

# Temperature Dependence of Densities and Speeds of Sound of Nitromethane + Butanol Isomers in the Range (288.15–308.15) K

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Densities and speeds of sound of the systems nitromethane + 1-butanol, nitromethane + 2-methyl-propan-1-ol, and nitromethane + 2-butanol were measured in the temperature range (288.15–308.15) K. Excess molar volumes are discussed and compared with those of other systems polar fluid + alcohol founded in the literature.

## Introduction

During the last years mixtures polar compound + alcohol have been studied by some authors.<sup>1–4</sup> The aim of the present work is to contribute to the study of such mixtures.

Nitromethane has been chosen as the polar component. Nitroalkanes are chemical compounds that are liquids at room temperature. They have high polarity, reflected in their high dipole moment and dielectric constant.<sup>5</sup> The alcohols chosen for the mixtures have been 1-butanol, 2-butanol, and 2-methyl-propan-1-ol. These mixtures present partial immiscibility near room temperature, specifically, at critical mole fraction at (290.34, 284.59, and 290.80) K,<sup>6,7</sup> respectively. For this reason we have studied them at higher temperatures to avoid difficulties due to effects related with the proximity of the upper critical point.

Some studies<sup>8</sup> have suggested that hydrogen bonding in nitroalkanes is very weak. Furthermore, the alcohols are characterized by their strong association by hydrogen bonds.

In this work densities and speeds of sound over the whole range of compositions, at atmospheric pressure, and in the temperature range (288.15–308.15) K were measured. From these experimental data we have obtained thermodynamic properties of these mixtures. These properties have been studied in order to establish the behavior of these systems with the composition and with the temperature. In addition we have compared this behavior with that of other polar compounds + alcohol systems found in the literature.

## Experimental Section

Nitromethane and 1-butanol (>99 mol % and >99.8 mol %, respectively) were supplied from Fluka, 2-methyl-propan-1-ol (>99.45 mol %) was supplied from Sigma-Aldrich, and 2-butanol (>99.45 mol %) was from Aldrich. All chemicals were partially degassed and dried over Fluka type 0.4 nm molecular sieves. All the mentioned purities are the values given by the manufacturer and were checked using the gas chromatograph Perkin-Elmer model 8700.

Densities  $\rho$  and speeds of sound  $u$  of the pure components and of the binary mixtures were measured using a DSA-48 densimeter and sound analyzer. This apparatus, con-

**Table 1. Selected Data of Densities  $\rho$  and Isobaric Thermal Expansivities  $\alpha$  for the Pure Liquids at the Temperature  $T$**

component	$T/K$	$\rho/g\cdot cm^{-3}$	
		this work	literature
nitromethane	288.15	1.143 28	1.143 18 <sup>10</sup>
	293.15	1.136 60	1.136 41 <sup>10</sup>
	298.15	1.129 90	1.129 58 <sup>10</sup>
	303.15	1.123 07	1.124 39 <sup>10</sup>
	308.15	1.116 14	1.115 92 <sup>10</sup>
1-butanol	288.15	0.813 24	
	293.15	0.809 43	0.809 56 <sup>5</sup>
	298.15	0.805 62	0.805 75 <sup>5</sup>
	303.15	0.801 79	
	308.15	0.797 93	
2-methyl-propan-1-ol	288.15	0.805 44	
	293.15	0.801 62	0.801 6 <sup>5</sup>
	298.15	0.797 77	0.797 8 <sup>5</sup>
	303.15	0.793 87	
	308.15	0.789 90	
2-butanol	288.15	0.810 51	
	293.15	0.806 48	0.806 52 <sup>5</sup>
	298.15	0.802 39	0.802 41 <sup>5</sup>
	303.15	0.798 19	
	308.15	0.793 88	
		$\alpha/10^{-3}K^{-1}$	
nitromethane	298.15	1.18	1.24 <sup>5</sup>
1-butanol	298.15	1.01	1.024 <sup>5</sup>
2-methyl-propan-1-ol	298.15	0.96	0.95 <sup>5</sup>
2-butanol	298.15	0.95	0.948 <sup>5</sup>

nected to a personal computer, has two cells. Calibration was done using *n*-heptane (>99.8 mol %) from Fluka and pure water (MilliQ). The experimental procedure was described in detail in a previous work.<sup>9</sup> The temperature was controlled through a solid-state thermostat that uses the Peltier effect, and the precision in the temperature was  $\pm 0.005$  K. The precision is estimated to be about  $\pm 2 \times 10^{-5}$  for mole fraction  $x$ ,  $\pm 1 \times 10^{-5} g\cdot cm^{-3}$  for  $\rho$ , and  $\pm 0.02 m\cdot s^{-1}$  for  $u$ .

