Solubility and Liquid−Liquid Equilibrium of Aqueous Systems of Iodoethane with Methanol, Ethanol, or 1-Propanol at Temperature 298.15 K and Pressure 101.2 kPa

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A study to attain the solubility and liquid−liquid equilibrium (LLE) data for the ternary mixtures of water + alcohol + iodoethane (where alcohol = methanol, or ethanol, or 1-propanol) was carried out at temperature 298.15 K and pressure of 0.1 MPa. The consistency of the binodal and phase diagram data were well ascertained by Hand and Othmer−Tobias empirical equations. The NRTL and UNIQUAC thermodynamic models were shown to yield accurate values for the LLE of the three systems. Plait point, distribution coefficient, solvent selectivity, and binary interaction parameters are reported for each ternary system. The selectivity of water for methanol in the ternary studied system is very high. The removal of methanol from the azeotropic binary system of methanol + iodoethane by means of water is potentially effective to yield pure iodoethane at ambient temperature. The immiscibility region of the system decreases significantly with increasing of the alcohol molecular chain.

Introduction

Iodoethane (ethyl iodide) finds important applications in pharmaceutical and chemical industries. It is used as an ethylating agent to pharmaceutical substances such as therapeutic drugs and in organic synthesis as solvent, intermediate agent for numerous chemicals, in dyes and pigments, fumigants, sterilant, antiseptics, or for the activation of silver catalysts. Iodoethane allows ultratrace level determination of phenylurea herbicides in natural waters and their degradation during drinking water treatment and transport and in lakes.[1] Mixtures of iodoethane with methanol are appropriate isosolvents in bimolecular nucleophilic substitution and synthesis reactions for charge-transporting and light-emitting materials, of bio-organic compounds such as phosphines and amines.[2−4]

An efficient recovery of the expensive iodoethane from product streams requires precise knowledge of thermodynamic properties and phase diagrams.[5−7] We studied the liquid−vapor phase diagrams of (methanol + iodoethane) and (methanol + toluene + iodoethane).[8] Now we report liquid−liquid equilibrium (LLE) data of the ternary aqueous mixtures of iodoethane, methanol, ethanol, and 1-propanol at the temperature of 298.15 K and pressure of 101.2 kPa.

The ternary systems present a type I liquid−liquid phase diagram in which the binary system (water + iodoethane) is partially miscible. The experimental data were well reproduced by NRTL and UNIQUAC equations with an average standard deviation equal to 0.9 %. Data on these ternary systems are lacking in the literature.

Experimental Section

Methanol, lot 425813; ethanol, lot 349619; 1-propanol, lot 1361444; and iodoethane, lot 1174423 were purchased from Fluka, and 2-propanol, lot 51880 was purchased from Riedel-deHaën. The chemicals were stored over A3 molecular sieves and were analyzed for purity by gas−liquid chromatography. Laboratory triple-distilled water was used throughout the study. Densities of the pure chemical components were measured at the temperature 298.15 K with an Anton-Paar vibrating-tube densimeter DMA5000 and agreed with literature values to ± 0.5 $kg \cdot m^{-3}$. The calibrating substance for the densimeter was cyclohexane (ρ = (774.04 ± 0.03) $kg \cdot m^{-3}$, T = 298.15 K).[14] The mass fraction purity and density values of the pure chemical components[14] are given in Table 1.

Table 1. Component Mass Fraction Purity and Density, ρ, Values of the Pure Components

		ρ(298.15 K)/($kg \cdot m^{-3}$)	
component	mass fraction	exptl	lit.[14]
water	0.9999	997.07	997.05
heptane	0.995	680.0	679.5
methanol	0.997	787.0	786.4
ethanol	0.999	785.2	784.9
1-propanol	0.995	799.7	799.6
2-propanol	0.995	781.5	781.3
iodoethane	0.997	1923.8	1924.4

Mole fractions of the heterogeneous mixtures were determined from the mass of the pure component using an Ohaus Explorer balance with a precision of ± 0.1 mg. The uncertainty in the mole fractions of the prepared mixtures were estimated to be ± $3 \cdot 10^{-4}$.

