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# Densities, viscosities, excess molar volumes, and refractive indices of acetonitrile and 2-alkanols binary mixtures at different temperatures: Experimental results and application of the Prigogine–Flory–Patterson theory

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## ABSTRACT

Densities, viscosities, and refractive indices of mixing of acetonitrile with 2-propanol, 2-butanol, 2-pentanol, 2-hexanol and 2-heptanol, have been measured as a function of composition at 293.15, 298.15, 303.15 and 308.15 K and ambient pressure. The excess molar volumes, viscosity and refractive index deviations calculated and fitted to Redlich–Kister polynomials. From the experimental data, partial molar volumes,  $\bar{V}_{m,i}$  and partial molar volumes at infinite dilution,  $\overline{V}_{m,i}^{o}$  were also calculated. The latter values are interesting from a theoretical point of view since at infinite dilution the only interactions present are solute solvent interactions. For mixtures of acetonitrile with used 2-alkanols, over the entire range of mole fractions,  $\Delta \eta$  is negative and both,  $V_m^E$  and  $\Delta n_D$  are positive. The effect of temperature and chain-length of the 2-alkanols on the excess molar volumes, viscosity and refractive index deviations of its mixtures with acetonitrile are discussed in terms of molecular interaction between unlike molecules. The experimental results have been used to test the applicability of the Prigogine–Flory–Patterson (PFP) theory.

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## 1. Introduction

The thermodynamic and transport properties of liquids and liquid mixtures have been used to understand the molecular interactions between the components of the mixture and also for engineering applications concerning heat transfer, mass transfer and fluid flow [1]. Density, viscosity and refractive index data of binary liquid mixtures are very important from theoretical point of view, to understand liquid theory. Acetonitrile, alkanols, and their binary mixtures find applications as solvent in chemistry and modern technology [2].

A survey of literatures shows that there are very few reports on the density, viscosity, and refractive index of acetonitrile+2alkanols. This paper is a part of an ongoing research effort to measure and characterize the properties of mixtures containing 2alkanols [3–5]. We present, here, densities, viscosities, refractive indices, excess molar volumes, viscosity and refractive index deviations of mixing for the binary mixtures of {acetonitrile+2-alkanols} at the temperatures of 293.15, 298.15, 303.15 and 308.15 K. To the best of our knowledge, no much data are reported for mixtures with acetonitrile and 2-alkanols at the comparable conditions of this study.

## 2. Experimental

# 2.1. Materials purities and suppliers

Acetonitrile (mass fraction > 0.99), 2-propanol (mass fraction 0.99), 2-butanol (mass fraction 0.99), 2-pentanol (mass fraction > 99), 2-hexanol (mass fraction > 0.99) and 2-heptanol (mass fraction > 0.99) were purchased from Merck and used without further purifications. The experimental densities, viscosities and refractive indices at 298.15 K of the pure materials are presented in Table 1 along with the corresponding literature values [2,3,6–8].

## 2.2. Apparatus and procedure

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Densities of the pure liquids and their mixtures at various temperatures were measured with an Anton Paar digital densimeter (Model DMA 4500) operated in the static mode, with an accuracy of  $\pm 1 \times 10^{-5}$ . Viscosities were measured with an Ubbleohde viscometer with an accuracy of  $\pm 2 \times 10^{-5}$ . The equation for viscosity, according to Poiseuille's law, is

$$\eta = \rho \left( kt - \frac{c}{t} \right) \tag{1}$$



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# Table 1

Experimental and literature values of densities  $\rho$ , viscosities  $\eta$ , and refractive indices  $n_D$ , of acetonitrile, 2-propanol, 2-butanol, 2-pentanol, 2-hexanol and 2-heptanol at 298.15 K.

Compound	$\rho (\mathrm{g}\mathrm{cm}^{-3})$	$ ho ( m gcm^{-3})$		η (mPa s)		n <sub>D</sub>	
	Exp.	Lit.	Expt.	Lit.	Expt.	Lit.	
Acetonitrile	0.77664	0.7766[7]	0.3369	0.342[2]	1.3411	1.34163[7]	
2-Propanol	0.78098	0.78126[7]	2.0439	2.0436[2]	1.3745	1.3752[7]	
2-Butanol	0.80256	0.80260[7]	3.1318	3.1150[6]	1.3948	1.3950[7]	
2-Pentanol	0.80524	0.80540[7]	3.4785	3.47[8]	1.4045	1.4044[7]	
2-Hexanol	0.81014	0.81025[3]	4.1	4.204[3]		1.4116	
2-Heptanol	0.81333	0.8134[7]	5.3305	5.346[3]		1.4188	

where *k* and *c* are the viscometer constants *t* and  $\eta$  are the efflux time and dynamic viscosity, respectively. The *k* and *c* parameters were obtained by measurements on double distilled water and benzene at 298.15 K. The temperature in the cell was regulated to  $\pm 0.01$  K.

Refractive indices were measured using a high accuracy Abbe refractometer with an accuracy of  $\pm 4 \times 10^{-5}$ . The measurement method relies on an optical detection of the critical angle at the wavelength of the sodium D line (589.6 nm). The mixtures were prepared by weighing known masses of pure liquids in air tight, narrow-mouth ground stoppered bottles taking due precautions to minimize evaporation losses. All the mass measurements were performed on an electronic balance (Mettler AE 163, Switzerland) accurate to 0.01 mg. The possible error in the mole fraction is estimated to be less than  $\pm 1 \times 10^{-4}$ .

## 3. Results and discussion

## 3.1. Densities and excess molar volumes

The excess molar volumes of the solutions of molar composition x were calculated from the densities of the pure liquids and their mixtures according to the following equation

$$V_m^E = \sum_{i=1}^N x_i M_i (\rho^{-1} - \rho_i^{-1})$$
<sup>(2)</sup>

where  $\rho$  is the density of the mixture,  $\rho_i$  is the density of pure component *i*,  $x_i$  is the mole fraction,  $M_i$  is the molar mass of component *i*, and *N* stands for the number of components in the mixture.

The corresponding  $V_m^E$  values of binary mixtures of  $[x_1 \text{ acetoni-trile}+(1-x_1) 2\text{ -alkanols}]$  measured at different temperatures are plotted against mole fraction of acetonitrile at 298.15 K in Fig. 1.



**Fig. 1.** Excess molar volumes  $V_m^E$  vs. mole fraction of acetonitrile for acetonitrile binary mixtures with (**a**) 2-propanol, ( $\diamond$ ) 2-butanol, (**b**) 2-pentanol, (**c**) 2-hexanol, (**c**) 2-heptanol at 298.15 K. The solid curves were calculated from coefficients of Eq. (3) given in Table 2.

Each set of results were fitted using a Redlich–Kister polynomial [9] which for binary mixtures is

$$Y^{E} = x_{1}(1 - x_{1}) \sum_{k=0}^{N} A_{k}(1 - 2x_{1})^{k}$$
(3)

where  $Y^E \equiv V_m^E$  or  $\Delta \eta$  or  $\Delta n_D$  and  $x_1$  is the mole fraction of acetonitrile,  $A_k$  are adjustable parameters obtained by least-squares method, and k is the degree of the polynomials.

In each case, the optimum number of coefficients was ascertained from an examination of the variation of standard deviation  $\sigma$  with

$$\sigma = \left[\frac{\sum (Y_{\text{exp.}} - Y_{\text{cal.}})^2}{(n-p)}\right]^{1/2}$$
(4)

where  $Y_{\text{exp.}}$  and  $Y_{\text{cal.}}$  are the experimental and calculated values of the property *Y*, respectively, and *n* and *p* are the number of experimental points and number of parameters retained in the respective equations.

Table 2 presents the values of the parameters  $A_k$  together with the standard deviation  $\sigma$ . The coefficients  $A_k$  were used to calculate the solid curves in Fig. 1. Excess molar volumes are positive for mixtures of acetonitrile with 2-alkanols over the whole range of mole fractions. Fig. 1 shows that,  $V_m^E$  at equimolar concentrations of acetonitrile, increases from 2-propanol up to 2-heptanol, as the length of the alkanols chain increases.

The same behavior is obtained at other temperatures, except that the values of  $V_m^E$  become more Positive with increase in temperature.

The observed  $V_m^E$  can be considered as arising from two types of interactions between the components: (i) physical interaction consist mainly dispersion forces and making a positive contribution, and (ii) chemical or specific interaction resulting in a volume decrease. The latter includes charge transfer forces, forming and/or



**Fig. 2.** Plot of excess molar volume  $V_m^E$  against mole fraction of acetonitrile for the  $\{x_1 \text{ acetonitrile} + (1 - x_1) \text{ 2-propanol}\}$  mixtures. (•) Experimental; (--) calculated by using PFP theory.

### Table 2

Parameters and standard deviations of Eqs. (3) and (4) for acetonitrile + 2 alkanols at different temperatures.

		Temperature	A <sub>0</sub>	<i>A</i> <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	σ
Acetonitrile + 2-propanol	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	293.15	0.6394	-0.1539	0.0088	-0.4421	0.003
		298.15	0.8407	-0.1006	-0.1343	-0.4601	0.006
		303.15	0.9144	-0.0960	-0.0460	-0.3896	0.005
		308.15	1.028	-0.1214	-0.2983	-0.2862	0.001
	$\Delta \eta (\mathrm{mPas})$	293.15	-2.9410	-1.9301	-1.4723	-0.6149	0.009
		298.15	-2.4568	-1.4489	-1.4642	-0.9840	0.004
		303.15	-2.048	-1.1176	-1.1363	-0.7532	0.003
		308.15	-1.7352	-0.9349	-0.8138	-0.5752	0.003
	$\Delta n_D$	293.15	0.0125	-0.0102	0.0015	0.0014	0.00005
		298.15	0.0208	-0.0051	-0.0048	- 0.0009	0.0001
		303.15	0.0169	0.0012	0.0082	-0.0138	0.0002
		308.15	0.0238	0.0022	0.0039	-0.0202	0.0003
Acetonitrile + 2-butanol	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	293.15	1.2481	-0.1305	-0.4009	0.7341	0.007
		298.15	1.3547	-0.0223	0.0973	0.1967	0.006
		303.15	1.3926	-0.0316	0.1749	-0.1837	0.003
		308.15	1.4622	0.0016	-0.2378	-0.3579	0.005
	$\Delta\eta~(\mathrm{mPa}\mathrm{s})$	293.15	-5.3910	-3.5409	-4.4644	-4.2187	0.009
		298.15	-4.1111	-2.5578	-2.9842	-2.6724	0.001
		303.15	-3.1527	-1.8637	-1.9971	-1.6378	0.006
		308.15	-2.6069	-1.5344	-1.6050	-1.2956	0.0002
	$\Delta n_D$	293.15	0.0289	0.0101	0.0068	-0.0030	0.00005
		298.15	0.0305	-0.0023	-0.0009	-0.0077	0.00005
		303.15	0.0358	0.0104	-0.0040	-0.0173	0.00008
		308.15	0.0369	-0.0159	0.0124	-0.0187	0.0001
Acetonitrile + 2-pentanol	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	293.15	1.2982	-0.1878	-0.0156	-0.0087	0.004
		298.15	1.340	-0.2918	-0.026	-0.1584	0.003
		303.15	1.4179	-0.2064	-0.0431	0.0163	0.005
		308.15	1.4581	-0.2232	-0.0476	-0.0351	0.002
	$\Delta\eta$ (mPa s)	293.15	-5.6808	-3.6033	-4.088	-3.3281	0.024
		298.15	-4.3811	-2.8846	-2.4687	-1.082	0.047
		303.15	-3.2071	-1.8007	-1.5014	-0.7396	0.006
		308.15	-2.6469	-1.4531	-1.3176	-0.8693	0.005
	$\Delta n_D$	293.15	0.0527	-0.0102	-0.0095	0.0192	0.0001
		298.15	0.0568	-0.0063	0.0158-	-0.0079	0.0001
		303.15	0.0609	-0.0073	-0.0105	-0.0069	0.0009
		308.15	0.0669	-0.0396	-0.0301	0.0483	0.0009
Acetonitrile + 2-hexanol	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	293.15	1.3656	-0.3098	-0.2335	-0.0135	0.001
		298.15	1.4115	-0.3362	-0.2574	-0.0239	0.002
		303.15	1.4122	-0.2496	0.0207	-0.4043	0.003
		308.15	1.4452	-0.2402	-0.2829	-0.3496	0.004
	$\Delta \eta$ (mPa s)	293.15	-6.4860	-3.6654	-3.5826	-2.7317	0.030
		298.15	-4.8490	-2.6035	-2.1334	-1.3399	0.010
		303.15	-3.8441	-1.9671	-1.6201	-0.9541	0.007
		308.15	-2.9752	-1.4529	0.9902	-0.4597	0.003
	$\Delta n_D$	293.15	0.0616	-0.0197	0.0048	-0.0193	0.0004
		298.15	0.0731	-0.0190	-0.0026	0014	0.0002
		303.15	0.0831	0.0279-	-0.0002	0.0075	0.0005
		308.15	0.0902	-0.0189	0.0233	-0.0450	0.0002
Acetonitrile + 2-heptanol	$V_m^E$ (cm <sup>3</sup> mol <sup>-1</sup> )	293.15	1.3669	-0.3139	0.0617	-0.3491	0.006
-		298.15	1.4065	-0.1915	-0.0562	-0.5971	0.009
		303.15	1.4232	-0.2107	-0.1502	-0.3058	0.005
		308.15	1.5212	-0.0152	-0.3250	-1.1118	0.007
	$\Delta\eta$ (mPa s)	293.15	-8.1686	-4.6000	-3.2429	-2.3763	0.028
		298.15	-6.3674	-3.2978	-2.5122	-2.3887	0.020
		303.15	-4.8318	-2.3522	-1.4507	-1.3395	0.019
		308.15	-3.6669	-1.5195	-0.8862	-1.1093	0.017
	$\Delta n_D$	293.15	0.0774	-0.0285	-0.0025	-0.0097	0.0003
		298.15	0.0839	-0.0177	0.0081	-0.0351	0.0003
		303.15	0.0907	-0.0139	0.0046	-0.0523	0.0002
		308.15	0.0907	-0.0139	0.0046	-0.0523	0.0003