## Results and Discussion

The automatic system to measure densities and speeds of sound of the pure liquids and mixtures allows us to obtain data at many temperatures. Because of this we give only data at selected temperatures. In Table 1 we present densities  $\rho$  of the pure liquids and their comparison with literature data. Isobaric thermal expansivities  $\alpha$  at 298.15 K were calculated from differentiation of the density

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**Table 2. Selected Data of Sound Velocity  $u$  and Adiabatic Compressibility  $\kappa_S$  for the Pure Liquids at the Temperature  $T$** 

component	$T/K$	$u/m\cdot s^{-1}$	$\kappa_S/(T Pa^{-1})$	
			this work	literature
nitromethane	283.15	1378.06	457.89	
	288.15	1358.46	473.97	
	293.15	1338.51	491.08	
	298.15	1318.72	508.93	
	303.15	1298.82	527.83	
1-butanol	308.15	1279.64	547.15	
	288.15	1273.12	758.65	
	293.15	1255.94	783.22	
	298.15	1238.99	808.60	
	303.15	1222.08	835.10	
2-methyl-propan-1-ol	308.15	1205.79	861.97	866 <sup>5</sup>
	288.15	1220.64	833.28	
	293.15	1203.56	861.18	
	298.15	1186.72	890.07	
	303.15	1170.08	920.07	
2-butanol	308.15	1153.86	950.87	950 <sup>5</sup>
	283.15	1263.90	768.59	848.4 <sup>11</sup>
	288.15	1246.38	794.22	
	293.15	1228.38	821.75	
	298.15	1210.43	850.62	
303.15	1192.47	881.05		
308.15	1174.89	912.54		

equation, and their values for the pure liquids are also given in this table.

In Table 2 we give selected speeds of sound  $u$  and isentropic compressibilities  $\kappa_S$  of the pure liquids compared with literature data. We have calculated  $\kappa_S$  from the Laplace equation:

$$\kappa_S = \frac{1}{\rho u^2} \quad (1)$$

1-Butanol has a higher density, lower isentropic compressibility, and lower isobaric thermal expansivity than the other two alcohols studied. This is expected since the steric hindrance of alkyl groups disturbs the formation of hydrogen bonds on the nonprimary alcohols.<sup>12–14</sup>

Densities and speeds of sound of the mixtures are presented in Table 3. Isentropic compressibilities were calculated for the mixtures using also eq 1. We have fitted simultaneously as a function of composition and temperature these three magnitudes according to the expression:

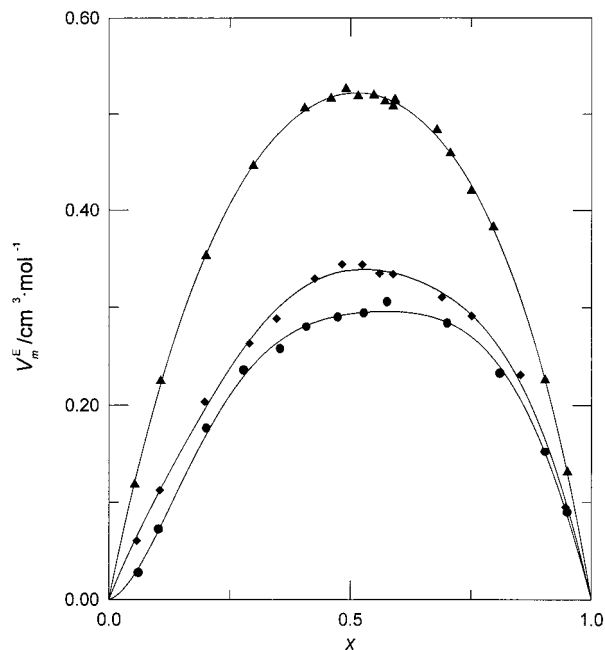
$$Y = \sum_{i=1}^m \sum_{j=1}^n A_{ij} \times 10^{1-j} x^{j-1} (TK - T_0)^{j-1} \quad (2)$$

