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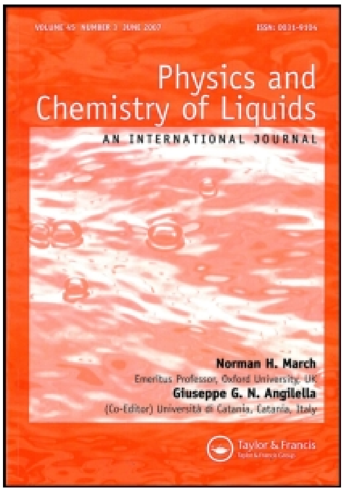

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Mixing properties and modelling of methanol with chlorobenzene and bromobenzene at 293, 303, and 313 K

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Refractive index, ultrasonic velocity and density for the binary mixtures of methanol with chlorobenzene and bromobenzene at 293, 303, and 313 K have been measured over the entire composition range. The values of refractive index (n), ultrasonic velocity (u), and density (ρ) were used to compute deviation in molar refraction (ΔR_m) and deviation in isentropic compressibility ($\Delta\kappa_s$). The results of deviation were fitted to the Redlich–Kister polynomial equation to derive the binary coefficients and standard deviation. Both the systems exhibited negative values of ΔR_m and $\Delta\kappa_s$ over the entire composition range. The density, ultrasonic velocity and refractive index were correlated to first order polynomial with respect to mole fraction. Experimental data of physical properties (refractive index, isentropic compressibility and density) were compared with the results obtained by theoretical estimation procedures.

Keywords: molar refraction; isentropic compressibility; methanol; chlorobenzene; bromobenzene

1. Introduction

The physical properties of binary mixtures have been studied for many reasons, one of the most important facts is that these properties may provide information about the molecular interactions between the components of the mixtures, to develop new theoretical models, and also to carry out engineering applications in the process industry [1–3]. Many chemical food, pharmacological and other industries need to know physical properties of non ideal mixtures which could be involved in process design. For this reason, it is necessary to pay attention to the device and equipment design and operational magnitudes to obtain an adequate and optimized process. In recent years, there has been considerable interest in theoretical and experimental investigation of the excess thermodynamic properties of binary mixtures. The interaction between the molecules can be established from the study of the characteristic departure from ideal behavior of some physical properties (i.e. volume, compressibility, viscosity, refractive index etc.).

This article is devoted to the study of different thermodynamic properties of mixtures containing the methanol, which forms the basis for many products including silicons, refrigents adhesive etc, and it may also be used as fuel source in fuel cells. Aryl halides (chlorobenzene, bromobenzene) having the special kind of structure,

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nucleophilic substitution proceeds readily and can be used for synthetic purpose. The possibility of intramolecular hydrogen bonding with in alcohol molecule and their tendency to form new hydrogen bonds with other molecules produce interesting solution behavior.

In our laboratory, the thermodynamic properties of binary mixtures of alcohols with organic solvents have been studied in order to investigate the intermolecular interactions and the internal structure of mixed binary solvents. In continuing of our program on the thermodynamic, acoustic, and transport properties of mixtures of alcohol with organic solvents, the present article reports refractive index, ultrasonic velocity and density for binary mixtures containing methanol with chlorobenzene and bromobenzene, respectively, at temperatures $T = 293$, 303, and 313 K. The experimental data of refractive index, ultrasonic velocity and density for both the mixtures were used to compute the corresponding derived magnitudes, deviation in molar refraction (ΔR_m) and deviation in isentropic compressibility ($\Delta \kappa_S$) and fitted to Redlich–Kister polynomial equation. The results of refractive index, ultrasonic velocity and density measurement were fitted to a first order polynomial with respect to mole fraction of methanol. The experimental data were compared with the results obtained by mixing rule proposed by Lorentz–Lorenz and Oster for refractive index, the collision factor theory and Nomoto's relation for isentropic compressibility, and equation of state for density.