Iodoethane is easily oxidized to iodine by atmospheric oxygen, and it also undergoes photodecomposition that causes free iodine to form, resulting in pale-rose-colored samples. Therefore, solubility and tie-line measurements were realized in the absence of day light. The measurement of the binodal curves of (water + alcohol + iodoethane) mixtures were performed by titration in a double-jacketed equilibration cell at the temperature (298.15 ± 0.03) K[9] using tungsten filament lighting.

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Table 2. Experimental Solubility Data for the Ternary System of Water (1) + Alcohol (2) + Iodoethane (3) at T = 298.15 K and p = 0.1 MPa

x_1	x_2	x_3	x_1	x_2	x_3
Water (1) + Methanol (2) + Iodoethane (3)					
0.098	0.292	0.609	0.241	0.634	0.125
0.112	0.345	0.542	0.268	0.631	0.101
0.124	0.403	0.473	0.293	0.624	0.082
0.129	0.464	0.406	0.314	0.617	0.069
0.145	0.502	0.353	0.338	0.604	0.057
0.160	0.555	0.284	0.061	0.159	0.780
0.176	0.585	0.239	0.385	0.575	0.040
0.184	0.604	0.212	0.428	0.542	0.030
0.199	0.619	0.183	0.451	0.525	0.024
0.217	0.628	0.154	0.489	0.493	0.018
Water (1) + Ethanol (2) + Iodoethane (3)					
0.039	0.148	0.833	0.402	0.432	0.166
0.080	0.231	0.689	0.447	0.426	0.128
0.120	0.281	0.599	0.483	0.417	0.100
0.146	0.325	0.529	0.529	0.397	0.074
0.166	0.351	0.482	0.569	0.375	0.056
0.239	0.392	0.369	0.596	0.360	0.043
0.270	0.411	0.318	0.636	0.333	0.031
0.306	0.426	0.268	0.662	0.315	0.023
0.345	0.435	0.221	0.671	0.311	0.019
0.393	0.432	0.175	0.697	0.291	0.012
Water (1) + 1-Propanol (2) + Iodoethane (3)					
0.025	0.125	0.851	0.347	0.407	0.246
0.056	0.191	0.752	0.416	0.406	0.178
0.100	0.251	0.650	0.468	0.393	0.139
0.134	0.309	0.557	0.510	0.378	0.113
0.165	0.343	0.492	0.555	0.355	0.090
0.197	0.372	0.431	0.598	0.331	0.072
0.219	0.383	0.398	0.641	0.303	0.056
0.254	0.396	0.350	0.693	0.265	0.042
0.291	0.403	0.307	0.726	0.241	0.033

For the tie-line measurements, the feed-immiscible mixtures were vigorously stirred in stoppered ampules for 8 h, and the ampules were then submerged in the cryostat bath, which controls the temperature to ± 0.03 K and allowed phase equilibrium to be attained for three days at the desired temperature.[10−13] Samples from the equilibrated phases were then taken from each phase using glass hypodermic syringes and were kept in bottles protected from light. A gas chromatograph (Perkin-Elmer, model: Clarus 500) was used to determine the mole fractions of phases. The chromatograph was equipped with a thermal conductivity detector and a packed column (Porapak p, 80/100 mesh, 1 m length). The internal standard calibration method was used for phase-mole fraction analysis. The gas chromatograph was calibrated by means of standard mixtures. The internal standard was 2-propanol.

The tie-line samples were examined under the following conditions: temperature: injector = 513.2 K; column = 393.2 K; detector = 473.2 K. The uncertainty in temperatures was ± 0.5 K. The carrier gas was nitrogen with a flow rate of 14.3 $\mathrm{mL \cdot min^{-1}}$ in the column. The component mean retention time was water = 0.99 min, methanol = 1.72 min, ethanol = 4.54 min, 2-propanol = 10.12 min, 1-propanol = 12.32 min, and iodoethane = 17.95 min. The mean uncertainty in the measurements of phase mole fractions was ± 0.003.

Results and Data Correlation

The mixtures of (water + alcohol + iodoethane) present partial miscibility with phase α being rich in water and phase β being rich in iodoethane. The experimental solubilities and tie-line values at 298.15 K and pressure of 101.2 kPa are given in Tables 2 and 3, respectively.