where  $x$  is the mole fraction of nitromethane,  $T$  is the absolute temperature, and  $T_0$  is 280.15 K.  $Y$  can be density  $\rho/g\cdot cm^{-3}$ , speed of sound  $u/m\cdot s^{-1}$ , or isentropic compressibility  $\kappa_S/(T Pa^{-1})$ . All the measured data were used in the fitting process. The coefficients  $A_{ij}$  were obtained using Marquardt<sup>15</sup> algorithm and are given in Tables 4–6.

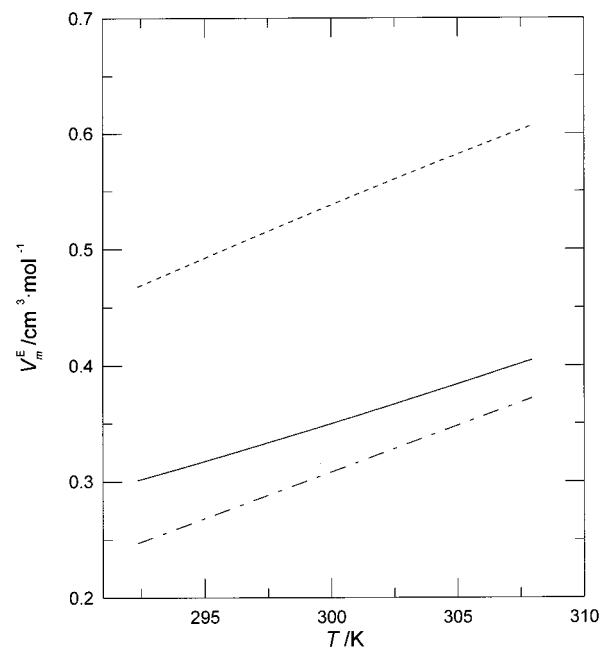
We have calculated also excess molar volumes  $V_m^E$ . These quantities were fitted simultaneously to temperature and mole fraction to the Redlich–Kister polynomials:

$$V_m^E/cm^3\cdot mol^{-1} = x(1-x) \sum_{i=1}^5 \sum_{j=1}^3 A_{ij} \times 10^{1-j} (2x-1)^{j-1} (TK - T_0)^{j-1} \quad (3)$$

The coefficients  $A_{ij}$  were obtained also using Marquardt algorithm and are given in Table 7. Also, all the measured data were used in the fitting process.



**Figure 1.** Excess molar volumes  $V_m^E$  at 298.15 K against composition  $x$ : ( $\blacklozenge$ )  $x$  nitromethane +  $(1-x)$  1-butanol; ( $\bullet$ )  $x$  nitromethane +  $(1-x)$  2-methyl-propan-1-ol; ( $\blacktriangle$ )  $x$  nitromethane +  $(1-x)$  2-butanol.



**Figure 2.** Excess molar volumes  $V_m^E$  at equimolar composition against temperature  $T/K$ : (—)  $x$  nitromethane +  $(1-x)$  1-butanol; (---)  $x$  nitromethane +  $(1-x)$  2-methyl-propan-1-ol; (- · -)  $x$  nitromethane +  $(1-x)$  2-butanol.

