



The isobaric vapor liquid equilibria of ethyl acetate + acetonitrile + bis(trifluoromethylsulfonyl)imide-based ionic liquids at 101.3 kPa



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ABSTRACT

We investigated the isobaric vapor liquid equilibria (VLE) of the binary system ethyl acetate + acetonitrile, the ternary system ethyl acetate + acetonitrile + 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide([EMIM][NTf₂]), as well as ethyl acetate + acetonitrile + 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide([HMIM][NTf₂]) at 101.3 kPa in a modified Othmer still. The experimental data were correlated with the e-NRTL activity coefficient model, and the parameters were obtained with a good consistency. The results indicated that ionic liquids([EMIM][NTf₂] and [HMIM][NTf₂]) produced a consistent salting-out effect of ethyl acetate, resulting in the incremental relative volatility of ethyl acetate to acetonitrile and even eliminated the azeotropic phenomenon when the mole fraction of ILs was up to 0.05.

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1. Introduction

Increasing concern about environmental issues has recently directed the attention of the scientific community to novel processes based on greener technologies, especially for solvent mixtures containing azeotrope [1]. Ionic liquids (ILs), not only due to their remarkable physicochemical properties but also for their recyclability, have attracted researchers' interest for their application on azeotropic distillation [2–18]. He et al. [5] investigated the solubility of difluoromethane (R-32), 1,1-difluoroethane (R-152a), and pentafluoroethane (R-125) in [HMIM][NTf₂], and found that the solubility are in sequence of R-152a > R-32 > R-125. By means of studying the vapor liquid equilibria (VLE) data, excess enthalpies (H^E) of binary systems with 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide(alkyl = ethyl, [EMIM][NTf₂]; alkyl = butyl, [BMIM][NTf₂]; alkyl = hexyl, [HMIM][NTf₂]; alkyl = octyl, [OMIM][NTf₂]), and prediction of γ^∞ using modified UNIFAC(Dortmund), Gmehling et al. [11] proposed that ionic liquids can be used to separate the azeotropic mixtures. Therefore, the ILs

were considered good candidate solvents for the purification of acetonitrile.

Acetonitrile is a key solvent in the chemical industries [19,20], which can be used as extraction solvents to separate butadiene, solvents to synthesize fiber and recrystallize steroid drugs, intermediates to produce medicine(vitamin B₁) and some spices. However, acetonitrile is difficult to be fully purified by using conventional distillation processes [21,22], particularly for the azeotropic system of ethyl acetate and acetonitrile [23,24]. Water [23] and n-hexane [24] are used as extraction solvent to extraction separation the azeotrope, but there is no further application due to the difficult solvent separation to recycle. By using ILs, the purification of acetonitrile becomes more facile [25,26]. ILs [EMIM][OTf] [25] and [BMIM][PF₆] [26] both can eliminate azeotropy when concentration are up to 0.05. The ionic liquids make the separation azeotrope of ethyl acetate and acetonitrile realized with properties of reused, low concentration, low energy consumption, and pollution-free to the environment. However, how ILs effectuates the separation of azeotrope is deserving research yet. It is also worthwhile to develop a better utilization of ILs in the separation of mixtures.

In this work, we studied on the isobaric VLE of ethyl

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Table 1
Specifications of used chemical samples with boiling point of the pure components at 101.3 kPa.

Chemical name	Source	Initial purity	Purification method	Final purity		T_b /K		Analysis method
				Final water content (KF ^d)	Final purity of substance	This work	Reference	
ethyl acetate	Tianjin Jinke Fine Chemical Industry Research Institute, China	0.995 (GC ^c)	none	0.00025	0.9950(GC ^c)	350.15	349.90 [26] 350.26 [27]	GC ^c , KF ^d
acetonitrile	Tianjin Fuchen Chemical Reagents Factory, China	0.998 (GC ^c)	none	0.00024	0.9980(GC ^c)	354.65	354.30 [26] 354.80 [27]	GC ^c , KF ^d
[EMIM][NTf ₂] ^a	Shanghai Cheng Jie Chemical Co. LTD, China	0.98 (LC ^e)	vacuum with rotary evaporator (433.15 K, 0.1 kPa, 8 h)	0.00051	0.9995(LC ^e)			LC ^e , KF ^d
[HMIM][NTf ₂] ^b	Shanghai Cheng Jie Chemical Co. LTD, China	0.98 (LC ^e)	vacuum with rotary evaporator (433.15 K, 0.1 kPa, 8 h)	0.00051	0.9995(LC ^e)			LC ^e , KF ^d

^a [EMIM][NTf₂] = 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide.

^b [HMIM][NTf₂] = 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide.

^c GC = gas chromatography.

^d KF = Karl Fischer titration.