Table 3. Experimental Liquid−Liquid Equilibrium Data for the Ternary System of Water (1) + Alcohol (2) + Iodoethane (3) at T = 298.15 K and p = 0.1 MPa

water-rich phase		iodoethane-rich phase	
x_1^{α}	x_2^{α}	x_1^{β}	x_2^{β}
Water (1) + Methanol (2) + Iodoethane (3)			
0.323	0.615	0.101	0.342
0.374	0.581	0.072	0.224
0.462	0.515	0.051	0.146
0.541	0.447	0.033	0.090
0.597	0.392	0.025	0.071
0.690	0.299	0.012	0.041
0.776	0.215	0.008	0.029
0.850	0.139	0.004	0.011
0.154[a]	0.540[a]	0.154	0.540
Water (1) + Ethanol (2) + Iodoethane (3)			
0.443	0.425	0.069	0.236
0.528	0.393	0.064	0.187
0.582	0.362	0.047	0.162
0.661	0.307	0.023	0.130
0.747	0.251	0.010	0.099
0.817	0.178	0.008	0.073
0.843	0.148	0.007	0.066
0.901	0.096	0.005	0.032
0.200[a]	0.378[a]	0.201	0.380
Water (1) + 1-Propanol (2) + Iodoethane (3)			
0.684	0.278	0.250	0.401
0.737	0.227	0.208	0.374
0.775	0.202	0.180	0.351
0.807	0.178	0.156	0.328
0.848	0.137	0.134	0.316
0.892	0.094	0.105	0.281
0.909	0.079	0.095	0.264
0.938	0.054	0.087	0.238
0.964	0.029	0.071	0.206
0.396[a]	0.410[a]	0.396	0.410

[a] Plait point.

The LLE results are correlated satisfactorily by the Hand equation[15]

$$\ln(x_2^{\beta}/x_3^{\beta}) = A + B\ln(x_2^{\alpha}/x_1^{\alpha}) \tag{1}$$

and by the Othmer−Tobias equation[16]

$$\ln\{(1 - x_3^{\beta})/x_3^{\beta}\} = A_1 + B_1\ln\{(1 - x_1^{\alpha})/x_1^{\alpha}\} \tag{2}$$

where x_i^{φ} is the mole fraction of component i in the phase φ. The fitting parameters of eqs 1 and 2 were determined using a linear-least-squares method, and they are reported in Table 4. The plait-point mole fractions of the ternary mixtures were estimated by the Othmer−Tobias method[15] and are reported in Table 3. The solubility and LLE data are plotted on a triangular diagram in Figure 1, whereas the LLE results with the Othmer−Tobias values are shown in Figure 2.

The distribution coefficient, $d_i = (x_i^{\alpha}/x_i^{\beta})$, of components 1 and 2 in the two liquid−liquid phase regions is used to estimate the selectivity, S, of the solvent iodoethane to extract the solute alcohol from its aqueous ternary mixtures. The selectivity values are calculated from the expression: $S = (x_1^{\alpha}x_2^{\beta}/x_1^{\beta}x_2^{\alpha})$, and they are found to be large at ambient temperature, which suggests a process toward a complete extraction of the alcohols from iodoethane mixtures and recovery of pure iodoethane. Table 5 assembles experimental values of distribution coefficients and selectivities. The ternary LLE of the azeotrope methanol (1) + iodoethane (2) (T = 313.2 K: p_{az} = 57.7 kPa, $x_{1,\mathrm{az}}$ = 0.485)[8] presents selectivities of water for the methanol: $16 \le (x_2^{\alpha}x_3^{\beta}/x_2^{\beta}x_3^{\alpha})$ 1190. Accordingly, the extraction of methanol from the azeotropic

Table 4. Parameters of Hand and Othmer−Tobias Equations from Liquid−Liquid Equilibrium Data of Water (1) + Alcohol (2) + Iodoethane (3) at T = 298.15 K and p = 0.1 MPa

Hand equation			Othmer−Tobias equation		
A	B	R^2	A_1	B_1	R^2
Water (1) + Methanol (2) + Iodoethane (3)					
−1.767 ± 0.077	1.532 ± 0.085	0.982	−1.580 ± 0.059	1.527 ± 0.066	0.989
Water (1) + Ethanol (2) + Iodoethane (3)					
−1.086 ± 0.057	0.987 ± 0.046	0.987	−1.028 ± 0.045	0.974 ± 0.038	0.991
Water (1) + 1-Propanol (2) + Iodoethane (3)					
0.446 ± 0.087	0.519 ± 0.041	0.959	0.918 ± 0.094	0.613 ± 0.047	0.961

binary system is definitely potential by means of water to yield pure iodoethane.