Excess isobaric thermal expansivities  $\alpha^E$  were determined at 298.15 K following the ideality criterion of Benson and Kiyohara,<sup>16</sup> which is the most frequent used for this purpose:

$$\alpha^E = \alpha - (\phi\alpha_1 + (1-\phi)\alpha_2) \quad (4)$$

where  $\phi$  is the volume fraction of component 1, defined by

$$\phi = \frac{\rho}{\rho_1} xM_1 / (xM_1 + (1-x)M_2) \quad (5)$$

**Table 3. Selected Data of Densities  $\rho$  and Speeds of Sound  $u$  for the Studied Mixtures**

$x$	$\rho/\text{g}\cdot\text{cm}^{-3}$					$u/\text{m}\cdot\text{s}^{-1}$				
	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K	288.15 K	293.15 K	298.15 K	303.15 K	308.15 K
$x$ Nitromethane + $(1-x)$ 1-Butanol										
0.056 70		0.82000	0.816 09	0.812 08	0.808 05		1255.86	1238.64	1221.53	1205.03
0.103 78		0.82925	0.825 17	0.821 04	0.816 88		1255.12	1238.01	1220.76	1203.96
0.197 35		0.84872	0.844 44	0.840 02	0.835 66		1254.38	1236.86	1218.87	1202.62
0.290 57		0.87012	0.865 62	0.860 99	0.856 34		1253.87	1236.36	1219.03	1201.74
0.346 86		0.88404	0.879 43	0.874 78	0.870 13		1254.30	1237.41	1218.59	1202.14
0.425 91		0.90500	0.900 05	0.895 04	0.890 00		1253.82	1236.96	1219.93	1203.02
0.482 52		0.92115	0.916 01	0.910 81	0.905 62		1254.03	1237.24	1221.17	1204.63
0.524 56		0.93390	0.928 61	0.923 30	0.917 98		1255.68	1238.16	1222.92	1206.35
0.559 49		0.94502	0.939 63	0.934 24	0.928 78		1256.76	1240.56	1224.36	1208.18
0.587 64		0.95421	0.948 73	0.943 20	0.937 71		1257.09	1241.01	1225.21	1209.97
0.689 09		0.98996	0.984 27	0.978 52	0.972 77		1267.10	1251.14	1235.51	1219.22
0.750 78		1.01394	1.008 07	1.002 18	0.996 29		1277.35	1260.39	1244.39	1227.41
0.852 46		1.05815	1.051 89	1.045 59	1.039 26		1300.15	1282.17	1264.12	1246.13
0.946 35		1.10580	1.099 35	1.092 86	1.086 02		1326.53	1307.10	1287.76	1268.97
$x$ Nitromethane + $(1-x)$ 2-Methylpropan-1-ol										
0.060 62		0.813 54	0.809 49	0.805 40	0.801 23		1207.31	1190.09	1173.06	1156.43
0.102 90		0.822 00	0.817 82	0.813 66	0.809 39		1208.61	1191.31	1174.10	1157.54
0.201 28		0.842 84	0.838 43	0.833 95	0.829 49		1212.29	1194.89	1177.60	1160.96
0.279 91		0.861 13	0.856 48	0.851 81	0.847 12		1215.04	1197.91	1180.70	1164.06
0.355 32		0.880 32	0.875 47	0.870 62	0.865 70		1218.01	1201.28	1184.44	1168.08
0.409 67		0.894 98	0.889 97	0.884 96	0.879 88		1220.51	1204.37	1187.69	1171.36
