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# Experimental isobaric vapor–liquid equilibrium at atmospheric and sub-atmospheric pressures, excess molar volumes and deviations in molar refractivity from 293.15 K to 318.15 K of diisopropyl ether with methanol and isopropyl alcohol

# Soujanya J.ª, Satyavathi B.ª,\*, Sankarshana T.<sup>b</sup>

<sup>a</sup> Chemical Engineering Division, Indian Institute of Chemical Technology, Tarnaka, Hyderabad, Andhra Pradesh 500 007, India
<sup>b</sup> College of Technology, Osmania University, Hyderabad, Andhra Pradesh 500 007, India

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## ABSTRACT

Experimental isobaric vapor–liquid equilibrium data for the binary systems, diisopropyl ether + isopropyl alcohol and methanol + diisopropyl ether at the local atmospheric pressure of 94.79 kPa and at subatmospheric pressures of (53.3, 66.7, 79.9) kPa were obtained over the entire composition range using a Sweitoslawsky-type ebulliometer. The experimental temperatures were compared with predictions made using Wilson, NRTL, UNIQUAC, UNIFAC, Peng–Robinson (PR) and Soave–Redlich–Kwong (SRK) equations of state (EoS) with Wong–Sandler (WS) mixing rules. Model parameters along with the deviations in temperature have been presented. Experimental temperatures were found to be in good agreement with the predicted values. NRTL model was found to represent the VLE behavior of these systems better than the other models used. Density and refractive indices of mixtures are reported from 293.15 K to 318.5 K.

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# 1. Introduction

The binary systems studied experimentally in this work, diisopropyl ether (DIPE)+isopropyl alcohol (IPA) and methanol+DIPE are part of the study of the vapor-liquid equilibrium (VLE) behavior of the ternary system, methanol+ DIPE + IPA. DIPE is a potential eco-friendly gasoline additive [1] and an important solvent in the industry. It is found in the downstream of various industries such as in acetone manufacturing [2] and it can be synthesized from isopropanol. In the present study we have experimentally investigated the isobaric vaporliquid equilibrium behavior of these binary systems at the local atmospheric pressure and sub-atmospheric pressures. Densities and refractive indices of the mixtures at various compositions have been measured from 293.15 K to 318.5 K. The work reported here is in continuation with our previous studies of phase equilibria and properties of industrially important streams containing alcohols, hydrocarbons and halogenated organics [3–5]. Chamorro et al. [1] have reported an azeotrope for the DIPE + IPA binary system as part

\* Corresponding author.

Tel.: +91 9666226355/40 27191399; fax: +91 40 27193626.

E-mail addresses: drsatyavathib@gmail.com, bsatyavthi@gmail.com (S. B.).

of the isothermal VLE data of the binary and ternary systems containing DIPE, IPA and *n*-heptane at 313.15 K and Lladosa et al. [6] have studied this system at 30 and 101.3 kPa. Frakova et al. [7] have reported isothermal VLE data for the methanol + DIPE system at 320 and 330 K.

## 2. Experimental

## 2.1. Materials Used

Methanol (>99.8 mass %, HPLC grade) provided by SD Fine Chemicals, India and diisopropyl ether (>98.5 mass %, GC grade) and isopropyl alcohol (>99.8 mass %, HPLC grade) supplied by Sigma–Aldrich were used for experimentation. The chemicals were stored in dessicators to prevent absorption of moisture and were used without any further purification. The final purity of the compounds was measured by a ZB-5 column using FID detector on a Shimadzu 2010 gas chromatograph. The densities and refractive indices of the pure components measured at 298.15 K are compared with literature values [8–12] in Table 1.

## 2.2. Apparatus

A Sweitoslawsky-type ebulliometer, similar to the one described by Hala et al. [13], was used for VLE measurements.





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Chemcial	IUPAC name	T (K)	ho ( $ imes$ 10 <sup>3</sup> kg m <sup>-3</sup> )		$n_D$	
			This work	Reference	This work	
Methanol	Methanol	298.15	0.78662	0.78656 <sup>a</sup> 0.78637 <sup>b</sup>	1.32666	
DIPE	2,2'-Oxybispropane	298.15	0.71830	0.71854 <sup>b</sup> 0.71823 <sup>c</sup> 0.71820 <sup>d</sup> 0.7183 <sup>e</sup>	1.3653	
IPA	2-propanol	298.15	0.78245	0.7827 <sup>e</sup> 0.78126 <sup>b</sup> 0.78130 <sup>f</sup>	1.37522	

Table 1 Co

DIPE: diisopropyl ether.