The LLE state is described by the thermodynamic equation

$$\gamma_i^{\alpha} x_i^{\alpha} = \gamma_i^{\beta} x_i^{\beta}, \quad (T, p, \text{constant}) \qquad (3)$$

where $\gamma_i^{\varphi}$and x_i^{φ} are the activity coefficient and mole fraction of component i in liquid phase φ, respectively.

The activity coefficient models of nonrandom two liquid (NRTL)[17] and the universal quasi-chemical (UNIQUAC)[18] were used to correlate the measured LLE data by minimizing the following objective function

$$F(x_i^{\varphi}) = \sum_{l}^{M} \sum_{i}^{3} \sum_{\varphi}^{2} (\Delta x_i^{\varphi})^2 \qquad (4)$$

with $\Delta x_i^{\varphi} = (x_i^{\varphi} - x_{i,\text{calcd}}^{\varphi})$ where x_i^{φ} and $x_{i,\text{calcd}}^{\varphi}$ denote the experimental and calculated mole fraction of component i in

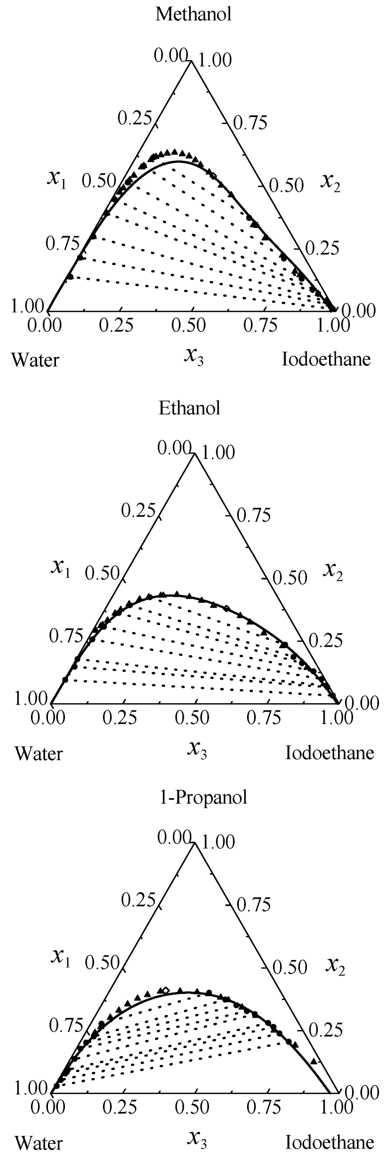

Figure 1. Experimental solubility and liquid−liquid equilibrium for the systems of water (1) + alcohol (2) + iodoethane (3) at 298.15 K: ▲, solubility; ●, LLE; ◇, plait point; ···, tie line; −, NRTL equation.

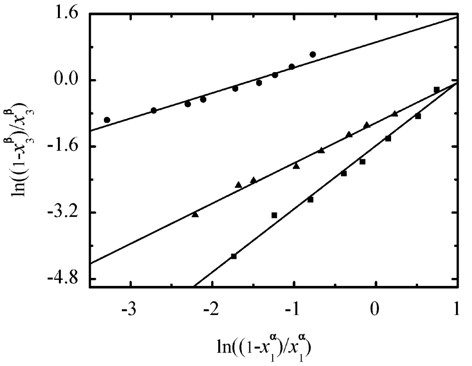

Figure 2. Liquid−liquid equilibrium data correlation by Othmer−Tobias for the systems of water (1) + alcohol (2) + iodoethane (3) at 298.15 K and p = 0.1 MPa: ■, methanol; ▲, ethanol; ●, 1-propanol; −, eq 2.