0.474 07		0.913 60	0.908 39	0.903 15	0.897 84		1224.16	1208.64	1192.24	1175.80
0.528 33		0.930 31	0.924 95	0.919 59	0.914 14		1228.66	1213.52	1197.34	1181.18
0.576 24		0.945 82	0.940 29	0.934 80	0.929 23		1233.44	1218.47	1202.46	1186.41
0.701 39		0.990 96	0.985 20	0.979 25	0.973 34		1253.63	1238.38	1221.64	1205.33
0.810 60		1.036 89	1.030 73	1.024 58	1.018 34		1281.62	1264.11	1246.41	1229.17
0.904 90		1.082 61	1.076 17	1.069 72	1.063 18		1310.64	1291.76	1272.91	1254.78
0.950 15		1.107 20	1.100 60	1.094 00	1.087 35		1325.12	1305.48	1285.90	1267.30
$x$ Nitromethane + $(1-x)$ 2-Butanol										
0.052 27	0.820 05	0.815 84	0.811 56	0.807 19	0.802 71	1247.22	1228.83	1210.51	1192.15	1174.28
0.105 95	0.830 34	0.825 96	0.821 52	0.817 00	0.812 38	1247.55	1228.96	1210.44	1191.96	1173.97
0.199 92	0.849 98	0.845 34	0.840 64	0.835 87	0.831 00	1248.54	1229.95	1211.29	1192.76	1174.37
0.298 38	0.872 73	0.867 84	0.862 86	0.857 84	0.852 73	1250.55	1232.35	1213.93	1195.54	1177.51
0.404 68	0.900 17	0.894 95	0.889 68	0.884 36	0.878 97	1253.27	1235.81	1217.89	1199.67	1181.86
0.459 04	0.915 55	0.910 17	0.904 76	0.899 28	0.893 75	1255.83	1238.79	1221.10	1203.04	1185.18
0.490 29	0.924 71	0.919 24	0.913 75	0.908 22	0.902 62	1257.67	1240.85	1223.27	1205.31	1187.64
0.515 62	0.932 54	0.927 01	0.921 45	0.915 86	0.910 18	1259.48	1242.83	1225.34	1207.45	1189.64
0.547 97	0.942 74	0.937 12	0.931 46	0.925 78	0.920 04	1262.20	1245.61	1228.15	1210.28	1192.68
0.570 97	0.950 26	0.944 58	0.938 88	0.933 14	0.927 35	1264.47	1247.98	1230.57	1212.75	1195.23
0.587 71	0.955 85	0.950 14	0.944 40	0.938 63	0.932 79	1266.44	1249.87	1232.50	1214.70	1197.15
0.591 70	0.957 12	0.951 38	0.945 63	0.939 83	0.933 98	1266.71	1250.15	1232.76	1214.91	1197.32
0.678 93	0.988 24	0.982 30	0.976 34	0.970 33	0.964 25	1277.82	1261.13	1243.62	1225.69	1207.83
0.706 51	0.998 91	0.992 93	0.986 92	0.980 86	0.974 75	1282.86	1265.98	1248.34	1230.33	1212.75
0.750 42	1.016 70	1.010 61	1.004 51	0.998 35	0.992 12	1292.32	1274.74	1256.73	1238.51	1220.57
0.796 26	1.036 25	1.030 08	1.023 86	1.017 58	1.011 25	1302.51	1284.39	1265.99	1247.52	1229.47
0.903 47	1.087 93	1.081 52	1.075 08	1.068 54	1.061 94	1331.48	1312.19	1292.91	1273.67	1255.02
0.950 10	1.113 44	1.106 90	1.100 31	1.093 64	1.086 90	1345.08	1325.29	1305.64	1286.06	1267.00

