



(Liquid + liquid) equilibria in ternary aqueous mixtures of phosphoric acid with organic solvents at $T = 298.2$ K

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ABSTRACT

(Liquid + liquid) equilibrium (LLE) data for the ternary mixtures of {water (1) + phosphoric acid (2) + organic solvents (3)} were determined at $T = 298.2$ K and atmospheric pressure. The organic solvents were cyclohexane, 2-methyl-2-butanol (*tert*-amyl alcohol), and isobutyl acetate. All the investigated systems exhibit Type-1 behaviour of LLE. The immiscibility region was found to be larger for the (water + phosphoric acid + cyclohexane) ternary system. The experimental LLE results were correlated with the NRTL model, and the binary interaction parameters were obtained. The reliability of the experimental tie-line results was tested through the Othmer–Tobias and Bachman correlation equations. Distribution coefficients and separation factors were evaluated over the immiscibility regions and a comparison of the extracting capabilities of the solvents was made with respect to these factors. The experimental results indicate the superiority of cyclohexane as the preferred solvent for the extraction of phosphoric acid from its aqueous solutions.

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1. Introduction

Studies of phase equilibria of ternary systems are very important in both theoretical and industrial applications. Precise LLE data of aqueous mixtures with organic solvents are needed in the evaluation of industrial units for solvent extraction processes. The accurate interpretation of phase equilibria and thermodynamic behaviour for the different ternary mixtures is a fundamental and important key to improving solvent extraction techniques [1–9].

Phosphoric acid is one of the most widely used inorganic acids, which has many industrial applications. The pure phosphoric acid is extensively used as an additive in the food industry. Therefore, the efficient separation of phosphoric acid from aqueous solutions, by solvent extraction technique, is of considerable economic importance in the chemical industry [10–12].

The type of solvent is one of the most important factors, which influence the equilibrium characteristics of extraction of the acid from aqueous solutions. Many organic solvents have been tested as extractants for the recovery and purification of phosphoric acid from water. Heavy alcohols, ketones and ethers have mainly been used for extraction of phosphoric acid from aqueous solutions [13–20].

From practical and economical aspects, the search for new and suitable organic solvents for the separation of phosphoric acid from water is a current study. We have recently reported [21] LLE results for the aqueous mixtures of phosphoric acid with 1-butanol and butyl acetate at $T = 308.2$ K, where a Type 1 (liquid + liquid) phase diagram was obtained for both the ternary systems. As a continuation of that previous work, we present the LLE results for the three ternary systems (water + phosphoric acid + cyclohexane), (water + phosphoric acid + isobutyl acetate), (water + phosphoric acid + 2-methyl-2-butanol) at $T = 298.2$ K. These organic solvents widely used as extractants to determination of LLE data for many ternary mixtures [22–29].

In order to evaluate the extracting capability of the solvents for the separation of the acid from aqueous solutions with (liquid + liquid) extraction, the separation factor (S) was calculated. The experimental LLE values were correlated using the non-random two-liquid (NRTL) model of Renon and Prausnitz [30] and the interaction parameters were obtained. The LLE values were then analyzed in terms of root mean square deviations (RMSD) between experimental and calculated compositions in both equilibrium phases.

2. Experimental

2.1. Materials

Cyclohexane and 2-methyl-2-butanol with stated mass fraction purity higher than 0.99 were obtained from Merck. The isobutyl

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TABLE 1
Experimental and NRTL ($\alpha = 0.3$) correlated tie-line data, in mole fraction, in the aqueous and organic phase for {water (1) + phosphoric acid (2) + solvent (3)} at $T = 298.2$ K.

Water-rich phase (aqueous phase)				Solvent-rich phase (organic phase)			
x_1 (water)		x_2 (phosphoric acid)		x_1 (water)		x_2 (phosphoric acid)	
Exp.	NRTL	Exp.	NRTL	Exp.	NRTL	Exp.	NRTL
(Water + phosphoric acid + cyclohexane)							
0.9029	0.9267	0.0745	0.0509	0.0459	0.0445	0.0354	0.0509
0.8745	0.9067	0.1007	0.0699	0.0457	0.0473	0.0498	0.0699
0.8465	0.8892	0.1306	0.0863	0.0489	0.0496	0.0608	0.0863
0.8176	0.8614	0.1570	0.1123	0.0530	0.0530	0.0845	0.1123
0.7859	0.8385	0.1847	0.1334	0.0560	0.0552	0.0987	0.1334
(Water + phosphoric acid + isobutyl acetate)							
0.9120	0.9415	0.0764	0.0486	0.0626	0.0595	0.0276	0.0486
0.8817	0.9147	0.1080	0.0728	0.0639	0.0668	0.0539	0.0728
0.8602	0.8883	0.1294	0.1002	0.0674	0.0743	0.0756	0.1002
0.8388	0.8779	0.1494	0.1120	0.0842	0.0774	0.1005	0.1120
0.8019	0.8511	0.1625	0.1349	0.0840	0.0829	0.1087	0.1322
(Water + phosphoric acid + 2-methyl-2-butanol)							
0.9066	0.9073	0.0759	0.0759	0.5642	0.5716	0.0862	0.0809
0.8825	0.8803	0.1013	0.1027	0.5805	0.5820	0.1045	0.1027
0.8647	0.8632	0.1199	0.1195	0.5911	0.5916	0.1211	0.1195
0.8450	0.8436	0.1320	0.1385	0.5948	0.6054	0.1357	0.1385
0.8265	0.8272	0.1569	0.1541	0.6211	0.6209	0.1578	0.1541

acetate, with stated mass fraction purity higher than 0.98, was supplied by Merck. For the study of the equilibrium data, analytical grade phosphoric acid containing 85 wt% (Merck) was used. The purity of the acid was checked through acidimetric titration with 1 N NaOH. Deionised and redistilled water was used throughout all the experiments. All materials were used as received without any further purification.