2. Experimental section

The chemicals used were obtained from Ranbaxy Fine Chemicals Limited. All the chemicals used were purified by standard procedure, discussed by Perrin and Armarego [4]. The purities of all the chemicals were ascertained by the constancy of their boiling point during final distillation and also by literature comparisons [5] of their densities and refractive indices at 293 K. These values agreed well within the precision of experimental error.

Mixtures were prepared by weighing the liquids in specially designed ground glass stoppered bottles, taking extreme precautions to minimize preferential evaporation. A Sartorius (BP121S) single pan balance having a stated precision of 0.1 mg was used through out. The maximum possible error in the mole fraction is estimated to be ±0.0001.

Refractive index was measured using Abbe's refractometer provided by Optical Technologies, New Delhi. The refractometer was calibrated by measuring the refractive index of triply distilled water and benzene at $T = 293$ K. The accuracy in the refractive index measurement was 0.001 unit. Temperature was controlled by circulating water around the prisms of the refractometer from thermostatically controlled adequately stirred water bath. The sample mixtures were directly injected into the prism assembly of the instrument by means of an air tight hypodermic syringe. An average of four to five measurements was taken for each sample mixture.

The ultrasonic velocity of pure components and their mixtures were measured by variable path interferometer provided by Mittal Enterprises, New Delhi (Model M-83). It consists of a high frequency generator and a measuring cell. The calibration of ultrasonic interferometer was done by measuring the velocity in AR grade benzene and carbontetrachloride. The measured values of ultrasonic velocity (u) for benzene and carbontetrachloride were compared from the literature values [5] of (u) at 298 K and $-\mathrm{d}u/\mathrm{d}t$. The maximum estimated error in ultrasonic velocity measurement has been found to be ±0.08%. The temperature was controlled by circulating water around the liquid cell from thermostatically controlled adequately stirred water bath (accuracy ±0.1°C).

The density has been measured using a single capillary pyknometer with an accuracy of ±0.5. For each solution, four to five density measurements were taken and the results were averaged.

3. Results and discussion

Tables 1 and 2 list the experimental values of refractive index, ultrasonic velocity, density, isentropic compressibility, deviation in molar refraction and deviation in isentropic compressibility.

Table 1. Thermodynamic properties of methanol + chlorobenzene binary mixtures at different temperatures.

x_1	n	u (m s^{-1})	ρ (g cm^{-3})	κ_s (TPa^{-1})	ΔR_m	$\Delta\kappa_s$ (TPa^{-1})
$T = 293$ K						
0.0000	1.524	1286	1.1058	546.82	0.00	0.00
0.2808	1.496	1245	1.0665	604.92	−3.42	−73.34
0.4676	1.472	1216	1.0292	657.10	−4.81	−108.61
0.6010	1.447	1194	0.9939	705.75	−5.27	−122.41
0.7009	1.427	1177	0.9605	751.54	−5.03	−123.39
0.7783	1.409	1164	0.9288	794.64	−4.44	−116.51
0.8405	1.391	1153	0.8985	837.19	−3.68	−103.09
0.8913	1.374	1141	0.8697	883.20	−2.82	−80.85
0.9335	1.358	1132	0.8423	926.49	−1.91	−57.32
0.9693	1.344	1124	0.8162	969.77	−0.94	−30.79
1.000	1.330	1116	0.7911	1014.94	0.00	0.00
$T = 303$ K						
0.0000	1.521	1256	1.1095	521.60	0.00	0.00
0.2808	1.493	1219	1.0560	569.86	−3.43	−139.94
0.4676	1.468	1192	1.0190	620.30	−4.86	−194.91
0.6010	1.443	1172	0.9837	671.36	−5.30	−211.66
0.7009	1.423	1157	0.9504	723.41	−5.05	−206.66
0.7783	1.406	1143	0.9189	778.66	−4.42	−185.97
0.8405	1.388	1132	0.8888	831.92	−3.66	−159.23
0.8913	1.371	1122	0.8601	886.49	−2.79	−125.62
0.9335	1.355	1114	0.8329	950.54	−1.87	−80.62
0.9693	1.340	1107	0.8068	998.98	−0.93	−44.23
1.000	1.325	1101	0.7819	1055.05	0.00	0.00
$T = 313$ K						
0.0000	1.515	1212	1.0820	629.17	0.00	0.00
0.2808	1.488	1182	1.0440	685.59	−3.42	−75.15
0.4676	1.465	1161	1.0070	736.73	−4.78	−111.55
0.6010	1.441	1145	0.9725	784.33	−5.21	−126.45
0.7009	1.420	1132	0.9394	830.72	−5.00	−126.86
0.7783	1.402	1120	0.9081	877.87	−4.41	−115.98
0.8405	1.383	1111	0.8783	922.42	−3.68	−100.58
0.8913	1.366	1103	0.8499	967.12	−2.81	−79.68
0.9335	1.349	1096	0.8229	1011.65	−1.92	−54.92
0.9693	1.339	1091	0.7971	1053.99	−0.92	−29.36
1.000	1.321	1086	0.7724	1097.74	0.00	0.00