$\alpha$  is calculated from analytical differentiation from eq 2, subscripts denote properties of the pure products, and  $M$  is the molecular weight.

In Figure 1 we present excess molar volumes against composition at 298.15 K for the three systems. The excess molar volumes of all systems are positive over the whole composition range. The system nitromethane + 2-butanol shows a higher  $V_m^E$  value than the other ones, and the composition dependence of  $V_m^E$  for the three systems is parabolic. In Figure 2 is presented this quantity against temperature. For the three systems the excess molar volumes increase with an increase of temperature; an almost linear temperature dependence is observed. The mixture containing 1-butanol appears to be less sensitive to temperature changes.

Excess isobaric thermal expansivities at 298.15 K are represented in Figure 3. Also the mixture containing 2-butanol has higher excess thermal expansivities than those of the other two systems.

The behavior of the excess molar volumes of these three systems can be explained as a balance between positive contributions, due to hydrogen bond rupture and dispersive

**Table 4. Coefficients  $A_{ij}$  of Eq 2 and Standard Deviations  $s$  for the Density  $\rho$** 

$j$	$i$				
	1	2	3	4	5
$x$ Nitromethane + $(1-x)$ 1-Butanol ( $s = 0.000\ 14\ \text{g}\cdot\text{cm}^{-3}$ )					
1	0.819 30	0.186 92	0.094 86	-0.002 89	0.054 11
2	-0.006 97	-0.013 63	0.038 19	-0.059 70	0.029 81
3	-0.000 18	0.002 16	-0.009 60	0.014 37	-0.007 01
$x$ Nitromethane + $(1-x)$ 2-Methylpropan-1-ol ( $s = 0.000\ 18\ \text{g}\cdot\text{cm}^{-3}$ )					
1	0.811 72	0.192 96	0.094 69	-0.01533	0.069 80
2	-0.007 53	-0.010 53	0.028 13	-0.039 75	0.016 33
3	-0.000 06	0.001 24	-0.007 09	0.010 15	-0.004 29
$x$ Nitromethane + $(1-x)$ 2-Butanol ( $s = 0.00015\ \text{g}\cdot\text{cm}^{-3}$ )					
1	0.816 96	0.175 31	0.144 64	-0.085 84	0.102 65
2	-0.007 70	-0.007 62	0.003 69	-0.001 61	0.000 01
3	-0.000 18	0.000 55	-0.001 34	0.001 56	-0.000 67

interactions between unlike molecules, and negative contributions due to packing effects.<sup>10</sup> Complex interactions between unlike molecules<sup>2</sup> may also have an effect in  $V_m^E$ .

**Table 5. Coefficients  $A_{ij}$  of Eq 2 and Standard Deviations  $s$  for the Speed of Sound  $u$** 

$j$	$i$							
	1	2	3	4	5	6	7	8
$x$ Nitromethane + (1 - $x$ ) 1-Butanol ( $s = 0.6 \text{ m}\cdot\text{s}^{-1}$ )								
1	1299.90	39.09	-680.29	4330.12	-13026.09	19118.10	-12924.96	3234.50
2	-33.76	-20.17	244.42	-1575.15	4940.90	-7492.40	5334.50	-1437.90
$x$ Nitromethane + (1 - $x$ ) 2-Methylpropan-1-ol ( $s = 0.3 \text{ m}\cdot\text{s}^{-1}$ )								
1	1247.41	80.40	-236.04	528.69	-804.25	670.20	417.77	-514.14
2	-33.59	-10.74	3.25	202.72	-500.80	563.45	-427.84	163.95
$x$ Nitromethane + (1 - $x$ ) 2-Butanol ( $s = 0.5 \text{ m}\cdot\text{s}^{-1}$ )								
1	1274.92	34.03	-184.36	602.38	-863.84	470.93	520.75	-464.81
2	-35.81	-20.79	126.00	-381.06	827.09	-1049.09	609.31	-115.23

**Table 6. Coefficients  $A_{ij}$  of Eq 2 and Standard Deviations  $s$  for the Isentropic Compressibility  $\kappa_S$** 

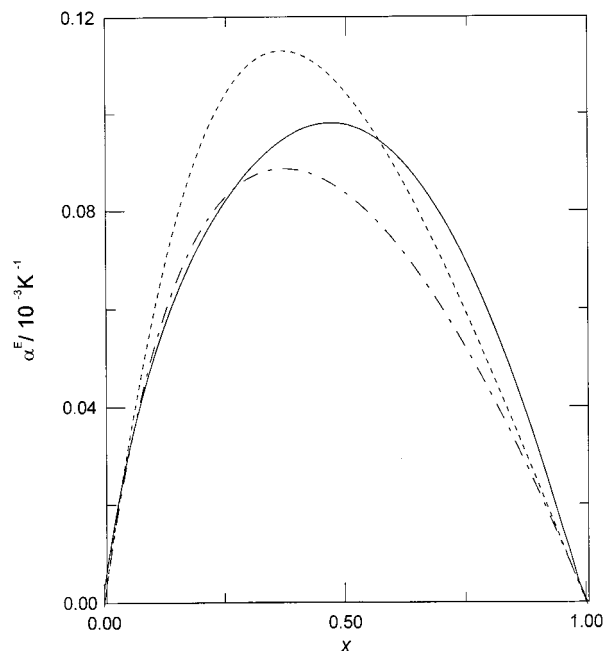
$j$	$i$				
	1	2	3	4	5
$x$ Nitromethane + (1 - $x$ ) 1-Butanol ( $s = 1.2 \text{ T Pa}^{-1}$ )					
1	720.2	-140.3	-41.0	-151.0	60.4
2	47.4	-84.9	337.1	-422.7	152.2
3	1.2	25.8	-108.9	130.9	-46.9
$x$ Nitromethane + (1 - $x$ ) 2-Methylpropan-1-ol ( $s = 0.9 \text{ T Pa}^{-1}$ )					
1	791.4	-341.7	649.8	-1191.1	538.7
2	51.7	7.5	-189.7	313.2	-151.9
3	1.9	3.1	7.0	-26.8	16.5
$x$ Nitromethane + (1 - $x$ ) 2-Butanol ( $s = 0.7 \text{ T Pa}^{-1}$ )					
1	754.12	-241.10	332.10	-697.77	300.08
2	53.86	-34.80	-0.84	21.27	-8.53
3	1.28	17.94	-47.27	50.71	-21.07