^e LC = liquid chromatography.

acetate + acetonitrile + [EMIM][NTf₂]/[HMIM][NTf₂] at 101.3 kPa. We analyzed the separating effect of ILs([EMIM][NTf₂] and [HMIM][NTf₂]) on the azeotrope, and correlated the experimental data of equilibrium with the e-NRTL model to obtain the important parameters.

2. Experimental

2.1. Materials

Ethyl acetate(≥99.50%, mass fraction) and acetonitrile(≥99.80%, mass fraction) were purchased from Tianjin Jinke Fine Chemical Industry Research Institute, and Tianjin Fuchen Chemical Reagents Factory, China, respectively. ILs([EMIM][NTf₂] and [HMIM][NTf₂]; ≥98.00%, mass fraction) were obtained from Shanghai Chengjie Chemical Co. Ltd, China.

Ethyl acetate and acetonitrile were used without further treatment and analyzed by gas chromatography(GC) and Karl Fischer

titration(KF). [EMIM][NTf₂] and [HMIM][NTf₂] were purified under vacuum with a rotary evaporator(433.15 K, 0.1 kPa, 8 h) and analyzed by liquid chromatography(LC) and KF. The specifications of used chemicals were summarized in Table 1.

2.2. Apparatus and procedure

A modified Othmer still (CE-2), which was supplied by Peiyang Chemical ENG. Co.(China), was used to measure the VLE data. The modified Othmer still included the injection port, sample connection, thermometer socket and condenser interface, which had the advantage of simple structure, convenient operation, accurate temperature control and precise results at atmospheric pressure. More details about this apparatus were described in previous literatures [25,26,28–31]. The amounts of ethyl acetate and acetonitrile in liquid-phase and vapor-phase were determined by gas chromatography (SP7800, China) with the following operating conditions: injector temperature at 443.15 K, oven temperature at

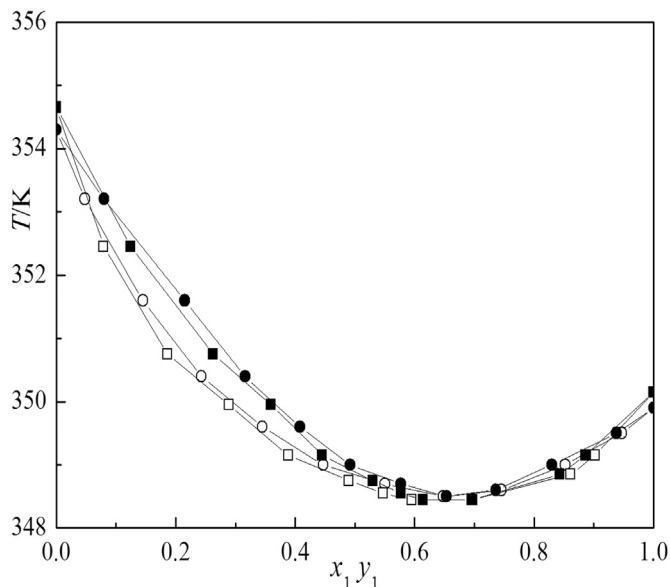


Fig. 1. Comparison of T -(x_1 , y_1) diagram for ethyl acetate(1) + acetonitrile(2) at 101.3 kPa this work: \square -, x_1 ; \blacksquare -, y_1 ; Ref [26]: \circ -, x_1 ; \bullet -, y_1 .

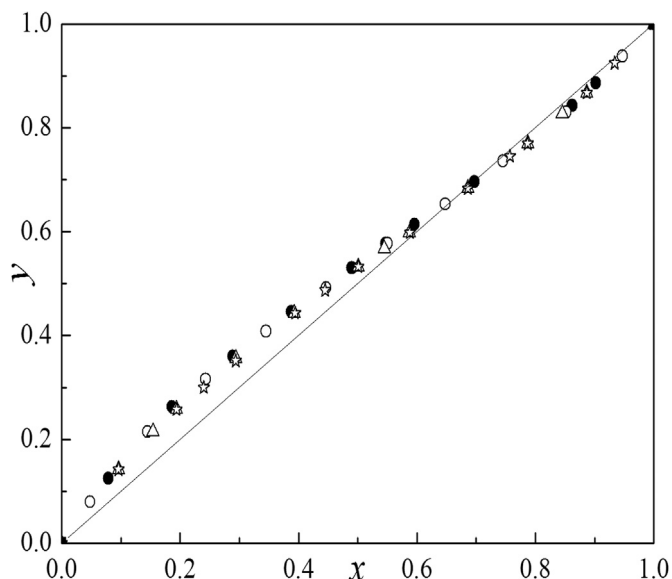


Fig. 2. VLE(x_1 - y_1) comparison of ethyl acetate(1) + acetonitrile(2) at 101.3 kPa this work, \bullet ; Ref [25], \triangle ; Ref [26], \circ ; Ref [32], \star .

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