Table 2. Thermodynamic properties of methanol + bromobenzene binary mixtures at different temperatures.

x_1	n	u (m s^{-1})	ρ (g cm^{-3})	κ_s (TPa^{-1})	ΔR_m	$\Delta\kappa_s$ (TPa^{-1})
$T = 293$ K						
0.0000	1.560	1178	1.497	481.38	0.00	0.00
0.3528	1.518	1167	1.381	531.70	−4.65	−137.92
0.5504	1.484	1157	1.280	583.61	−5.90	−191.44
0.6775	1.457	1149	1.192	635.45	−5.79	−207.41
0.7657	1.432	1143	1.114	687.10	−5.18	−202.82
0.8305	1.408	1138	1.045	738.92	−4.91	−185.58
0.8802	1.388	1132	0.9830	793.88	−3.51	−157.14
0.9195	1.364	1128	0.9276	847.27	−2.75	−124.72
0.9552	1.353	1124	0.8714	908.34	−1.57	−82.69
0.9778	1.341	1121	0.8323	956.11	−0.84	−46.98
1.0000	1.330	1116	0.7911	1014.94	0.00	0.00
$T = 303$ K						
0.0000	1.554	1137	1.4830	481.38	0.00	0.00
0.3528	1.514	1133	1.3670	531.70	−4.57	−75.33
0.5504	1.480	1128	1.2670	583.61	−5.83	−110.88
0.6775	1.451	1124	1.1790	635.45	−5.79	−124.98
0.7657	1.426	1120	1.1020	687.10	−5.19	−126.63
0.8305	1.404	1115	1.0330	738.92	−4.36	−116.50
0.8802	1.385	1112	0.9721	793.88	−3.44	−101.09
0.9195	1.367	1109	0.9172	847.27	−2.54	79.73
0.9552	1.350	1105	0.8615	908.34	−1.52	−55.92
0.9778	1.338	1103	0.8228	956.11	−0.79	−29.00
1.0000	1.325	1101	0.7819	1014.94	0.00	0.00
$T = 313$ K						
0.0000	1.550	1118	1.4670	545.36	0.00	0.00
0.3528	1.510	1114	1.3520	596.01	−4.59	−144.23
0.5504	1.476	1110	1.2530	647.74	−5.86	−201.65
0.6775	1.447	1106	1.1660	701.12	−5.81	−218.48
0.7657	1.422	1102	1.0890	756.15	−5.21	−212.16
0.8305	1.400	1098	1.0210	812.40	−4.38	−191.71
0.8802	1.381	1094	0.9607	869.72	−3.45	−161.85
0.9195	1.363	1092	0.9064	925.20	−2.55	−128.07
0.9552	1.346	1090	0.8511	988.93	−1.52	−84.06
0.9778	1.334	1088	0.8129	1039.21	−0.79	−46.26
1.0000	1.321	1086	0.7724	1097.74	0.00	0.00

The deviation in molar refraction ΔR_m, was calculated from the Lorentz–Lorenz [6] equation:

$$\Delta R_m = R_m - \sum_{i=1}^{2} R_i \phi_i, \tag{1}$$

where R_i and R_m are the molar refraction of pure components and mixture, respectively and ϕ_i is the volume fraction of the pure components ($i = 1, 2$), given as:

$$\phi_i = \frac{x_i V_i}{\sum_{i=1}^{2} x_i V_i},$$

where $x_i = M_i/\rho_i$.