**Table 7. Coefficients  $A_{ij}$  of Eq 3 and Standard Deviations  $s$  for the Excess Molar Volumes  $V_m^E$** 

$j$	$i$				
	1	2	3	4	5
$x$ Nitromethane + (1 - $x$ ) 1-Butanol ( $s = 0.006 \text{ cm}^3\cdot\text{mol}^{-1}$ )					
1	0.9281	0.0270	0.6861	1.0912	-0.0595
2	0.2084	0.1451	-0.3745	-0.6161	0.1295
3	0.0145	-0.0356	0.0665	0.1277	-0.0177
$x$ Nitromethane + (1 - $x$ ) 2-Methylpropan-1-ol ( $s = 0.006 \text{ cm}^3\cdot\text{mol}^{-1}$ )					
1	0.5962	-0.0478	1.0639	1.1799	-1.0546
2	0.3207	0.2092	-0.3056	-0.3981	0.0241
3	-0.0001	-0.0499	0.0497	0.0610	0.0441
$x$ Nitromethane + (1 - $x$ ) 2-Butanol ( $s = 0.006 \text{ cm}^3\cdot\text{mol}^{-1}$ )					
1	1.3877	0.1217	0.5673	0.4207	0.0805
2	0.4130	0.0032	-0.0080	-0.2278	-0.0414
3	-0.0140	-0.0152	-0.0145	0.0320	0.0450

We can compare the results obtained for these three systems with other experimental data for polar compound + alcohol mixtures. In Table 8 we present some equimolar values of  $V_m^E$  at 298.15 K for nitroalkane + alcohol systems. Observing the systems nitromethane + 1-alcohol, we can see the excess molar volume is higher when the alkyl chain of the alcohol is longer. This effect also takes place in other polar compound + alcohol systems.<sup>3,4</sup>

In Table 8, it can be seen that, at the same concentration and temperature, all excess magnitudes studied in the mixtures with nitroethane + alcohol are smaller than those for the mixture with nitromethane + the same alcohol. Consequently, for all these mixtures if the alkyl chain of the nitroalkane increases, the excess properties decrease.

**Figure 3. Excess isobaric thermal expansivities  $\alpha^E$  at 298.15 K against composition  $x$ : (—)  $x$  nitromethane + (1 -  $x$ ) 1-butanol; (---)  $x$  nitromethane + (1 -  $x$ ) 2-methylpropan-1-ol; (- · -)  $x$  nitromethane + (1 -  $x$ ) 2-butanol.****Table 8. Excess Molar Volume  $V_m^E$  at 298.15 K of Nitroalkane + Alcohol Systems at Equimolar Composition**

	$V_m^E/\text{cm}^3\cdot\text{mol}^{-1}$	
	nitromethane	nitroethane
methanol	-0.173 <sup>17</sup>	
ethanol	0.011 <sup>17</sup>	
1-propanol	0.236 <sup>10</sup>	
2-propanol	0.240 <sup>10</sup>	
1-butanol	0.338	0.222 <sup>9</sup>
2-methylpropan-1-ol	0.294	0.183 <sup>9</sup>
2-butanol	0.522	0.408 <sup>9</sup>

This effect is also observed for other systems and might be due to the fact that, although in the gas phase the molecular dipole moments of the nitroalkanes are nearly the same (3.5 D), in the condensed liquid phase the effective polarity<sup>18</sup> is greater for the smaller nitroalkane. As the alkyl chain of the nitroalkane increases, the polar groups are more diluted and their interactions are therefore weakened.

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