IPA: isopropyl alcohol.

 $u(\rho): \pm 0. \text{ kg m}^{-3}$ .

 $u(n_D)$ : ±0.00001. Ref. [8].

<sup>b</sup> Ref. [9].

<sup>c</sup> Ref. [10].

<sup>d</sup> Ref. [11].

<sup>e</sup> Ref. [6].

<sup>f</sup> Ref. [12].

The details of the construction of the ebulliometer and the experimental method used in the present study are as described by Vittal Prasad et al. [5]. The ebulliometer is connected to a vacuum pump and a nitrogen gas cylinder, along with a closed end manometer in line to maintain the pressure to within 0.05 kPa of the desired value. This is done by adjusting the opening of the needle valve of the gas cylinder or by opening the bypass line of the vacuum pump. A WIKA digital thermometer (Model CTH6200,  $\pm$  0.05 K) calibrated by point-to-point comparison with a WIKA hand-held calibrator (Model CEP3000) is used for measuring the equilibrium temperatures with an uncertainty of  $\pm 0.05$  K. The thermometer is placed in the thermowell containing glycerol to note the equilibrium temperature for the (vapor + liquid) mixture

Table	2

Vapor pressures of IPA.				
$P_i^0(kPa)$	<i>T</i> (K)			
14.02	312.63			
16.09	315.22			
18.94	318.35			
21.65	320.97			
24.56	323.46			
26.99	325.36			
29.69	327.30			
32.53	329.19			
36.08	331.35			
38.28	332.60			
40.49	333.80			
43.63	335.42			
45.88	336.52			
48.77	337.86			
51.47	339.06			
54.24	340.23			
56.82	341.27			
59.59	342.35			
62.14	343.30			
65.69	344.58			
67.60	345.24			
70.27	346.13			
73.16	347.08			
75.65	347.87			
78.35	348.70			
81.05	349.51			
83.80	350.31			
86.40	351.05			
96.28	353.69			

 $u(T) = \pm 0.05 \text{ K}.$ 

impinging on the thermowell from the Cottrell tube of the ebulliometer. The equilibrium temperature is recorded after steady-state conditions, judged by the constancy of temperature and uniformity of the drop rate maintained for at least 1800s. The mixtures to be studied were prepared gravimetrically by weighing the required amounts of the pure liquids and stirring them well to make homogeneous mixtures before charging the mixtures into the still. A Mettler balance, capable of recording weights to the uncertainty of  $\pm 0.0001$  g, was used. After the mixture is charged in to the ebulliometer, vacuum is applied gradually and then the heating rate is slowly increased and adjusted to produce the required boil-up rate so that a drop count of about 30 drops per minute is achieved. This is in accordance with the suggestion of Hala et al. [13]. The VLE experiment is first done at the lowest pressure. After the measurement of the equilibrium temperature at this pressure, vacuum is released and the pressure increased to the

> Table 3 Vapor pressures of methanol.

$P_i^0(kPa)$	T (K)
26.55	306.91
29.52	309.10
32.46	311.09
35.65	313.08
37.80	314.34
40.63	315.91
43.23	317.27
44.63	317.98
48.35	319.77
51.40	321.15
53.97	322.26
56.89	323.47
59.55	324.53
62.25	325.56
64.90	326.54
67.50	327.47
70.07	328.36
72.95	329.32
75.66	330.20
78.35	331.05
81.05	331.87
83.76	332.67
86.46	333.45
96.35	336.15

 $u(T) = \pm 0.05 \text{ K}.$ 

Reference 1.3267<sup>a</sup> 1.32652<sup>b</sup> 1.3655<sup>c</sup> 1.3655<sup>d</sup> 1.3652<sup>e</sup> 1.3754<sup>e</sup> 1.3752<sup>b</sup> 1.3750<sup>f</sup>

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