The deviations in isentropic compressibility ($\Delta\kappa_s$) have been evaluated using the following equations [7]:

$$\Delta\kappa_s = \kappa_s - \sum_{i=1}^{2} \kappa_{si} x_i, \tag{2}$$

where κ_{si} and κ_s are the isentropic compressibility of pure components and mixture, respectively and x_i is the mole fraction of pure components ($i = 1, 2$).

The deviation in molar refraction (ΔR_m) and isentropic compressibility ($\Delta\kappa_s$) with mole fraction can be expressed by Redlich–Kister equation [8]:

$$\Delta Y = x_1 x \sum a_i (x_2 - x_1)^i, \tag{3}$$

where ΔY refers to deviation in ΔR_m or $\Delta\kappa_s$. The adjustable parameters a_i was determined by a least squares method by fitting the experimental values to equation (3).

The root mean square deviation (σ) is defined as:

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

where n is the number of data points and m is the number of coefficients.

The values of a_i along with the standard deviation (σ) between the experiment and fitted values of the respective function are summarised in Table 3.

The experimental density, refractive index and ultrasonic velocity data were correlated to a first order polynomial with respect to mole fraction of methanol

$$Z = \alpha + \beta x_1, \tag{5}$$

where Z refers to ρ, n and u, x_1 is the mole fraction of methanol, α and β represent the coefficients. The values of coefficients α and β were determined by least-squares method

Table 3. Adjustable parameters a_i with the standard deviations σ (Y^E) for deviation in molar refraction (ΔR_m) and deviation in isentropic compressibility ($\Delta\kappa_s$) for both the binary mixtures.

Functions	T (K)	a_0	a_1	a_2	a_3	a_4	σ
Methanol + chlorobenzene							
ΔR_m	293	−28.25	−11.82	27.54	105.93	60.73	0.0059
	303	−19.57	−0.73	−6.49	36.48	28.37	0.0093
	313	−19.74	8.84	−5.42	−0.85	1.020	0.0124
$\Delta\kappa_s$ (TPa^{-1})	293	−4.63	4.16	−0.057	−5.89	−8.49	0.0074
	303	−4.66	3.36	−1.08	−2.31	−3.76	0.0048
	313	−4.66	2.83	−0.99	−0.26	−2.36	0.0052
Methanol + bromobenzene							
ΔR_m	293	−24.32	4.53	−1.11	23.69	11.37	0.0578
	303	−19.51	12.93	−31.82	−54.59	−31.26	0.0024
	313	−21.56	11.17	−15.09	−19.81	−12.78	0.0044
$\Delta\kappa_s$ (TPa^{-1})	293	−7.19	5.03	−3.31	0.13	−6.12	0.0062
	303	−7.39	4.51	−1.89	4.69	−3.33	0.0069
	313	−7.25	8.27	−7.51	−25.65	−26.16	0.0067

Table 4. Coefficients α and β and the root mean square deviation (σ) for binary systems from first order polynomial equation.