breaking of H bonds and other complex forming interactions. It is well-known that both acetonitrile and 2-alkanols are associated in liquid state. Acetonitrile contains molecules with strong parallel and antiparallel orientations and this strongly ordered structure is stabilized by dipole–dipole interactions [10], where as 2-alkanols are associated through the hydrogen bonding of their hydroxyl groups.

Molecular association decreases with increase in chain-length of 2-alkanol. The increase in  $V_m^E$  with the increase in chain-length of 2-alkanol implies that acetonitrile-2-alkanol interaction is relatively

# Table 3

Densities  $\rho$ , viscosities  $\eta$ , refractive indices  $n_D$ , of mixing for the binary mixtures as a function of the mole fraction  $x_1$  of acetonitrile.

<i>x</i> <sub>1</sub>	$\rho (\mathrm{g}\mathrm{cm}^{-3})$	$\bar{V}_{m,1}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_{m,2} \ ({ m cm}^3 \ { m mol}^{-1})$	η (mPa s)	n <sub>D</sub>
Acetonitrile(1)+2-propand	ol (2) at 293.15 K				
0.0000	0.78519			2.3511	1.3766
0.0496	0 78497	52 771	76 534	1 9715	1 3757
0.0906	0.78472	52.88	76.527	1 6877	1 3751
0.0500	0.78472	52.042	70.327	1.0077	1.3731
0.1529	0.78431	52.943	70.514	1.3082	1.3/3/
0.2022	0.78390	52.944	/6.51/	1.1/59	1.3/26
0.2783	0.78336	52.888	76.531	0.9608	1.3705
0.3678	0.78271	52.801	76.575	0.7912	1.3677
0.4768	0.78202	52.713	76.65	0.6502	1.3640
0.6132	0.78153	52.636	76.726	0.5100	1.3590
0.7714	0.78113	52.578	76.858	0.4156	1.3528
0 9207	0 78126	52 517	77 272	0 3716	1 3469
1,0000	0.78204	521017	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	0 3542	1 3436
1.0000	0.70204			0.5542	1.5450
At 298.15 K					
0.0000	0.78098			2.0439	1.3745
0.0496	0.78076	53.258	76.937	1.6909	1.3733
0.0906	0 7803	53 394	76 939	1 4612	1 3724
0.1520	0.7707	52 /69	76.020	1 2074	1 2712
0.1525	0.7757	53.400	70.323	1.2074	1.3713
0.2022	0.7797	55,400	70.95	1.044	1.5/02
0.2783	0.7792	53.374	/6.945	0.8677	1.3687
0.3678	0.77765	53.254	77.009	0.7248	1.3667
0.4768	0.77879	53.126	77.121	0.6062	1.3635
0.6132	0.77620	53.006	77.239	0.4735	1.3591
0.7714	0.77579	52.935	77.403	0.3840	1.3528
0.9207	0.77595	52.878	77.774	0.3499	1.3452
1 0000	0 77664			0 3369	1 3411
				0.0000	
At 303.15 K					
0.0000	0.77671			1.7583	1.3724
0.0496	0.77632	53,7846	77.3646	1.4742	1.3715
0.0906	0 77584	53 8653	77 3658	1 2875	1 3707
0.1520	0.77512	52 9010	77 2629	1,0602	1 2604
0.1525	0.77313	53.6515		0.0267	1.3034
0.2022	0.77434	53.6040	77.3722	0.9507	1.2004
0.2783	0.77397	53./64/	//.3918	0.7975	1.3666
0.3678	0.77288	53.6389	77.4536	0.6615	1.3641
0.4768	0.77184	53.5155	77.5639	0.5492	1.3608
0.6132	0.77113	53.3939	77.684	0.4429	1.3561
0.7714	0.77052	53.3163	77.8716	0.3617	1.3500
0.9207	0.77059	53.2502	78.2738	0.3311	1.3433
1.0000	0.77121			0.3254	1.3390
At 308.15 K					
0.0000	0.77236			1.5315	1.3703
0.0496	0.77186	54.224	77.8059	1.2958	1.3694
0.0906	0.77131	54.3317	77.8052	1.1500	1.3687
0 1529	0 77057	54 3794	77 7908	0.9576	1 3679
0.2022	0.76002	54 2607	77.700	0.8460	1 2670
0.2022	0.70992	54.3007	77,752	0.8400	1.3070
0.2783	0.76898	54.2052	77.8124	0.7168	1.3057
0.3678	0.76780	54.1254	77.8884	0.6057	1.3637
0.4768	0.76644	53.9689	78.0409	0.5051	1.3605
0.6132	0.76575	53.7788	78.2157	0.4111	1.3557
0.7714	0.76526	53.6666	78.4583	0.3442	1.3491
0.9207	0.76518	53.6311	78.7756	0.3202	1.3417
1.0000	0.76575			0.3082	1.3371
Acetonitrile(1)+2-buanol (	2) at 293.15 K				
0.0000	0.80657			3.9119	1.3966
0.0844	0.80453	53.459	91.909	2.5031	1.3952
0 1644	0.8025	53 263	91 951	1 6545	1 3930
0.2516	0.80041	53 153	91 981	1 3764	1 3899
0.3369	0 79833	53.066	92.013	1 0890	1 3860
0.3303	0.75655	53,000	02.000	0.850	1,3000
0.5292	0.7000	52.522	92.090	0.0004	1.5804
0.5382	0.79335	52.707	92.241	0.953	1.3/51
0.6425	0.7907	52.613	92.498	0.5565	1.3686
0.7610	0.7881	52.487	92.791	0.4636	1.3610
0.8715	0.78592	52.452	92.845	0.3984	1.3534
0.9588	0.78348	52.488	92.513	0.3663	1.3467
1.0000	0.78204			0.3542	1.3436
At 298.15 K					
0.0000	0.80256			3.1318	1.3946
0.0844	0.80028	54.045	92.369	2.1353	1.3918
0.1644	0.79807	53.784	92.417	1.5742	1.3893
0 2516	0 79579	53 582	92 474	1 2185	1 3865
0 3369	0 79363	53 431	92 532	0 9920	1 3830
0.4444	0.70006	53. <del>1</del> 31 53.20	02.631	0.7027	1.3030
0.4444	0.79090	33.200	52.021	0.7357	1.5/82

# Table 3 (Continued)

<i>x</i> <sub>1</sub>	$ ho (\mathrm{g}\mathrm{cm}^{-3})$	$\bar{V}_{m,1}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_{m,2} (\mathrm{cm}^3 \mathrm{mol}^{-1})$	η (mPa s)	n <sub>D</sub>
0.5382	0.7885	53.152	92.738	0.6498	1.3734
0.6425	0.78567	53.045	92.919	0.5180	1.3674
0.7610	0.78265	52.938	93.164	0.4216	1.3597
0.8715	0.77999	52.871	93.405	0.3868	1.3518
0.9588	0.77771	52.861	93.581	0.3632	1.3448
1.0000	0.77664			0.3369	1.3411
At 303 15 K					
0.0000	0.79826			2.5340	1.3924
0.0844	0 79595	54 407	92 865	1 7943	1 3902
0 1644	0 79374	54 216	92 893	1 3829	1 3886
0.2516	0 79138	54 012	92 945	1 0822	1 3860
0 3369	0 78907	53 837	93.018	0.8873	1 3829
0.4444	0.78617	53.66	93.131	0.7129	1.3779
0 5382	0.78362	53 544	93 245	0 5936	1 3722
0.6425	0.78073	53.444	93.393	0.4865	1.3656
0.7610	0.77745	53.347	93.613	0.4019	1.3575
0.8715	0.77443	53.271	93.943	0.3612	1.3495
0.9588	0.77205	53.244	93.374	0.3414	1.3426
1.0000	0.77121			0.3254	1.3390
4+ 200 15 1/					
AL 508.15 K	0 70306			2 1723	1 2005
0.0000	0.79590	54 855	03 368	1 5718	1.3905
0.1644	0.78927	54 669	93 391	1 2127	1.3870
0.2516	0.78527	54.005	02.45	0.0642	1,2025
0.2310	0.78077	54.346	02 52	0.9042	1.3023
0.3309	0.78437	54.052	33.33 02.657	0.6524	1.3753
0.5282	0.78135	52.025	02 774	0.0324	1.3733
0.5382	0.77609	53.555	02 012	0.3475	1.3713
0.0425	0.77207	52 7/2	93.912 0/ 110	0.4355	1 35039
0.8715	0.76899	53 665	94.113	0.3730	1 3510
0.0588	0.76651	53 628	95.049	0.3238	1 3/23
1 0000	0.76575	55.028	33.043	0.3238	1 3371
1.0000	0.70373			0.3002	1.5571
Acetonitrile(1)+2-pentano	ol (2) at 293.15 K				
0.0000	0.80929			4.2982	1.4060
0.1160	0.80675	53.427	108.933	2.5440	1.4035
0.1727	0.80546	53.342	108.946	2.0931	1.4020
0.2827	0.80279	53.181	109	1.5337	1.3981
0.3546	0.80101	53.072	109.049	1.2618	1.3951
0.4458	0.79866	52.94	109.136	1.0078	1.3908
0.5366	0.79626	52.815	109.249	0.8100	1.3858
0.6488	0.79309	52.689	109.438	0.6391	1.3779
0.7671	0.78952	52.589	109.7	0.5048	1.3674
0.8793	0.78603	52.522	110.002	0.4119	1.3561
0.9578	0.78359	52.489	110.244	0.3705	1.3478
1.0000	0.78204			0.3542	1.3430
At 298.15 K					
0.0000	0.80524			3.4785	1.4045
0.1160	0.80261	53.783	109.485	2.1703	1.4012
0.1727	0.80125	53.699	109.502	1.8045	1.3999
0.2827	0.79855	53.553	109.543	1.3619	1.3965
0.3546	0.79668	53.462	109.586	1.1248	1.3941
0.4458	0.79417	53.343	109.669	0.9044	1.3901
0.5366	0.7916	53.217	109.787	0.7392	1.3848
0.6488	0.78828	53.069	109.997	0.5884	1.3764
0.7671	0.78454	52.952	110.301	0.4715	1.3657
0.8793	0.78088	52.883	110.621	0.3910	1.3548
0.9578	0.77828	52.855	110.82	0.3537	1.3461
1.0000	0.77664			0.3369	1.3411
At 303.15 K					
0.0000	0.77671			1.7583	1.3724
0.1160	0.77632	53.784	77.364	1.4742	1.3715
0.1727	0.77584	53.865	77.365	1.2875	1.3707
0.2827	0.77513	53.891	77.363	1.0692	1.3694
0.3546	0.77454	53.864	77.372	0.9367	1.3684
0.4458	0.77397	53.764	77.391	0.7975	1.3666
0.5366	0.77288	53.638	77.453	0.6615	1.3641
0.6488	0.77184	53.515	77.563	0.5492	1.3608
0.7671	0.77113	53.393	77.684	0.4429	1.3561
0.8793	0.77052	53.316	77.871	0.3617	1.3500
0.9578	0.77059	53.25	78.273	0.3311	1.3433
1.0000	0.77121			0.3254	1.3390