Table 5. Distribution Coefficient, d_i, and Selectivity, S, from Liquid−Liquid Equilibrium Data of Water (1) + Alcohol (2) + Iodoethane (3) at 298.15 K

d_1	d_2	S
Water (1) + Methanol (2) + Iodoethane (3)		
3.2	1.8	1.8
5.2	2.6	2.0
9.1	3.5	2.6
16.3	4.9	3.3
24.2	5.6	4.3
58.7	7.3	8.1
100.0	7.4	13.4
223.8	13.2	17.0
Water (1) + Ethanol (2) + Iodoethane (3)		
6.4	1.8	3.6
8.3	2.1	3.9
12.3	2.2	5.5
28.3	2.4	11.9
71.8	2.5	28.4
105.9	2.4	43.2
120.3	2.2	54.0
176.7	3.0	59.7
Water (1) + 1-Propanol (2) + Iodoethane (3)		
2.7	0.7	3.9
3.5	0.6	5.8
4.3	0.6	7.5
5.2	0.5	9.5
6.3	0.4	14.6
8.5	0.3	25.4
9.6	0.3	32.0
10.8	0.2	47.5
13.6	0.1	96.4

Table 6. Structural Molecular Parameters $(r,q)^{19}$ for the UNIQUAC Model

component	r	q
water	0.9200	1.400
methanol	1.4311	1.432
ethanol	2.1055	1.972
1-propanol	2.7799	2.513
iodoethane	2.8395	2.830

Table 7. Binary Interaction Parameters for the NRTL and UNIQUAC Models and Plait Point Deviations Δx_i^{cs} at $T = 298.15$ K

	NRTL ($\alpha = 0.200$)		UNIQUAC	
components $i-j$	$\Delta\lambda_{ij}$ $\mathrm{J \cdot mol^{-1}}$	$\Delta\lambda_{ji}$ $\mathrm{J \cdot mol^{-1}}$	Δu_{ij} $\mathrm{J \cdot mol^{-1}}$	Δu_{ji} $\mathrm{J \cdot mol^{-1}}$
Water (1) + Methanol (2) + Iodoethane (3)				
1−2	5342.9	−9083.9	1270.9	−8120.9
1−3	25 953.8	6502.4	6860.4	1428.2
2−3	5043.6	−279.1	147.9	2095.5
rmsd %	1.5		1.6	
Δx_1^{cs}, Δx_2^{cs}	0.007	0.005	0.009	0.002
Water (1) + Ethanol (2) + Iodoethane (3)				
1−2	8511.9	−5437.3	4000.5	−2384.0
1−3	17 055.3	8987.4	6707.4	9241.0
2−3	2127.1	624.2	−705.7	2973.7
rmsd %	0.5		0.5	
Δx_1^{cs}, Δx_2^{cs}	0.009	0.010	0.010	0.013
Water (1) + 1-Propanol (2) + Iodoethane (3)				
1−2	−6740.2	508.3	406.3	534.8
1−3	12 898.3	4547.6	1904.8	6846.0
2−3	−3626.9	−8802.9	2531.6	−1084.4
rmsd %	0.6		1.1	
Δx_1^{cs}, Δx_2^{cs}	0.048	0.027	0.013	0.004

phase φ for l tie-line number, respectively. The UNIQUAC structural parameters of the pure chemicals[19] are summarized in Table 6. The nonrandomness parameter, α_{ij}, in the NRTL equation was fixed to 0.200. The standard deviation of the LLE data fitting was estimated from the equation

$$\sigma(x_i^{\varphi}) = \left[\sum_{l}^{M}\sum_{i}^{3}\sum_{\varphi}^{2}(\Delta x_i^{\varphi})^2/6M\right]^{0.5} \tag{5}$$

The average value of $\sigma(x_i^{\varphi})$ of correlation for the three systems and the tow models is equal to 0.9 %, whereas the mean value of $\sigma(x_i^{\varphi})$ for calculated phase-mole fractions was less than 1 % for both liquid phases by the two correlative models. Table 7 lists the optimized binary interaction parameters for NRTL and UNIQUAC equations together with comparison between the experimental and correlated mole fractions of the critical mixtures, $\Delta x_i^{cs} = (x_i^{cs} - x_{i,\mathrm{calcd}}^{cs})$. The correlated values of the LLE state by NRTL for the systems of water (1) + alcohol (2) + iodoethane (3) at 298.15 K are shown in Figure 1, whereas the measured and calculated distribution coefficient and selectivity data of the alcohol in ternary aqueous and organic phases are plotted in Figures 3 and 4. The deviation values of mole fractions, Δx_i^{φ}, and the standard deviations, $\sigma(x_i^{\varphi})$, for the investigated systems using the NRTL model are presented in Table 8 and are illustrated in Figure 5.