Parameters	T (K)	α	β	σ
Methanol + chlorobenzene				
u (m s^{-1})	293	1297.27	−174.74	0.8188
	303	1267.89	−162.93	0.7210
	313	1222.88	−133.82	0.6745
n	293	1.5718	−0.2210	0.0030
	303	1.5681	−0.2207	0.0029
	313	1.5654	−0.2225	0.0032
ρ (g cm^{-3})	293	1.1942	−0.3624	0.0060
	303	1.1829	−0.3605	0.0057
	313	1.1701	−0.3576	0.0056
Methanol + bromobenzene				
u (m s^{-1})	293	1196.52	−73.759	0.8101
	303	1153.70	−48.38	0.8166
	313	1132.42	−43.12	0.6739
n	293	1.6375	−0.2885	0.0042
	303	1.6310	−0.2842	0.0037
	313	1.6269	−0.2842	0.0037
ρ (g cm^{-3})	293	1.7470	−0.8825	0.0124
	303	1.7308	−0.8764	0.0122
	313	1.7124	−0.8682	0.0121

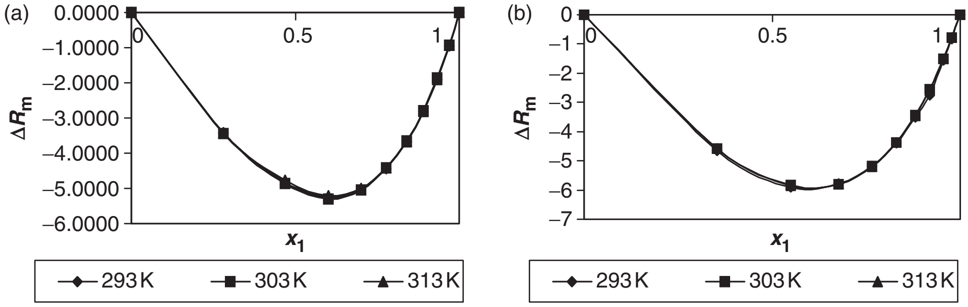

Figure 1. (a) Deviation in molar refraction *vs*. composition for methanol + chlorobenzene mixtures at varying temperature. (b) Deviation in molar refraction *vs*. composition for methanol + bromobenzene mixtures at varying temperature.

and are summarised along with the root mean square deviation (σ) between the experimental and fitted values of the respective functions in Table 4.

Figures 1(a) and (b) and 2(a) and (b) show the graphical variations of deviation in molar refraction (ΔR_m) and deviation in isentropic compressibility ($\Delta\kappa_s$) against mole fraction of methanol (x_1) for both the systems at 293, 303, and 313 K. The values of ΔR_m and $\Delta\kappa_s$ are found to be negative over the entire range of composition for both the systems indicating the presence of strong intermolecular interaction between unlike molecules. The minima of ΔR_m and $\Delta\kappa_s$ values for both the systems occur at around $x_1 = 0.6$–0.7 mole fraction of methanol. The ΔR_m and $\Delta\kappa_s$ values for methanol +bromobenzene mixture are

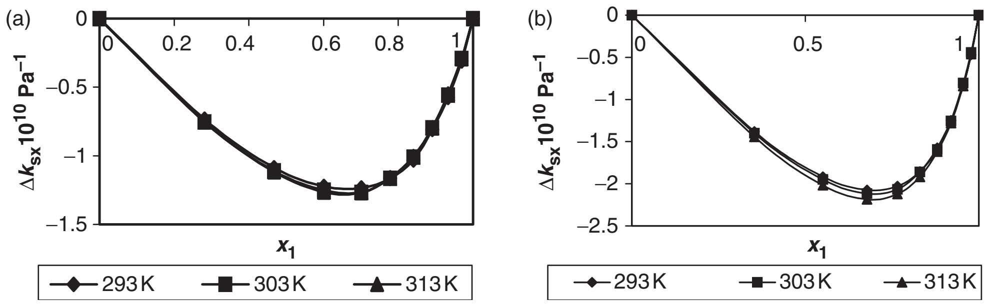

Figure 2. (a) Deviation in isentropic compressibility *vs.* composition for methanol + chlorobenzene mixture at varying temperature. (b) Deviation in isentropic compressibility *vs.* composition for methanol + bromobenzene mixture at varying temperature.