# Table 3 ( Continued )

SUBSIDJUNIT <t< th=""><th><i>x</i><sub>1</sub></th><th><math> ho ({ m gcm^{-3}})</math></th><th><math>\bar{V}_{m,1}</math> (cm<sup>3</sup> mol<sup>-1</sup>)</th><th><math>\bar{V}_{m,2}</math> (cm<sup>3</sup> mol<sup>-1</sup>)</th><th>η (mPa s)</th><th>n<sub>D</sub></th></t<>	<i>x</i> <sub>1</sub>	$ ho ({ m gcm^{-3}})$	$\bar{V}_{m,1}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_{m,2}$ (cm <sup>3</sup> mol <sup>-1</sup> )	η (mPa s)	n <sub>D</sub>
0.00000.7286J.52847.8631.29831.39940.17710.71110.43377.78951.29981.39940.17210.71110.43377.78920.44601.39700.45460.76885.42657.78120.74891.39770.45470.767805.12737.88830.49771.38270.57700.767505.35667.84380.44411.35770.6770.767505.36667.44380.34421.34970.6770.76185.16117.87750.2021.31710.6770.76185.3671.25591.40071.40070.6780.76185.3671.25591.40071.40030.6780.76185.37712.5691.40071.40030.78150.67675.36712.56931.40071.40030.78160.381712.56931.40071.40030.78160.37782.26131.26731.40071.3070.78160.377812.56730.76161.3371.40160.78160.378712.56731.40271.40311.40160.78160.379712.67831.49271.3021.30100.78160.79282.528712.66730.76281.49270.78160.79282.528712.67831.49671.3020.78160.79282.528712.67831.49671.3020.78160.79282.528712.67831.4967 </td <td>308.15 K</td> <td></td> <td></td> <td></td> <td></td> <td></td>	308.15 K					
0.100         0.7186         9.4234         7.7405         1.2868         1.3684           0.3572         0.7713         5.4331         7.7805         0.1500         1.367           0.3524         0.7767         5.4331         7.787         0.3768         1.367           0.3555         0.77870         5.125         7.788         0.6301         1.367           0.556         0.77870         5.125         7.788         0.6301         1.360           0.671         0.6575         3.378         7.215         0.411         1.360           0.671         0.6575         3.378         7.215         0.4301         1.3605           0.6757         0.7638         3.537         1.2358         0.3407         1.4103           0.6767         0.7638         3.537         1.2558         2.3677         1.403           0.6763         0.8344         5.2377         1.25678         1.6859         1.403           0.4346         0.8611         5.2579         1.2578         1.6829         1.404           0.4448         0.8664         5.2597         1.2578         1.6829         1.404           0.4448         0.8664         5.2599         1.26271	0.0000	0.77236			1.5315	1.3703
0.1720.778154.3377.8051.5061.3670.32420.7780754.3677.8050.40731.3670.32460.7678054.3877.7720.40411.3670.35460.7678054.3877.8040.40571.3670.64850.7664451.96872.640.40671.3670.64850.7678051.06472.4580.44111.38570.67710.7657351.06472.4580.44111.38570.67810.7657851.06472.4580.44111.38570.66950.767551.06472.4580.43021.377Actional (1) 2.1 synt, St.51.501.413550.3871.4250.09640.814153.38722.5082.12771.4610.09610.814352.28712.56282.12771.4610.25740.8614152.28712.56282.12771.4610.25740.8613152.28112.523541.02621.3870.75840.8003152.28112.59341.02631.3870.75840.861452.78912.64230.43781.3010.75790.776413.6771.3671.3670.75790.776413.6781.3671.3670.75790.776413.77812.24230.43781.3010.75790.776413.77812.2630.47491.3670.75790.776413.77812.2610.3781.301	0.1160	0.77186	54.224	77.805	1.2958	1.3694
0.2827         0.77907         54.379         77.79         0.576         1.3670           0.4426         0.70808         54.265         77.812         0.7080         1.3670           0.4426         0.70808         54.265         77.812         0.7081         1.3670           0.4436         0.70675         53.778         76.215         0.411         1.3570           0.4771         0.70757         53.778         76.215         0.4141         1.3570           0.5731         0.75818         53.611         72.775         0.2022         1.3171           0.6661         0.76726         53.362         12.559         1.4697         1.4101           0.6171         0.76756         53.362         12.559         1.4697         1.4101           0.6181         0.3177         12.559         1.4697         1.4101           0.7574         0.8681         53.362         12.5678         1.4597         1.4010           0.4450         0.5671         12.62678         1.4597         1.4021         1.4597           0.4450         0.5671         12.6278         1.4597         1.2023         1.4597           0.4450         0.5671         12.62778         1.62673<	0.1727	0.77131	54.331	77.805	1.1500	1.3687
0.5360.7690254.3677.7020.4601.36770.33640.7690354.3277.3620.076811.36770.33640.7670354.7277.3620.076131.36770.37810.767353.76677.46280.44111.35770.87930.767353.66677.46780.44111.35770.87930.767353.66677.46780.34021.34771.00000.767353.67677.46780.34021.34771.00000.767353.871.25.7981.40731.40730.87370.761853.871.25.7981.40731.40140.8130.810253.871.25.7931.40141.40140.3480.809352.811.25.7931.40131.40140.3480.809352.811.26.7940.70761.38770.73800.7281652.871.26.4210.38291.36130.73800.7281652.5871.26.4210.38271.36130.73800.7281653.7991.26.4210.38281.40141.10000.738753.7991.26.2112.39281.40141.10000.738753.7991.26.4710.38271.36280.73810.7381253.7891.26.4710.38281.36100.73840.7381253.7891.26.4710.38281.36100.73850.7381253.7891.26.4710.38461.37300.73850.73812	0.2827	0.77057	54.379	77.79	0.9576	1.3679
d.4450.78885.42657.7.8120.71880.60571.3670.53660.778.040.05751.366778.040.05711.3620.57870.765755.566678.0450.04421.3890.5780.75585.567678.0450.04421.3890.5780.75585.567678.0450.04421.3810.5780.75585.567678.0570.3021.3810.6660.14425.137772.5781.5591.4350.6640.11245.31871.255971.5691.4370.53400.66675.316712.56781.23771.3670.53400.666975.316712.56781.23771.3670.53400.66075.316712.56781.27711.3670.53400.60035.2587126.5730.44431.3620.53740.64035.2587126.5730.44431.3620.53750.7284126.730.44441.3620.537612.26381.4491.4051.3670.53800.61045.76812.62381.4491.4020.43810.96973.366512.62331.4491.4020.43930.37923.341122.6421.3571.3500.5390.73882.257812.62381.4491.4020.44410.96913.565126.2331.4491.4020.43930.97923.349122.6421.357 <td< td=""><td>0.3546</td><td>0.76992</td><td>54.36</td><td>77.792</td><td>0.8460</td><td>1.3670</td></td<>	0.3546	0.76992	54.36	77.792	0.8460	1.3670
0.5186     0.7780     54.125     72.888     0.8617     1.3672       0.6486     0.76674     3.5368     72.878     0.4171     1.3577       0.67575     3.5276     72.278     0.4171     1.3577       0.67676     3.5378     72.278     0.4171     1.3577       0.67676     3.5378     72.258     0.2020     1.3417       1.6000     0.5757     5.3587     1.2559     3.4607     1.4135       0.6964     0.8124     5.3387     1.25.599     3.4607     1.4135       0.6964     0.8124     5.3387     1.25.598     1.26771     1.407       0.75746     0.80071     5.3387     1.25.598     1.26771     1.367       0.4453     0.80111     5.3997     1.25.788     1.0662     1.3975       0.4583     0.80031     5.2.51     1.26.571     0.5778     1.3570       0.4583     0.80031     5.2.548     1.26.547     0.6629     1.3973       0.5790     0.79429     5.2.494     1.66.493     0.3542     1.3979       0.5770     0.79429     5.2.698     1.26.271     2.3878     1.4065       0.5784     0.49174     5.3765     1.26.281     2.3814     1.4065       0.5785     0.2669	0.4458	0.76898	54.265	77.812	0.7168	1.3657
0.6458         0.7674         5.3678         7.8.04         0.5051         1.3065           0.6771         0.7675         5.3778         7.8.458         0.4111         1.3575           0.6739         0.76575         5.3666         7.8.458         0.4142         1.3491           0.0000         0.79575         5.559         7.757         0.2082         1.3297           Accommit(1)* 2-Accommit(2)* 2-Accommit(2)* 2-Accommit(1)* 2-Accommit(1)* 2-Accommit(2)* 2-Accommit(2)         5.359         7.877         1.4101           0.0100         0.41468         5.289         1.25.626         2.1777         1.4051           0.1446         0.80834         5.2289         1.25.626         2.1777         1.4051           0.1446         0.80834         5.25.87         1.26.621         0.3276         1.3917           0.1446         0.40907         5.351         1.26.642         1.3917         1.3917           0.7570         0.74429         2.2494         126.6421         0.3232         1.3916           0.7571         0.74429         2.3765         126.241         2.3236         1.3916           0.7571         0.74429         5.3761         126.241         2.3236         1.4967           0.	0.5366	0.76780	54.125	77.888	0.6057	1.3637
0.7671     0.7675     5.778     7.8.215     0.4111     1.3557       0.5778     0.7650     3.5.3676     7.8.458     0.1412     1.3497       0.5078     0.7650     3.5.3676     7.8.458     0.1412     1.3497       0.5078     0.7650     3.5.377     12.5.093     3.4907     1.415       0.5078     0.81212     5.3.377     12.5.093     2.4907     1.4015       0.574     0.81214     5.3.387     12.5.093     2.4907     1.4015       0.574     0.88154     5.289     12.5.673     1.6052     1.3917       0.454     0.8969     0.8121     2.5.373     12.5.673     1.6052     1.3917       0.454     0.89697     5.2.688     12.6.773     0.7454     1.3817       0.454     0.79976     5.2.688     12.6.771     0.4544     1.3817       0.454     0.79976     5.2.688     12.6.771     0.4544     1.3817       0.4574     0.4994     126.592     0.5228     1.3299       0.4730     0.7348     5.756     12.6.171     0.3754     1.3290       0.4740     0.72904     5.756     12.6.211     2.2339     1.4044       0.4740     0.8398     0.5756     12.6.211     2.2339     1.4056	0.6488	0.76644	53.968	78.04	0.5051	1.3605
0.87930.7852653.68678.6880.34221.34911.00000.95750.756183.63178.7570.32021.33711.00000.814085.33711.55.003.26021.40750.00110.810225.33711.55.002.26622.17771.40510.45460.809345.32891.25.6262.17771.40510.45460.809115.24871.25.7871.63791.36710.45460.800715.24871.25.7881.77711.38720.53660.202885.24871.26.9490.35731.33010.75800.72885.25.871.26.4210.36201.37910.75900.744295.24941.26.9490.35731.33010.76000.81741.25.7881.26.2331.40601.40620.95740.784295.24941.26.9490.35421.40660.96040.818145.37651.26.2331.40621.40620.95740.78495.35611.26.2331.40621.40620.95740.93985.26.871.25.2520.96621.38270.95780.93985.26.871.25.2520.96621.38270.95790.798025.35711.25.5220.96621.38270.95790.798025.35711.25.5220.96621.38270.95790.798025.35911.26.5230.49441.40620.95790.798025.35911.26.5230.494	0.7671	0.76575	53.778	78.215	0.4111	1.3557
0.87580.785183.53172.7750.30221.3371Accountic(1) -2-becam (2) at 29.15 K <td>0.8793</td> <td>0.76526</td> <td>53.666</td> <td>78.458</td> <td>0.3442</td> <td>1.3491</td>	0.8793	0.76526	53.666	78.458	0.3442	1.3491
1.0000.75750.8121.3270.0000.814055.33621.255983.48071.41030.01810.810225.3.6221.25.0382.1.0771.40510.025740.80345.3.2871.25.5781.1.7571.30750.44310.80115.2.9771.25.5781.1.7571.30750.44320.800315.2.9771.25.5781.1.7571.30750.44350.795765.2.6881.26.1570.77671.33710.47350.792885.2.5871.26.2310.58201.33100.67350.792885.2.5871.26.370.57621.33190.67350.792885.2.5871.26.370.57621.33190.67350.792885.2.5871.26.330.44443.6210.67350.792895.2.5871.26.331.46421.40520.67350.792815.3.5811.26.2381.44491.40220.63430.398725.3.5411.26.2381.44491.40220.63440.336251.26.2381.44491.40220.63430.798725.3.5411.26.3281.44491.40220.63440.336251.26.2381.43491.40280.63540.798725.3.5411.26.3281.44491.40220.63540.798725.3.5411.26.3281.44491.3010.63540.798725.3.5411.26.3281.44491.30210.63540.798745.2.687<	0.9578	0.76518	53.631	78.775	0.3202	1.3417
Actominit(1) 1-2-becamb         5150         1.4135           0.0900         0.8194         53.357         125.589         3.4807         1.4107           0.8131         0.8124         53.357         125.583         2.4692         1.4077           0.2574         0.8034         53.262         125.025         1.2833         1.4014           0.4363         0.8007         53.167         125.034         1.4072         1.3207           0.4364         0.80013         2.2351         125.034         1.4072         1.3207           0.4365         0.7978         5.2857         126.421         0.7972         1.3301           0.4365         0.7978         5.2357         126.423         0.4344         1.3627           0.4373         0.7819         5.2357         126.423         0.4344         1.3627           0.4364         0.7974         126.238         0.4444         1.3627         1.331           0.42051	1.0000	0.76575			0.3082	1.3371
10000         0.4188         1.5.59 </td <td>Acetonitrile(1)+2-hexanol</td> <td>(2) at 293.15 K</td> <td></td> <td></td> <td>5 4550</td> <td>4 4405</td>	Acetonitrile(1)+2-hexanol	(2) at 293.15 K			5 4550	4 4405
0.004         0.8149         3.3.82         1.2.5.20         2.490         1.419           0.2574         0.2684         3.289         1.2.5.20         2.177         1.455           0.4485         0.80607         5.3.167         1.25.789         1.2673         1.375           0.4485         0.80013         5.2.851         1.25.814         1.0062         1.3972           0.538         0.80013         5.2.851         1.25.814         1.0062         1.3973           0.7580         0.75288         5.2.857         1.26.471         0.7560         1.3373           0.7580         0.75288         5.2.857         1.26.391         0.4449         1.3021           0.8733         0.7319         52.1494         126.599         0.3542         1.3439           0.8733         0.73204         2.2356         1.62.018         2.2359         1.4069           0.4131         0.80614         53.766         1.26.233         1.246.22         1.3479         1.4052           0.4543         0.79812         53.861         1.26.233         0.4062         1.3377         1.3975           0.4543         0.79819         53.341         126.6402         1.3137         1.3955	0.0000	0.81214	52.207	135 500	5.1550	1.4135