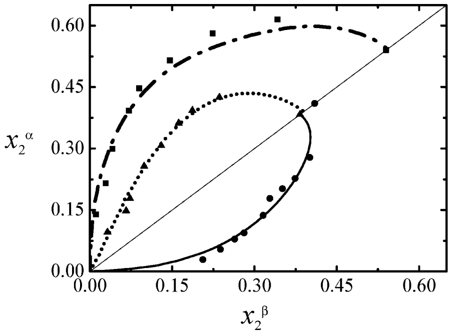

Figure 3. Distribution of alcohol in aqueous and organic phases for the systems water (1) + alcohol (2) + iodoethane (3) by NRTL correlation at 298.15 K: —, ■, methanol; ···, ▲, ethanol; —·—, ●, 1-propanol.

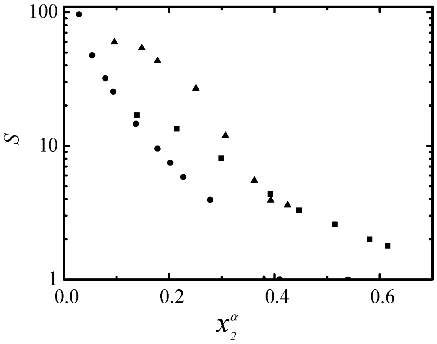

Figure 4. Selectivity from liquid−liquid equilibrium data for the systems water (1) + alcohol (2) + iodoethane (3) at 298.15 K: ■, methanol; ▲, ethanol; ●, 1-propanol.

Table 8. Deviations % and $\sigma(x_i^{\varphi})$ % for Predicting the Liquid−Liquid Equilibrium Data of Water (1) + Ethanol (2) + Iodoethane (3) at 298.15 K Using NRTL Model

water-rich phase			iodoethane-rich phase		
Δx_1^{α}	Δx_2^{α}	Δx_3^{α}	Δx_1^{β}	Δx_2^{β}	Δx_3^{β}
0.364	−0.243	−0.121	0.166	0.205	−0.372
−0.323	−0.036	0.358	−1.433	0.707	0.727
−0.184	0.046	0.138	−0.821	0.361	0.461
−0.044	0.030	−0.074	0.409	−0.236	−0.172
0.276	−0.389	0.113	1.006	−0.008	−0.999
−0.206	0.016	0.190	0.576	−0.656	0.081
−0.058	0.466	−0.408	0.517	−0.935	0.418
0.264	−0.169	−0.095	0.415	0.341	−0.755
$\sigma(x_i^{\varphi})$ %					
0.3	0.3	0.2	0.8	0.6	0.6

Moreover, the hygroscopic methanol and the photodecomposition of iodoethane have to be taken into account to assess an inner phase behavior of the system of water + methanol + iodoethane. This work reveals that the immiscibility region of the three systems decreases significantly with increasing of the alcohol molecular chain.

Conclusions

This work reports new and accurate solubility and LLE data for aqueous mixtures of iodoethane with methanol, ethanol, and

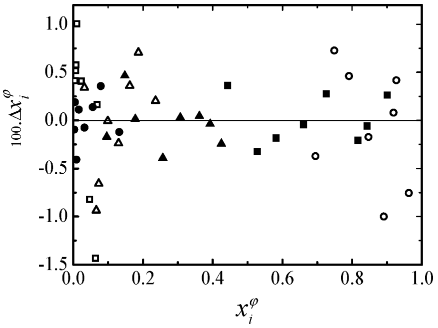

Figure 5. Deviations for predicting the liquid−liquid equilibrium data for water (1) + ethanol (2) + iodoethane (3) at 298.15 K using the NRTL equation. Solid symbols, water-rich phase; open symbols, iodoethane-rich phase: ■, □, water; ▲, △, ethanol; ●, ○, iodoethane.

1-propanol at 298.15 K and 101.2 kPa. The measured LLE values compared favorably to those of Hand and Other−Tobias equations together with the NRTL and UNIQUAC equations. The immiscibility region of the systems decreases significantly with increasing of the alcoholic molecular chain. The work outlines the high efficiency of liquid extraction of alcohols from iodoethane using water as solvent.

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