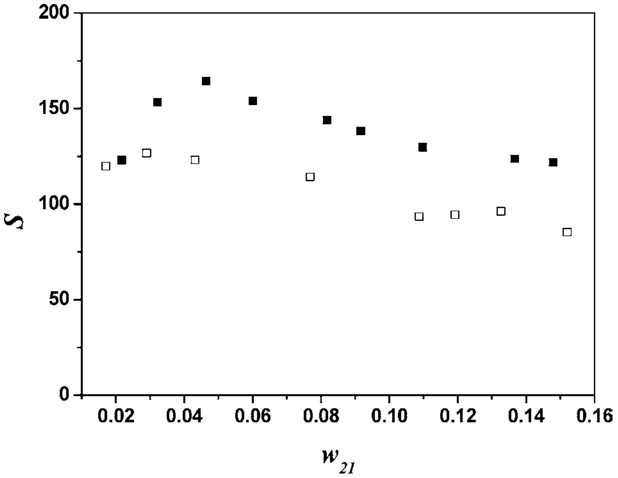

Figure 6. Separation factor, *S*, as a function of the mass fraction of pentane-2,4-dione in the aqueous phase, w_{21}, for the water (1) + pentane-2,4-dione (2) + ethyl ethanoate (3) system: ■, 298.15 K; □, 313.15 K.

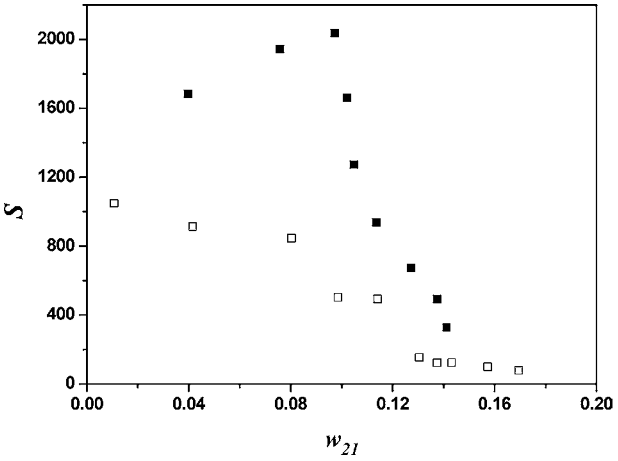

Figure 7. Separation factor, *S*, as a function of the mass fraction of pentane-2,4-dione in the aqueous phase, w_{21}, for the water (1) + pentane-2,4-dione (2) + cyclohexane (3) system: ■, 298.15 K; □, 313.15 K.

The reliability of experimentally measured tie-line data can be correlated by the Othmer−Tobias equation, by correlation factors (R^2) approximate to 1. Because the separation factor and selectivity in all cases are far more than 1, ethyl ethanoate and cyclohexane can be used to extract pentane-2,4-dione from water.

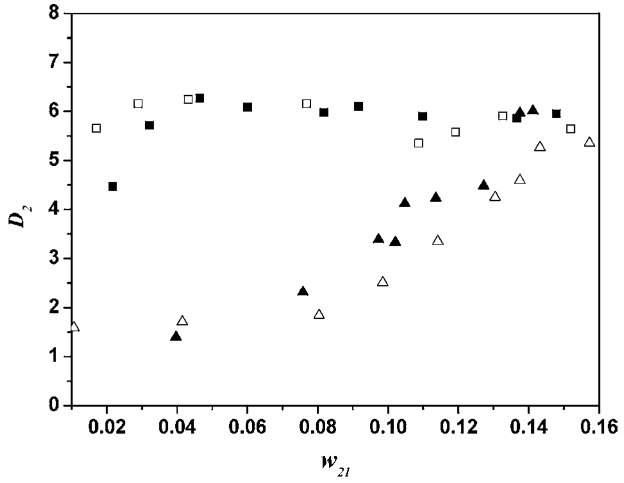

Figure 5. Distribution coefficient of pentane-2,4-dione, D_2, as a function of the mass fraction of pentane-2,4-dione in the aqueous phase, w_{21} for the systems of water (1) + pentane-2,4-dione (2) + ethyl ethanoate (3) (■, 298.15 K; □, 313.15 K); and water (1) + pentane-2,4-dione (2) + cyclohexane (3) (▲, 298.15 K; △, 313.15 K).

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