0.031         0.002         33.369         1.25.33         2.59.2         1.401           0.4436         0.80311         32.997         125.879         1.2763         1.391           0.5388         0.79676         52.898         126.573         0.7573         0.7373           0.6495         0.79676         52.898         126.573         0.7576         0.7382           0.6739         0.73204         2.5377         126.421         0.5362         1.3317           0.6790         0.73204         2.2494         126.73         0.4444         1.3621           0.000         0.73204         3.556         126.208         2.3352         1.4095           0.0954         0.88014         53.755         126.208         2.3352         1.4095           0.1131         0.36014         53.755         126.208         2.3352         1.4095           0.1313         0.36014         53.755         126.208         1.3377         1.397           0.1313         0.36014         53.755         126.208         1.3377         1.397           0.1313         0.36014         53.757         126.208         1.3377         1.392           0.1314         0.36014         53.75	0.0964	0.81214	53.387	125.599	3.4907	1.4103
12.31         0.30.32         3.5.67         1.2.673         1.2.07         1.4.07           0.4433         0.60013         52.879         1.25.789         1.273         1.3972           0.5388         0.80013         52.879         1.26.157         0.6766         1.3837           0.7580         0.77288         52.587         1.26.421         0.5520         1.3733           0.8733         0.74129         52.519         1.26.43         0.4444         1.3827           0.8759         0.74239         52.494         1.26.53         0.4444         1.3827           0.8000         0.81014         53.756         1.26.211         2.2385         1.400           0.0000         0.81014         53.756         1.26.211         2.2382         1.4002           0.1813         0.80614         53.756         1.26.218         2.3252         1.4002           0.4245         0.80814         53.756         1.26.218         1.2372         1.4022           0.4345         0.78872         53.516         1.26.218         1.2372         1.4022           0.4346         0.78872         53.516         1.26.218         1.2372         1.4022           0.4445         0.78872	0.1813	0.81022	53.302	125.003	2.0902	1.4077
0.138         0.800'         3.200'         1.2578         1.935 <th1.935< th="">         1.935         1.935         &lt;</th1.935<>	0.2574	0.80834	53.289	125.020	2.12/7	1.4051
0.538         0.8003         5.2881         1.26934         1.0052         1.3917           0.6486         0.9976         5.2698         125.157         0.7578         1.3397           0.7590         0.7592         52.597         126.421         0.5520         1.3391           0.5793         0.78429         52.494         126.573         0.4444         1.3301           0.0000         0.78220         1.3456         1.3456         1.3456           0.0000         0.78204         1.3456         1.3456         1.3456           0.0000         0.8104         53.769         126.208         2.9326         1.4095           0.1813         0.0614         53.756         126.211         2.2339         1.4076           0.2574         0.80419         53.861         126.233         1.8402         1.3817           0.2574         0.80419         53.851         126.233         0.8062         1.3975           0.2574         0.80419         53.287         127.051         0.338         1.3975           0.2574         0.79802         52.387         127.051         0.3361         1.344           0.6795         0.79802         52.387         127.051         0.3	0.3430	0.80007	52,007	125.078	1.0059	1,4014
0.6483         0.79576         52.688         1.0517         0.7576         1.3879           0.5780         0.7381         52.517         1.26471         0.3520         1.3279           0.6773         0.7429         52.519         1.26573         0.4444         1.3221           0.6700         0.78204         0.3542         1.346           0.0954         0.8014         5.756         1.26298         2.2335         1.4005           0.0954         0.8014         5.3756         1.26211         2.2339         1.4078           0.2574         0.80182         5.5651         1.26233         1.48402         1.4022           0.2574         0.80182         5.3561         1.26236         1.4749         1.4022           0.2433         0.7982         5.3334         1.26552         0.9062         1.3337           0.5380         0.79802         5.2887         1.27131         0.3538         1.341           0.6495         0.73000         3.3072         1.27611         0.3343         1.3440           0.7900         0.3736         1.27781         0.356         1.3411           0.8000         0.8074         1.26534         1.3610         1.444	0.4485	0.80311	52 951	125.785	1,2705	1.3972
0.7580         0.79288         52.587         10.6421         0.820         1.759           0.8733         0.78429         52.494         126.73         0.4444         1.350           0.0000         0.78204         126.949         0.3758         1.350           0.0000         0.8104         53.769         126.078         2.303         1.4469           0.0001         0.8104         53.769         126.208         2.323         1.4069           0.2574         0.00414         53.769         126.213         2.8429         1.4054           0.4346         0.00419         53.651         126.223         1.8402         1.4054           0.4346         0.07892         53.551         126.252         0.9062         1.337           0.4346         0.79802         53.072         126.785         0.6995         1.387           0.5750         0.79002         52.857         127.061         0.3581         1.348           0.8075         0.79002         52.857         127.061         0.3581         1.348           0.8079         0.7902         52.857         127.061         0.3581         1.348           0.8079         0.77064         727.61         0.5838 <td>0.5558</td> <td>0.79676</td> <td>52.608</td> <td>125.554</td> <td>0.7676</td> <td>1.3917</td>	0.5558	0.79676	52.608	125.554	0.7676	1.3917
0.4730         0.7819         5.539         1.0573         0.444         1.3621           0.6579         0.78204         0.3542         1.3660           0.000         0.78204         0.3542         1.3660           0.000         0.81014         5.756         1.262.08         1.3660           0.1813         0.80614         5.3756         1.262.28         1.4105           0.2574         0.80614         5.3756         1.262.28         1.4749         1.4026           0.2436         0.80182         5.5561         1.262.286         1.4749         1.4022           0.2443         0.79582         5.3211         1.265.52         0.9062         1.3843           0.7880         0.79882         5.2877         1.27.7813         0.4184         1.3950           0.6495         0.73900         5.3072         1.26.785         0.6995         1.3843           0.7800         0.78802         5.2.887         1.27.381         0.4184         1.3950           0.0570         0.77664         7.27.611         0.3362         1.3441         1.4062           0.0571         3.406         1.26.874         1.6100         1.4044         1.3925         1.3441         1.4062	0.7580	0.79288	52.535	126.137	0.5820	1 3730
00579         0.78429         52.494         126.949         0.3782         1.369           1.0000         0.78204         0.3542         1.349           0.2000         0.81014         -         4.100         1.416           0.0904         0.81014         53.769         1.262.08         2.3326         1.4096           0.1813         0.80014         53.756         1.262.01         2.3820         1.4096           0.1814         0.80014         53.756         1.262.02         1.3137         1.4092           0.4343         0.79872         53.384         1.262.402         1.3177         1.3927           0.4383         0.79882         52.2887         122.383         0.4184         1.3393           0.5759         0.79302         52.887         122.383         0.4184         1.3395           0.000         0.7064         -         0.336         1.3410         1.0400           0.0954         0.80613         -         3.41         1.4093           0.0954         0.7949         5.3908         126.874         1.600         1.4044           0.3543         0.7949         5.3908         126.874         1.6000         1.4044	0.8733	0.7819	52 519	126.73	0.4444	1.3733
International of the second	0.9579	0 78429	52,494	126 949	0 3758	1 3510
Access         Construction         Construction <thconstruction< th="">         Construction</thconstruction<>	1 0000	0.78204	52.757	120.545	0 3542	1 3436
0.000         0.81014	At 298.15 K	0.70201			0.00 12	115 15 0
0.09640.8081453,769126,2082.92261.40780.25740.8041953,365126,2331.84021.40780.25740.8041953,365126,2331.84021.40220.43450.7987253,384126,4021.13271.39750.53980.7958253,231126,5520.00621.33940.64950.7920953,072126,7850.60951.33730.75800.780252,287127,3830.41841.33550.55790.7790252,287127,6110.53541.34800.00000.80613-3.411.40930.00000.80613-3.411.40930.018130.819454,181126,8332.49141.40640.25760.7930954,068120,6771.10171.35760.02000.80613-3.3769120,6771.01141.40640.25740.7934954,068120,6771.01171.39790.43830.7937353,276127,5740.603961.33990.75800.773753,243128,550.4111.3560.05790.773753,243128,550.4111.3560.05790.773753,243127,5591.5481.40490.75800.778454,589127,4641.70841.40490.757454,549127,4641.70841.40490.75750.728453,3719128,050.4724<	0.0000	0.81014			4.100	1.4116
0.1813     0.80614     33,756     126,211     2.2839     1.4076       0.2574     0.80192     33,361     126,236     1.4749     1.4026       0.4483     0.79872     33,341     126,552     0.09052     1.3937       0.5798     0.79802     52,956     127,061     0.5384     1.3737       0.7580     0.78002     52,956     127,061     0.5384     1.3337       0.7580     0.77902     52,857     127,361     0.5384     1.3355       0.0000     0.77664	0.0964	0.80814	53.769	126.208	2.9326	1.4096
0.25740.8041953.685126.2331.84021.40540.33650.7801253.561126.2361.47491.40220.44830.7987253.384126.4021.13271.33750.53880.7980253.072126.7850.69951.33870.75800.780252.955127.0610.53841.33870.75800.780252.955127.0610.53841.33950.65730.77640.36831.34801.34800.00000.7764-3.061.34111.00000.806134.11.03130.809454.216126.8332.49141.40820.05440.3091454.181126.8441.61001.40420.25740.7999154.068126.8741.61001.40420.25740.7999153.075127.0510.3711.39790.53880.791353.599127.1930.821211.39250.64950.7874553.475127.6540.64091.33890.777453.265128.0110.39431.39690.78040.7773753.245128.0110.39431.39560.78740.797453.376127.47640.75141.39790.78640.7973753.245127.47640.75141.39790.78640.799754.552127.47640.75141.39790.78640.7978453.365128.6980.36311.3440<	0.1813	0.80614	53.756	126.211	2.2839	1.4078
0.3436     0.80182     53.561     126.286     1.4749     1.4022       0.4483     0.79572     53.384     126.402     1.1327     1.3924       0.6398     0.79582     53.231     126.552     0.6965     1.3337       0.7580     0.78802     52.956     127.061     0.5384     1.3370       0.8733     0.78308     52.857     127.611     0.3583     1.3480       0.0000     0.77664     0.336     1.3411       At 30.15 K     3.41     1.4063     0.2534     1.4014       0.0964     0.80043     54.216     126.833     2.4014     1.4062       0.1813     0.80194     54.181     126.847     1.6100     1.4064       0.4354     0.79749     53.908     126.942     1.3014     1.4021       0.4483     0.79749     53.908     126.942     1.3014     1.4021       0.4483     0.79749     53.908     126.942     1.3014     1.4021       0.4483     0.79749     53.3075     127.193     0.82121     1.3392       0.6495     0.78745     53.475     127.594     0.6409     1.389       0.6579     0.7733     53.245     127.4764     0.6331     1.356       0.6579     0.7734	0.2574	0.80419	53.685	126.233	1.8402	1.4054
0.44830.7987253.384126.4021.13271.139750.53980.739053.072126.7850.69951.39370.75800.780052.087127.0610.53841.33950.87330.7830852.087127.0810.35831.34800.0000.77640.3361.3411At 30.315 K3.41481.40023.4111.40020.00000.006133.4111.40023.4111.40020.00040.806133.4181126.8332.49141.40020.18130.8019454.181126.8431.96711.40640.25740.7999154.068126.8741.61001.40420.43460.7974953.090120.69421.01671.33970.53880.7943853.719127.0571.01671.33970.53880.7943853.799127.0570.03611.34000.43450.797453.266128.0110.39431.33960.57500.777453.266128.0110.39431.33960.69570.773753.245127.4640.50361.37400.00000.802627.75591.15481.40490.53880.786353.817128.0510.33111.34560.69590.787453.365128.0510.33631.34640.69590.787453.376127.4641.70841.40490.53880.786353.817128.0540.37511.336	0.3436	0.80182	53.561	126.286	1.4749	1.4022
0.53980.7958253.231126.520.90621.39370.75800.780252.956127.0610.53841.37300.75300.7790252.857127.6110.3581.34801.0000.7764-0.3361.34111.0000.7764-3.311.4801.0000.7764-3.411.40931.0000.806133.411.40930.95640.8040454.216126.8332.49141.40820.15140.8019454.181126.8471.51001.40440.25740.7999154.068126.83741.51001.40440.3580.7974953.908126.8421.30141.40230.53980.7913353.599127.1930.621211.39250.54850.784553.475127.3640.64091.38390.5590.7874553.475127.3640.64091.38390.5590.7874553.475127.3640.64091.38390.5580.7874553.475127.4641.40611.34500.5590.7874553.475127.4641.40811.40650.65790.773453.265127.4641.51841.40260.8130.7974454.583127.4641.51841.40260.8130.7978454.583127.4641.51841.40260.5380.7867353.875127.8640.75141.39250.6485 </td <td>0.4483</td> <td>0.79872</td> <td>53.384</td> <td>126.402</td> <td>1.1327</td> <td>1.3975</td>	0.4483	0.79872	53.384	126.402	1.1327	1.3975