2.2. Procedure

A 250 cm³ glass cell connected to a thermostat was used to measure the LLE values at $T = 298.2$ K. A water jacket was used to control the temperature of the cell to within $\pm 0.1\%$. We determined the equilibrium values preparing the ternary mixtures of known compositions. The prepared mixtures were placed in the extraction cell and were vigorously agitated by a magnetic stirrer for 4 h. The mixtures were then settled for 4 h at constant system temperature to separate completely into two liquid phases.

After separation, samples of both phases were transparent and were carefully collected from each phase and analyzed to determine their compositions. The concentrations of phosphoric acid in both phases were determined by potentiometric NaOH titration in the presence of phenolphthalein as an indicator. The water content of the organic phase was measured by the Karl–Fisher method [31] using a Mettler Toledo DL 38 Karl–Fisher titrator. The content in the aqueous phase and the amount of the organic solvents in both phases were determined by using a material balance [17]. All weighting was carried out with an analytical balance accurate to within ± 0.0001 g. The estimated uncertainties in the mole fractions were about 0.0005.

3. Results and discussion

3.1. Experimental LLE results

The experimental tie-line data for the ternary systems {water + phosphoric acid + organic solvents (cyclohexane, isobutyl acetate, and 2-methyl-2-butanol)} were determined at $T = 298.2$ K. The experimental and the correlated values for each ternary system are listed in table 1. The LLE phase diagrams for these ternary systems are plotted and are shown in figures 1 to 3.

Since the (water + organic solvent) mixture is the only pair that is partially miscible and two liquid pairs (phosphoric acid + water) and (phosphoric acid + solvent) are completely miscible, these investigated systems behave as a Type 1 LLE [32]. The type of organic solvent is one of the most important factors, which influence

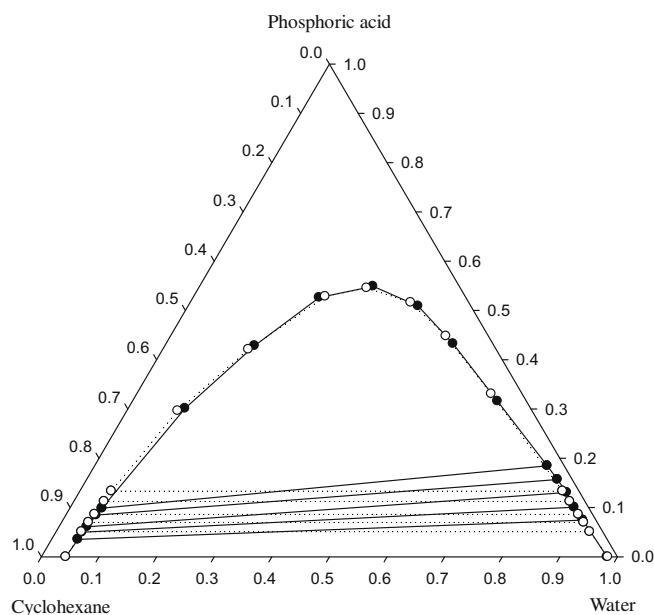


FIGURE 1. Ternary phase diagram for LLE of {water (1) + phosphoric acid (2) + cyclohexane (3)} at $T = 298.2$ K; (•) Experimental points; (○) NRTL calculated points ($\alpha = 0.3$).

the equilibrium characteristics and the immiscibility region of the investigated mixtures. As seen from the phase diagrams, the area of the two-phase region obviously depends on the mutual solubility of water and the organic solvent. In the ternary systems, water is the most soluble in the system containing 2-methyl-2-butanol but is the least soluble in isobutyl acetate or cyclohexane. The immiscibility region decreases in the order of the mixtures containing cyclohexane > isobutyl acetate > 2-methyl-2-butanol.

The efficient separation of phosphoric acid from aqueous solutions is an important concept in the chemical industries. In order to evaluate the extracting capability of the solvents (i.e., cyclohexane, isobutyl acetate, and 2-methyl-2-butanol) for the separation of phosphoric acid from aqueous solutions with (liquid + liquid) extraction, the separation factor (S) was calculated. The separation factor is defined as the ratio of distribution coefficients of the acid (D_2) to water (D_1), as follows:

$$S = \frac{D_2}{D_1}, \quad (1)$$

where D_1 and D_2 are the distribution coefficients of water and the acid, respectively. The distribution coefficients of water and phosphoric acid were calculated from the experimental results as follows:

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