0.6495         0.79209         53.072         126.785         0.6995         1.3870           0.7580         0.7802         52.887         127.061         0.5384         1.3730           0.8773         0.77902         52.857         127.611         0.5353         1.3480           0.000         0.7764         0.336         1.3411           At 303.15 K         3.41         1.4093           0.0000         0.80613         3.41         1.4093           0.0094         0.80404         54.216         126.834         2.4914         1.4062           0.02574         0.79991         54.068         126.874         1.6100         1.4044           0.2574         0.79991         54.068         126.874         1.6100         1.4044           0.2574         0.79991         54.068         126.874         1.6100         1.4044           0.2545         0.78745         53.475         127.057         1.0167         1.3979           0.5386         0.79133         53.599         127.193         0.82121         1.3925           0.4483         0.79845         53.475         127.364         0.6499         1.3340           0.5750         0.7337         53.	0.5398	0.79582	53.231	126.552	0.9062	1.3924
0.7580     0.78802     52.956     17.061     0.5834     1.3730       0.8733     0.78308     52.887     127.383     0.4184     1.3595       0.000     0.77664     0.336     1.3411       1.303.15 K     3.41     1.4080       0.0904     0.80613     3.41     1.4082       0.0904     0.80194     54.216     126.833     2.4914     1.4082       0.1813     0.80194     54.216     126.874     1.9671     1.4044       0.2574     0.79991     54.068     126.874     1.9671     1.4044       0.2534     0.79943     53.908     126.874     1.9014     1.4024       0.4483     0.79748     53.908     127.057     1.0167     1.3979       0.5388     0.79133     53.599     127.394     0.6049     1.3380       0.7580     0.78307     53.376     127.594     0.5036     1.3740       0.8733     0.77774     53.245     128.55     0.3411     1.3461       0.6000     0.8026     7.7137     53.243     128.55     0.3411     1.3461       0.1813     0.79784     54.552     127.472     2.1366     1.4069       0.2574     0.79574     54.552     127.472     2.1384     1.	0.6495	0.79209	53.072	126.785	0.6995	1.3837
0.8733     0.78308     52.887     127.813     0.4184     1.3950       0.0579     0.7764     0.3383     1.3480       1.0000     0.77664     0.3383     1.3411       At 30.151 K	0.7580	0.78802	52.956	127.061	0.5384	1.3730
0.9579     0.77902     52.857     127.611     0.3363     1.3410       1.0000     0.7664     0.336     1.3411       4.303.15 K	0.8733	0.78308	52.887	127.383	0.4184	1.3595
1.0000     0.77664     0.336     1.411       Af 30.151K       1.410       0.0000     0.80613      1.26.833     2.4914     1.4082       0.0813     0.80194     54.161     126.833     2.4914     1.4082       0.2813     0.80194     54.181     126.843     1.6600     1.4046       0.2574     0.79791     53.068     126.942     1.3014     1.4021       0.4436     0.79749     53.059     127.163     0.82121     1.3979       0.5398     0.79133     53.579     127.364     0.6409     1.3839       0.7580     0.7837     53.245     127.364     0.6409     1.3369       0.579     0.7737     53.245     128.51     0.3411     1.3450       0.509     0.7737     53.245     127.464     0.5036     1.3740       0.873     0.79784     54.552     127.472     2.1336     1.4006       0.2574     0.79544     54.552     127.464     1.7084     1.4061       0.2574     0.79574     54.552     127.464     1.7084     1.4026       0.4413     0.7988     54.317     127.464     1.7084     1.4026       0.518     0.43199     127.484     0.5114 <td< td=""><td>0.9579</td><td>0.77902</td><td>52.857</td><td>127.611</td><td>0.3583</td><td>1.3480</td></td<>	0.9579	0.77902	52.857	127.611	0.3583	1.3480
At 303.15 K       3.41       1.4093         0.00964       0.80404       54.216       126.833       2.4914       1.4093         0.1813       0.80194       54.181       126.834       1.9671       1.4064         0.2574       0.79991       54.068       126.874       1.6100       1.4044         0.3436       0.79749       53.098       126.942       1.3014       1.4021         0.4483       0.79138       53.599       127.193       0.82121       1.3925         0.6495       0.78745       53.475       127.594       0.5036       1.3340         0.8750       0.78307       53.266       128.011       0.3943       1.3596         0.5579       0.77737       53.243       128.55       0.34111       1.3450         0.0000       0.80206        2.819       1.4069         0.5754       0.7974       54.552       127.472       2.1336       1.4069         0.515 K         1.4064       1.4066       1.2574       0.79574       54.552       127.472       2.1336       1.4069         0.518 K         1.27.759       1.1548       1.4069         0.2574       0.79574 <td>1.0000</td> <td>0.77664</td> <td></td> <td></td> <td>0.336</td> <td>1.3411</td>	1.0000	0.77664			0.336	1.3411
0.0000       0.80613       3.41       1.4093         0.0964       0.80194       54.216       126.833       2.4914       1.4064         0.2574       0.79991       54.068       126.874       1.6100       1.4044         0.2574       0.79919       54.068       126.874       1.6100       1.4042         0.3436       0.79749       53.908       126.942       1.3014       1.4021         0.4483       0.79438       53.719       127.057       1.0167       1.3979         0.5398       0.78745       53.475       127.364       0.6409       1.3839         0.7580       0.78307       53.286       128.011       0.3943       1.3596         0.8733       0.77774       53.286       128.011       0.3943       1.3596         0.0579       0.77337       53.243       128.55       0.3411       1.3450         0.0000       0.80206       2.819       1.4077       0.964       1.7084       1.4061         0.2574       0.79574       54.529       1.27.474       1.7084       1.4061         0.2574       0.79588       54.126       127.77       0.9154       1.3925      0.6398       0.78265       53.719 <td< td=""><td>At 303 15 K</td><td></td><td></td><td></td><td></td><td></td></td<>	At 303 15 K					
0.0000         0.80404         54.216         126.83         2.4914         1.4082           0.1813         0.80194         54.181         126.84         1.9671         1.4082           0.2574         0.79991         54.068         126.874         1.5100         1.4044           0.336         0.79749         53.908         126.942         1.3014         1.4021           0.4483         0.79133         53.599         127.193         0.82121         1.3925           0.6495         0.78745         53.475         127.594         0.5036         1.3340           0.8570         0.77337         53.243         128.55         0.3411         1.3456           0.9579         0.77337         53.245         127.472         2.1336         1.4092           0.000         0.77121         -         0.325         1.3390         1.4077           0.0964         0.79997         54.552         127.472         2.136         1.4092           0.1813         0.79784         54.589         127.464         1.7084         1.4069           0.2574         0.79574         54.552         127.472         2.1336         1.4072           0.2543         0.79818         54.337	0.0000	0.80613			3 41	1 4093
0.1813         0.80194         54.181         126.84         1.9671         1.4064           0.2574         0.79991         54.068         126.942         1.3014         1.4021           0.3436         0.79749         53.908         126.942         1.3014         1.4021           0.4833         0.79438         53.719         127.057         1.0167         1.3972           0.6495         0.78307         53.376         127.594         0.6036         1.3740           0.8733         0.77774         53.246         128.011         0.3943         1.3596           0.5759         0.77337         53.243         128.55         0.3411         1.3450           0.0000         0.80206         2.819         1.4071           0.0964         0.79997         54.552         127.472         2.136         1.4066           0.2574         0.79574         54.552         127.472         2.136         1.4026           0.254         0.7984         54.589         127.464         1.7084         1.4061           0.2574         0.79574         54.532         127.464         1.7084         1.4026           0.4483         0.78868         54.126         127.7         0.9	0.0964	0.80404	54 216	126 833	2 4914	1 4082
0.2574         0.79991         54.068         126.874         1.6100         1.4044           0.3436         0.79749         53.008         126.942         1.3014         1.4021           0.4483         0.79438         53.719         127.057         1.0167         1.3979           0.5398         0.78133         53.599         127.193         0.82121         1.3925           0.6495         0.78307         53.376         127.594         0.5036         1.3740           0.8733         0.77774         53.286         128.011         0.3943         1.3596           0.5579         0.77337         53.243         128.55         0.3411         1.3450           0.0000         0.77121	0 1813	0 80194	54 181	126.84	1 9671	1 4064
0.3436         0.79749         53.908         126.942         1.304         1.4027           0.4483         0.79438         53.719         127.057         1.0167         1.3979           0.5398         0.79133         53.599         127.193         0.82121         1.3925           0.6495         0.78307         53.376         127.594         0.5036         1.3740           0.8733         0.77774         53.276         128.55         0.3411         1.3450           0.000         0.77337         53.243         128.55         0.3411         1.3450           0.000         0.77337         53.243         128.55         0.3411         1.3450           0.000         0.7737         54.552         127.472         2.1336         1.4069           0.813         0.79784         54.559         127.464         1.7084         1.4061           0.2574         0.79574         54.552         127.472         2.1336         1.4049           0.2436         0.79318         54.337         127.559         1.1548         1.4026           0.4438         0.79388         54.126         127.7         0.9154         1.3979           0.5398         0.78283         53.6	0.2574	0 79991	54.068	126.874	1 6100	1 4044
0.4483     0.79438     53.719     127.057     1.0167     1.3979       0.5398     0.79133     53.599     127.193     0.82121     1.3929       0.6495     0.78745     53.375     127.364     0.6409     1.3839       0.7580     0.78745     53.376     127.594     0.5036     1.3740       0.8733     0.7774     53.263     128.011     0.3943     1.3506       0.5579     0.77337     52.243     128.55     0.3411     1.3450       0.0000     0.80206     2.819     1.0407       0.0564     0.79974     54.552     127.472     2.1336     1.4069       0.1813     0.79784     54.589     127.464     1.7084     1.4069       0.2574     0.79984     54.549     127.464     1.7084     1.4049       0.3436     0.79918     54.337     127.759     1.1548     1.4026       0.4483     0.78988     54.126     127.7     0.9154     1.3979       0.5398     0.78673     53.617     128.056     0.4724     1.3745       0.4483     0.78988     54.126     127.7     0.9154     1.3979       0.5398     0.78673     53.618     128.906     0.3263     1.3469       0.59579	0.3436	0.79749	53.908	126.942	1.3014	1.4021
0.53980.7913353.599127.1930.821211.39250.64950.7814553.475127.3640.64091.38390.75800.7830753.276127.5940.50361.37400.87330.7777453.286128.0110.39431.3560.95790.773753.243128.550.34111.34501.00000.771212.8191.40770.96640.799454.552127.4722.13361.40690.18130.7978454.589127.4641.70841.40610.23740.7957454.397127.4581.41981.40610.23740.7957454.397127.4581.15481.40260.44830.7898854.126127.70.91541.39790.53980.7867353.974128.6640.59331.38440.75800.7783653.719128.0560.47241.37450.95790.7652353.618128.6380.37591.3640.0000.8171853.204128.9263.3651.44260.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.3651.41450.19470.8131653.378142.2053.3651.41450.19470.8131653.378142.2053.3651.41450.19470.8131653.378142.2053.3651.41450.25100.817853.04142.201 <td>0.4483</td> <td>0.79438</td> <td>53.719</td> <td>127.057</td> <td>1.0167</td> <td>1.3979</td>	0.4483	0.79438	53.719	127.057	1.0167	1.3979
0.6495       0.78745       53.475       127.364       0.6409       1.3839         0.7580       0.78307       53.376       127.594       0.5036       1.3740         0.8733       0.77774       53.246       128.011       0.3943       1.3596         0.9579       0.77337       53.243       128.55       0.3411       1.3450         0.0000       0.77121       0.325       1.390         At 308.15 K       2.819       1.4077         0.0000       0.80206       2.819       1.4077         0.0544       0.7997       54.552       127.472       2.1336       1.4069         0.1813       0.79784       54.499       127.464       1.7084       1.4049         0.2574       0.79318       54.337       127.559       1.1548       1.4049         0.3436       0.79318       54.337       127.864       0.7511       1.3925         0.5398       0.78673       53.974       127.864       0.5933       1.3844         0.7580       0.78283       53.817       128.064       0.5933       1.3849         0.5795       0.76823       53.618       128.996       0.3263       1.3469         0.5795       0.76823 <td>0.5398</td> <td>0.79133</td> <td>53.599</td> <td>127.193</td> <td>0.82121</td> <td>1.3925</td>	0.5398	0.79133	53.599	127.193	0.82121	1.3925
0.7580       0.78307       53.376       127.594       0.5036       1.3740         0.8733       0.77734       53.266       128.011       0.3943       1.3596         0.9579       0.77121       128.55       0.325       1.3390         At J08.15 K       2.819       1.4077         0.0964       0.79997       54.552       127.472       2.1336       1.4061         0.2574       0.79574       54.589       127.464       1.7084       1.4061         0.2574       0.79574       54.439       127.459       1.1548       1.4029         0.4833       0.79984       54.337       127.559       1.1548       1.4029         0.4843       0.79818       54.337       127.559       1.1548       1.4029         0.5398       0.78673       53.974       127.864       0.5933       1.3844         0.7580       0.77836       53.719       128.056       0.4724       1.3745         0.8733       0.77284       53.618       128.996       0.3263       1.3469         0.9579       0.76823       53.618       128.996       0.3263       1.4066         0.9579       0.76823       53.618       128.996       0.3263       1.	0.6495	0.78745	53.475	127.364	0.6409	1.3839
0.8733       0.7774       53.286       128.011       0.3943       1.3596         0.9579       0.77337       53.243       128.55       0.3411       1.3450         1.0000       0.77121	0.7580	0.78307	53.376	127.594	0.5036	1.3740
0.9579       0.77337       53.243       128.55       0.3411       1.3450         1.0000       0.77121       0.325       1.3300         At 308.15 K	0.8733	0.77774	53.286	128.011	0.3943	1.3596
1.0000       0.77121       0.325       1.3390         At 308.15 K       2.819       1.4077         0.0090       0.80206       2.819       1.4077         0.0964       0.79997       54.552       127.472       2.1336       1.4069         0.1813       0.79784       54.59       127.464       1.7084       1.4061         0.2574       0.79574       54.499       127.458       1.4198       1.4049         0.3436       0.79988       54.126       127.7       0.9154       1.33925         0.5438       0.78673       53.974       127.864       0.7511       1.33925         0.6495       0.78283       53.817       128.055       0.4724       1.3746         0.7580       0.77284       53.65       128.638       0.3759       1.3610         0.9579       0.76823       53.618       128.996       0.3263       1.3499         0.9579       0.7687.5       -       -       0.308       1.3371         0.9000       0.7757       -       1.3469       1.4206       1.4176         0.4000       0.8178       -       6.5198       1.4206       1.4145         0.1422       0.81497       53.429	0.9579	0.77337	53.243	128.55	0.3411	1.3450
At 308.15 K 0.0000 0.80206 2.819 1.4077 0.0964 0.79997 54.552 127.472 2.1336 1.4069 0.1813 0.79784 54.589 127.464 1.7084 1.4069 0.2574 0.79574 54.499 127.488 1.4198 1.4049 0.3436 0.79318 54.337 127.559 1.1548 1.4026 0.4483 0.78988 54.126 127.7 0.9154 1.3979 0.5398 0.78673 53.974 127.864 0.5933 1.3844 0.7580 0.77836 53.719 128.064 0.5933 1.3844 0.7580 0.77836 53.719 128.305 0.4724 1.3745 0.8733 0.77284 53.65 128.638 0.3759 1.3610 0.9579 0.76823 53.618 128.996 0.3263 1.3690 1.0000 0.81718 - 0.308 1.3371 Acetonitrile(1)+2-heptanol (2) at 293.15 K 0.0000 0.81718 53.429 142.194 4.3265 1.4147 0.1142 0.81497 53.429 142.194 4.3265 1.4147 0.1142 0.81497 53.429 142.205 3.3365 1.4145 0.1142 0.81497 53.429 142.205 3.3365 1.4145 0.1142 0.81497 53.304 142.201 2.7697 1.4124 0.3491 0.80924 53.144 142.301 2.1331 1.4094 0.4525 0.80632 52.854 142.407 1.5843 1.4042	1.0000	0.77121			0.325	1.3390
0.0000       0.80206       2.819       1.4077         0.0964       0.79997       54.552       127.472       2.1336       1.4069         0.1813       0.79784       54.589       127.464       1.7084       1.4069         0.2574       0.79574       54.499       127.488       1.4198       1.4049         0.3436       0.79318       54.337       127.559       1.1548       1.4026         0.4483       0.78988       54.126       127.7       0.9154       1.3979         0.5398       0.78673       53.974       127.864       0.7511       1.3925         0.6495       0.78233       53.817       128.064       0.5933       1.3844         0.7580       0.77283       53.618       128.305       0.4724       1.3745         0.8733       0.77284       53.65       128.638       0.3263       1.3469         1.0000       0.76575        1.3025       1.3469       1.3745         0.1142       0.81718       53.429       142.194       4.3265       1.4176         0.1142       0.8178       53.304       142.205       3.3365       1.4145         0.1442       0.81178       53.304       142.205	At 308.15 K					
0.09640.7999754.552127.4722.13361.40690.18130.7978454.589127.4641.70841.40610.25740.7957454.399127.4881.41981.40490.34360.7991854.337127.5591.15481.40260.44830.7898854.126127.70.91541.39790.53980.7867353.974127.8640.75111.39250.64950.7828353.817128.0640.59331.34440.75800.7728453.65128.6380.37591.36100.95790.7682353.618128.9960.32631.34691.0000.7675	0.0000	0.80206			2.819	1.4077
0.18130.7978454.589127.4641.70841.40610.25740.7957454.499127.4881.41981.40490.34360.7931854.337127.5591.15481.40260.44830.7898854.126127.70.91541.39790.53980.7867353.974127.8640.59331.38440.75800.7828353.817128.0640.59331.38440.75800.7783653.719128.3050.47241.37450.87330.7728453.65128.6380.37591.36100.95790.7682353.618128.9960.32631.34691.00000.765756.51981.42060.11420.817186.51981.42060.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41240.34910.8092453.144142.3012.13311.40420.45250.8063252.854142.5191.23871.3864	0.0964	0.79997	54.552	127.472	2.1336	1.4069
0.2574       0.79574       54.499       127.488       1.4198       1.4049         0.3436       0.79318       54.337       127.559       1.1548       1.4026         0.4483       0.78988       54.126       127.7       0.9154       1.3979         0.5398       0.78673       53.974       127.864       0.5933       1.3844         0.6495       0.78283       53.817       128.064       0.5933       1.3844         0.7580       0.77836       53.719       128.305       0.4724       1.3745         0.8733       0.77284       53.65       128.638       0.3759       1.3610         0.9579       0.76823       53.618       128.996       0.3263       1.3469         1.0000       0.76575        0.308       1.371         Acetonitrile(1)+2-heptami/2) at 293.15 K         0.308       1.3469         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.231       2.7697       1.4124         0.3491       0.80924       53.144<	0.1813	0.79784	54.589	127.464	1.7084	1.4061
0.34360.7931854.337127.5591.15481.40260.44830.7898854.126127.70.91541.39790.53980.7867353.974127.8640.75111.39250.64950.7828353.817128.0640.59331.38440.75800.7783653.719128.0550.47241.37450.87330.7728453.65128.6380.37591.36100.95790.7682353.618128.9960.32631.34691.00000.765750.3081.3371Acetonitrile(1)+2-heptam/(2) at 293.15 K0.00000.817186.51981.42060.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2053.33651.41450.34910.8092453.144142.3012.13311.40940.45250.8063252.854142.1991.23871.3986	0.2574	0.79574	54.499	127.488	1.4198	1.4049
0.44830.7898854.126127.70.91541.39790.53980.7867353.974127.8640.75111.39250.64950.7828353.817128.0640.59331.38440.75800.7783653.719128.3050.47241.37450.87330.7728453.65128.6380.37591.36100.95790.7682353.618128.6380.37591.36491.0000.765750.3081.3371Acetonitrile(1)+2-heptand (2) at 293.15 K0.0000.8171853.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41240.34910.8092453.144142.3012.13311.40940.45250.8063252.854142.5191.23871.3986	0.3436	0.79318	54.337	127.559	1.1548	1.4026
0.53980.7867353.974127.8640.75111.39250.64950.7828353.817128.0640.59331.38440.75800.7783653.719128.3050.47241.37450.87330.7728453.65128.6380.37591.36100.95790.7682353.618128.9960.32631.34691.0000.765750.3081.3371Acetonitrile(1)+2-heptanol (2) at 293.15 K0.0000.817186.51981.42060.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41240.34910.8092453.144142.3012.13311.40940.45250.8063252.854142.5191.23871.3986	0.4483	0.78988	54.126	127.7	0.9154	1.3979
0.64950.7828353.817128.0640.59331.38440.75800.7783653.719128.3050.47241.37450.87330.7728453.65128.6380.37591.36100.95790.7682353.618128.9960.32631.34690.0000.76570.3081.3371Acetonitrile(1)+2-heptanol (2) at 293.15 K6.51981.42060.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41240.34910.8092453.144142.3012.13311.40420.45250.8063252.854142.5191.23871.3986	0.5398	0.78673	53.974	127.864	0.7511	1.3925
0.7580       0.77836       53.719       128.305       0.4724       1.3745         0.8733       0.77284       53.65       128.638       0.3759       1.3610         0.9579       0.76823       53.618       128.996       0.3263       1.3469         1.0000       0.76575       0.308       1.3371         Acetonitrile(1)+2-heptanol (2) at 293.15 K       6.5198       1.4206         0.0000       0.81718       6.5198       1.4206         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.231       2.7697       1.4124         0.3491       0.80924       53.144       142.301       2.1331       1.4042         0.4525       0.80632       52.98       142.407       1.5843       1.4042         0.5436       0.80352       52.854       142.519       1.2387       1.3986	0.6495	0.78283	53.817	128.064	0.5933	1.3844
0.8733       0.77284       53.65       128.638       0.3759       1.3610         0.9579       0.76823       53.618       128.996       0.3263       1.3469         1.0000       0.76575       0.308       1.3371         Acetonitrile(1)+2-heptanol (2) at 293.15 K       6.5198       1.4206         0.0000       0.81718       6.5198       1.4206         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.231       2.7697       1.4124         0.3491       0.80924       53.144       142.301       2.1331       1.4094         0.4525       0.80632       52.98       142.407       1.5843       1.4094         0.5436       0.80352       52.854       142.519       1.2387       1.3986	0.7580	0.77836	53.719	128.305	0.4724	1.3745
0.9579       0.76823       53.618       128.996       0.3263       1.3469         1.0000       0.76575       0.308       1.3371         Acetonitrile(1)+2-heptanol (2) at 293.15 K       6.5198       1.4206         0.0000       0.81718       6.5198       1.4206         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.201       2.7697       1.4124         0.3491       0.80924       53.144       142.301       2.1331       1.4094         0.4525       0.80632       52.98       142.407       1.5843       1.4094         0.5436       0.80352       52.854       142.519       1.2387       1.3986	0.8733	0.77284	53.65	128.638	0.3759	1.3610
1.0000       0.76575       0.308       1.3371         Acetonitrile(1)+2-heptanol (2) at 293.15 K         0.0000       0.81718       6.5198       1.4206         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.231       2.7697       1.4124         0.3491       0.80924       53.144       142.301       2.1331       1.4094         0.4525       0.80632       52.98       142.407       1.5843       1.4094         0.5436       0.8052       52.854       142.519       1.2387       1.3986	0.9579	0.76823	53.618	128.996	0.3263	1.3469
Acetonitrile(1)+2-heptanol (2) at 293.15 K       6.5198       1.4206         0.0000       0.81718       6.5198       1.4206         0.1142       0.81497       53.429       142.194       4.3265       1.417         0.1947       0.81316       53.378       142.205       3.3365       1.4145         0.2510       0.81178       53.304       142.231       2.7697       1.4124         0.3491       0.80924       53.144       142.301       2.1331       1.4094         0.4525       0.80632       52.854       142.519       1.2387       1.3986	1.0000	0.76575			0.308	1.3371
0.11420.8149753.429142.1944.32651.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41450.34910.8092453.144142.3012.13311.40940.45250.8063252.98142.4071.58431.40420.54360.8035252.854142.5191.23871.3986	Acetonitrile(1)+2-heptanc	ol (2) at 293.15 K 0 81718			6 5198	1 4206
0.1120.014570.51425142.1344.52051.4170.19470.8131653.378142.2053.33651.41450.25100.8117853.304142.2312.76971.41240.34910.8092453.144142.3012.13311.40940.45250.8063252.98142.4071.58431.40420.54360.8035252.854142.5191.23871.3986	0.0000	0.81497	53 429	142 194	4 3265	1.4200
0.2510         0.81178         53.304         142.201         53.505         1.4143           0.2510         0.81178         53.304         142.231         2.7697         1.4124           0.3491         0.80924         53.144         142.301         2.1331         1.4042           0.4525         0.80632         52.98         142.407         1.5843         1.4042           0.5436         0.80352         52.854         142.519         1.2387         1.3986	0.1142	0.81316	53 378	142 205	3 3365	1.417
0.3491         0.80924         53.144         142.31         2.1637         14124           0.4525         0.80632         52.98         142.407         1.5843         1.4094           0.5436         0.80352         52.854         142.519         1.2387         1.3986	0.2510	0.81178	53 304	142.231	2 7697	1 4124
0.4525         0.80632         52.854         142.407         1.5843         1.4054           0.5436         0.80352         52.854         142.519         1.2387         1.3986	0 3491	0.80924	53 144	142 301	2 1331	1 4094
0.5436 0.80352 52.854 142.519 1.2387 1.3986	0.4525	0.80632	52.98	142.407	1.5843	1.4042
	0.5436	0.80352	52.854	142.519	1.2387	1.3986

## Table 3 ( Continued ).

<i>x</i> <sub>1</sub>	$\rho (\mathrm{g}\mathrm{cm}^{-3})$	$\bar{V}_{m,1}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\bar{V}_{m,2}$ (cm <sup>3</sup> mol <sup>-1</sup> )	$\eta$ (mPas)	$n_D$
0.6702	0.7989	52.726	142.732	0.8636	1.3881
0.7574	0.79518	52.651	142.938	0.6732	1.3793
0.8770	0.78927	52.551	142.392	0.5444	1.3637
0.9588	0.78477	52.492	142.907	0.3857	1.3516
1.0000	0.78204			0.3542	1.3436
At 298.15 K					
0.0000	0.81333			5.3303	1.4188
0.1142	0.81107	53.847	142.857	3.5832	1.4158
0.1947	0.80919	53.825	142.859	2.8206	1.4146
0.2510	0.80774	53.74	142.887	2.4016	1.4129
0.3491	0.80500	53.546	142.985	1.8531	1,4094
0.4525	0.80207	53.330	143.106	1.3949	1.4039
0.5436	0.79912	53.197	143.241	1.1061	1.3979
0.6702	0.79443	53.072	143.436	0.7855	1.3873
0 7574	0.79057	53 009	143 611	0.6191	1 3781
0.8770	0 78426	52,925	144 038	0.5120	1 3629
0.9588	0.77964	52.85	144 569	0.3652	1 3503
1.0000	0.77664	52.05	111.505	0.3369	1.3411
At 303.15 K					
0.0000	0.80944			4.3006	1,4165
0.1142	0.80706	54.218	143.553	3.0302	1.4134
0.1947	0.80514	54.171	143.557	2.4092	1.4127
0.2510	0.80362	54.1	143.59	2.0664	1.4118
0.3491	0.80093	53.911	143.663	1.6188	1.4093
0.4525	0.79779	53.716	143.791	1.2505	1.4029
0.5436	0.79469	53.587	143.939	0.9893	1.3973
0.6702	0.78988	53.424	144.167	0.7174	1.3863
0.7574	0.78600	53.346	144.356	0.5762	1.3774
0.8770	0.77950	53.275	144.724	0.4829	1.3620
0.9588	0.77436	53.231	145.088	0.3483	1.3481
1.0000	0.77121			0.3254	1.3390
At 308.15 K					
0.0000	0.80550			3.5285	1.4143
0.1142	0.80317	54.694	144.22	2.5779	1.4156
0.1947	0.80112	54.762	144.202	2.072	1.4141
0.2510	0.79949	54.667	144.237	1.8160	1.4126
0.3491	0.79653	54.384	144.363	1.4660	1.4079
0.4525	0.79331	54.09	144.546	1.1116	1.4022
0.5436	0.79011	53.93	144.724	0.8985	1.3958
0.6702	0.78523	53.801	144.896	0.6625	1.3845
0.7574	0.78116	53.751	145.018	0.5390	1.3744
0.8770	0.77415	53.687	145.41	0.4454	1.3576
0.9588	0.76893	53.61	146.029	0.3326	1.3452
1.0000	0.76575			0.3082	1.3371

weaker. Assuming the positive contribution due to H-bond breaking to be constant, the observed increase in  $V_m^E$  with increase in chainlength of 2-alkanol can be rationalized.

The positive  $V_m^E$  values for mixtures of acetonitrile with 2alkanol can be ascribed to dominance of disruption of H-bonds between alkanols over dipole–dipole interactions between 2alkanols and acetonitrile molecule.

Its be mentioned that  $V_m^E$  values for mixtures of acetonitrile with 1-alkanol also are positive and increase with increasing chainlength of 1-alkanols [13]. But difference in  $V_m^E$  between 2-alkanols and 1-alkanols are dependent on the position of the –OH group in the alkanol molecules.

The partial molar volumes  $\bar{V}_{m,i}$ , in these mixtures were calculated over the whole composition range using Eqs. (4) and (5) [11,12].

$$\bar{V}_{m,1} = V_m^E + V_{m,1}^* + (1-x) \left(\frac{\partial V_m^E}{\partial x}\right)_{T,P}$$
(5)

$$\bar{V}_{m,2} = V_m^E + V_{m,2}^* - x \left(\frac{\partial V_m^E}{\partial x}\right)_{T,P}$$
(6)

## Table 4

Partial molar volumes at infinite dilution  $\overline{V}_{m,i}^o$  , for acetonitrile + 2-alkanols at different temperatures.

	293.15 K	298.15 K	303.15 K	308.15 K			
Acetonitrile (1)+2-pr	Acetonitrile (1)+2-propanol (2)						
$\overline{V}_{m,1}^o$ (cm <sup>3</sup> mol <sup>-1</sup> )	52.947	53.479	53.938	54.439			
$\overline{V}_{m,2}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	77.11	77.657	78.146	78.706			
Acetonitrile (1)+2-bu	itanol (2)						
$\overline{V}_{m,1}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	53.458	53.954	54.361	54.807			
$\overline{V}_{m,2}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	92.813	93.51	94.121	94.712			
Acetonitrile (1)+2-pe	entanol (2)						
$\overline{V}_{m,1}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	53.499	53.874	54.328	54.739			
$\overline{V}_{m,2}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	110.11	110.704	111.32	111.948			
Acetonitrile (1)+2-he	exanol (2)						
$\overline{V}_{m,1}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	53.537	53.935	54.335	54.740			
$\overline{V}_{m,2}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	126.838	127.493	128.209	128.808			
Acetonitrile (1)+2-heptanol (2)							
$\overline{V}_{m,1}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	53.56	53.994	54.359	54.904			
$\overline{V}_{m,2}^{o}$ (cm <sup>3</sup> mol <sup>-1</sup> )	143.695	144.241	144.885	145.695			

where  $V_{m,1}^*$  and  $V_{m,2}^*$  are pure molar volumes of component 1, 2 respectively. Values of partial molar volumes  $\bar{V}_{m,i}$  are given in Table 3 and partial molar volumes at infinite dilution  $\overline{V}_{m,i}^o$ , are in Table 4.

The partial properties at infinite dilution are of interest since at the limit of infinite dilution the solute–solute interactions disappear and only interactions present are solute–solvent interactions. Since the partial molar volumes at infinite dilution of each component, are not very different from the corresponding molar volumes  $V_{m,i}^*$ , interaction between acetonitrile and alcohols is not very favorable.  $\overline{V}_{m,i}^o$  increases with chain-length of alkanols and slightly increase with temperature.

### 3.2. Theoretical analysis

The Flory's theory [14–18] and its extended forms [19–22] have been used extensively to predict excess properties of nonelectrolyte systems for different kinds of mixtures, including polar components [23–25]. The present work reports the applicability of the Prigogine–Flory–Patterson theory (PFP theory) to predict excess molar volume of binary mixtures of 2-alkanols with acetonitrile.

According to the PFP theory,  $V_m^E$ , calculations include three contributions: (i) interactional, which is proportional to the ( $\chi_{12}$ ) parameters; (ii) the free volume contribution which arises from the dependence of the reduced volume upon the reduced temperature as a result of the difference between the degree of expansion of the two components and (iii) the ( $P^*$ ) contribution, which depends both on the differences of internal pressures and differences of reduced volumes of the components. The  $V_m^E$  was calculated by means of the PFP theory using the following equation with the three contributions.

$$\frac{V_m^E}{(x_1V_1^*x_2V_2^*)} = \left(\frac{(\tilde{V}^{1/3} - 1)\tilde{V}^{1/3}\varphi_1\theta_2\chi_{12}}{((4/3)\tilde{V}^{1/3} - 1)P_1^*}\right)(x_1V_1^* + x_2V_2^*) 
- \frac{(\tilde{V}_1 - \tilde{V}_2)^2((14/9)\tilde{V}^{-1/3} - 1)\psi_1\psi_2}{((4/3)\tilde{V}^{1/3} - 1)\tilde{V}} (x_1V_1^* + x_2V_2^*) 
+ \frac{(\tilde{V}_1 - \tilde{V}_2)(P_1^* - P_2^*)\psi_1\psi_2}{P_1^*\varphi_2 - P_2^*\varphi_2} (x_1V_1^* + x_2V_2^*);$$
(7)

The  $\tilde{V}$  of the solution is obtained through the Flory's theory. The characteristic parameters  $V^*$  and  $P^*$  are obtained from thermal expansion coefficient, ( $\alpha_P$ ) and isothermal compressibility ( $\beta_T$ ). The thermal expansion coefficient ( $\alpha_i$ ) is used to calculate the reduced volume by equation:

$$\tilde{V}_i = \left(\frac{1 + (4/3)\alpha_i T}{1 + \alpha_i T}\right)^3;\tag{8}$$

Here, the molecular contact energy fraction is calculated by:

$$\psi_1 = \frac{\varphi_1 P_1^*}{\varphi_1 P_1^* + \varphi_2 P_2^*} \tag{9}$$

#### Table 5

Parameters of pure components used in Flory theory at 298.15 K.

Component	$P^*$ (J cm <sup>-3</sup> )	$V^*$ (cm <sup>-3</sup> mol <sup>-1</sup> )	<i>T</i> <sup>*</sup> (K)
Acetonitrile	456.106	41.6273	4946.39
2-Propanol	479.031	60.593	5163.6
2-Butanol	347.579	72.7335	5947.78
2-Pentanol	190.82	86.2095	5396.01
2-Hexanol	210.706	99.3931	5269.12
2-Heptanol	231.155	112.515	5279.53

with the hard-core volume fractions defined by:

$$\varphi_1 = \frac{x_1 V_1^*}{x_1 V_1^* + x_2 V_2^*} \tag{10}$$

The molecular surface fraction is calculated by:

$$\theta_2 = \frac{\varphi_2 S_2}{\varphi_2 S_2 + \varphi_1 S_1} \tag{11}$$

where  $S_i$  is the molecular fraction surface/volume ratio for the components determined by Bondi's method [26].

The values of pure parameters for the pure liquid components and the mixture are obtained by Flory theory [14]. The parameters for the pure liquid components derived using Flory theory are in Table 5.

The values of thermal expansion coefficient and isothermal compressibility for the pure components obtained from the literature. In order to obtain  $V_m^E$ , it is necessary to find the interactional parameter ( $\chi_{12}$ ) which was obtained by fitting the theory to experimental values of  $V_m^E$  for each one of the binary system. Table 6 presents the calculated equimolar values of the three contributions to  $V_m^E$  according to Eq. (7), together with the interactional parameter  $(\chi_{12})$ . An analysis of each of the three contributions to  $V_m^E$  shows that the interactional contribution is always positive in all binary mixtures of acetonitrile and 2-alkanol. The free volume effect, is negative and it seems to have little significance for the system studied. The third contribution due to different in internal pressure and in reduced volume of the components seems to be the most important to explain the  $V_m^E$  behavior, except 2-propanol for system studied. Figs. 2–6 show the excess molar values predicted by PFP theory for acetonitrile and 2-alkanols systems.

#### 3.3. Dynamic viscosities

The viscosity deviation can be calculated as

$$\Delta \eta = \eta - x_1 \eta_1 - x_2 \eta_2 \tag{12}$$

where  $\eta$  is the viscosity of mixture and  $\eta_1$  and  $\eta_2$  are pure components viscosity. The measured  $\eta$  values for binary systems at different temperatures are listed in Table 3.

The  $\Delta \eta$  values were fitted to Redlich–Kister equation (3) and the adjustable parameters and standard deviations are given in Table 2.

The viscosity deviation represents deviations from a rectilinear dependence of viscosity on mole fraction. The values of  $\Delta \eta$  that shown in Fig. 7, for the system containing 2-alkanols + acetonitrile, were asymmetrical and all negative throughout the whole concentration range at all the temperatures, with the more negative as the length of the alkanol chain increase.

Calculated values of three contributions of the PFP theory to  $V_m^E$  for (2-alkanols + acetonitrile) mixtures at 298.15 K.

System	$\chi_{12}$ (J cm <sup>-3</sup> )	Interactional	Free volume	$P^*$
$x_1$ [acetonitrile]+(1 – $x_1$ ) 2-propanol	23	0.2622	-0.0054	-0.0104
$x_1$ [acetonitrile] + $(1 - x_1)$ 2-butanol	19.2	0.1798	-0.0864	0.2350
$x_1$ [acetonitrile] + $(1 - x_1)$ 2-pentanol	2.4	0.02650	-0.0257	0.3764
$x_1$ [acetonitrile] + (1 – $x_1$ ) 2-hexanol	8.3	0.0963	-0.0158	0.2779
$x_1$ [acetonitrile] + (1 – $x_1$ ) 2-heptanol	8.6	0.0995	-0.0181	0.2734

Table 6



**Fig. 3.** Plot of excess molar volume  $V_m^E$  against mole fraction of acetonitrile for the  $\{x_1 \text{ acetonitrile} + (1 - x_1) 2\text{-butanol}\}$  mixtures. (•) Experimental; (--) calculated by using PFP theory.



**Fig. 4.** Plot of excess molar volume  $V_m^E$  against mole fraction of acetonitrile for the  $\{x_1 \text{ acetonitrile} + (1 - x) 2\text{-pentanol}\}$  mixtures. (•) Experimental; (--) calculated by using PFP theory.

The negative values of viscosity deviations for the binary systems investigated suggest that the viscosities of associates formed between unlike molecules are relatively less than those of the pure components. Also there are some reports on viscosity of acetonitrile + 1-alkanol [2,13]. Similar to 1-alkanol + acetonitrile mixtures, the values of viscosity deviation for 2-alkanols + acetonitrile also increase with the chain-length of 2-alkanols. However, the values of viscosity deviation for 1-alkanol mixtures are significantly higher



**Fig. 5.** Plot of excess molar volume  $V_m^E$  against mole fraction of acetonitrile for the  $\{x_1 \text{ acetonitrile} + (1 - x_1) 2\text{-hexanol}\}$  mixtures. (•) Experimental; (--) calculated by using PFP theory.



**Fig. 6.** Plot of excess molar volume  $V_m^E$  against mole fraction of acetonitrile for the  $\{x_1 \text{ acetonitrile } +(1-x_1) \text{ 2-heptanol}\}$  mixtures. (•) Experimental; (--) calculated by using PFP theory.



**Fig. 7.** Viscosity deviations of binary mixtures for acetonitrile with  $(\diamond)$  2-propanol, ( $\blacktriangle$ ) 2-butanol, ( $\blacksquare$ ) 2-pentanol, ( $\boxdot$ ) 2-hexanol, ( $\Box$ ) 2-heptanol at 298.15 K.

than those mixtures involving the corresponding 2-alkanols. Thus, the values of viscosity deviation are dependent on the position of the –OH group in the alkanol molecules.

Interaction between acetonitrile and 2 alkanols is said to involve a weak bond intermediate between a hydrogen bond and formation of an electron transfer complex. There is evidence for weak complex formation between acetonitrile and 2-alkanols.



**Fig. 8.** Refractive index deviations on mixing of acetonitrile with ( $\blacktriangle$ ) 2-propanol, ( $\bigcirc$ ) 2-butanol, ( $\bigcirc$ ) 2-betanol, ( $\bigcirc$ ) 2-hexanol, ()

## 3.4. Refractive index

Refractive index deviations were defined by

$$\Delta n_D = n_D - \{xn_{D,1}^* + (1-x)n_{D,2}^*\}$$
(13)

where  $n_D$  is the refractive index of the mixture,  $n_{D,i}^*$  is that corresponding to the pure component *i* and *x* is the mole fraction of component 1 in the mixture. The experimental refractive indices of the binary mixtures at different temperatures are listed in Table 3, and the values of  $\Delta n_D$  are shown in Fig. 8. The results were fitted by Eq. (3) and the adjustable parameters and standard deviations are given in Table 2.

It can be seen that the changes in refractive index of all 2-alkanol mixtures with acetonitrile are positive throughout the entire composition range, while the chain-length of the 2-alkanol increases the change in the refractive index becomes more positive. The same can be said about the change in refractive index of these mixtures at higher temperatures which were slightly more positive than they were at 293.15 K.

Fig. 8 shows that the maximum of refractive index deviations occur at equimolar concentration of acetonitrile with 2-alkanols, and becomes grater as temperature increases.

# Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.tca.2009.06.015.

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