more negative than methanol + chlorobenzene mixture. This may be explained on the basis of the fact that chlorine and bromine both are electronegative atoms and attached with the sp^2 hybridised carbon atom of benzene. An interaction of bromobenzene with methanol is greater because of the availability of more unshared pair of more electrons on bromine atom in bromobenzene as compared with chlorine atom in chlorobenzene. Since electrons are more closer to the nucleus and hence less available for the formation of hydrogen bond while in the case of bromine atom, the electrons are more available because these electrons in the outer most orbit are farther from the nucleus as bromine is much bigger atom than chlorine. Secondly, though both the chlorine and bromine atoms cause negative inductive effect but in both instances resonance or mesomeric effect is greater than inductive effect. Here, again unshared pair of electrons on bromine atom seems to be available more readily. The effect of temperature on ΔR_m and $\Delta\kappa_s$ for both the mixtures is insignificant. Similar trends in ΔR_m and $\Delta\kappa_s$ with mole fraction have been observed earlier [9–11]. These results are further supported by Fort and Moore [12].

4. Estimation of physical properties

In Tables 5–8, a comparison between the experimental and predicted values of physical properties (n, κ_s and ρ) are shown in terms of root mean square deviations.

The experimental refractive index data were compared with the estimated results for the mixing rules proposed by Lorentz–Lorenz (L-L) and Oster (Ost) [13], expressed by the equations respectively:

$$\frac{n^2-1}{n^2+2} = \sum_{i=1}^{2} \phi_i \left(\frac{n_i^2-1}{n_i^2+2}\right), \tag{6}$$

$$\left[\frac{(n^2-1)(2n^2+1)}{n^2}\right] V_m = \sum_{i=1}^{2} \frac{(n_i^2-1)(2n_i^2+1)}{n_i^2} x_i V_i, \tag{7}$$

where n and V_m are the refractive index and molar volume of mixture. n_i, V_i, and ϕ_i are the refractive index, molar volume and volume fraction of pure components ($i = 1, 2$).

The root mean square deviation for prediction of refractive index using L-L and Ost relation for both the mixtures are given in Table 5. It is observed that both the relations exhibit an excellent result for both the mixtures. However, the best correlation

Table 5. Root mean square deviations for estimation of refractive index with respect to corresponding experimental data for the binary mixtures at different temperatures.

T (K)	Lorentz–Lorenz	Oster
Methanol + chlorobenzene		
293	0.00061	0.00102
303	0.00045	0.00104
313	0.000262	0.001002
Methanol + bromobenzene		
293	0.001386	0.00069
303	0.001376	6.53×10^{-5}
313	0.001373	7.30×10^{-5}

Table 6. Root mean square deviations for estimation of isentropic compressibilities with respect to corresponding experimental data for the binary mixtures at different temperatures.

T (K)	CFT	Nomoto
Methanol + chlorobenzene		
293	0.4059	5.360
303	0.6057	5.616
313	0.8187	4.942
Methanol + bromobenzene		
293	0.3725	0.25560
303	0.7355	0.5695
313	1.0140	0.3842

Table 7. Critical values for pure compounds for the estimation of density.

Compound	P_c (Bar)	T_C (K)	Z_{RA}	ω_{SRK}	V^*	V_C
Methanol	80.9	512.6	0.2334	0.5536	0.1198	118
Chlorobenzene	45.2	632.4	0.2651	0.2461	0.3056	308
Bromobenzene	45.2	670.0	0.2637	0.2481	0.3204	324

representing our binary system data is found to be the Oster's relation with an average root mean square deviation of 6.53×10^{-5} for methanol + bromobenzene system.

The Schaffs–Nutsch–Kuhnkies (Collision Factor Theory) and Nomoto relation [13] has been applied for isentropic compressibilities prediction for both the binary mixtures. The Collision Factor Theory and Nomoto relation in terms of isentropic compressibility are given by the following equations:

$$\kappa_S = \left(\frac{1}{\rho^2}\right)\left(\frac{\sum_{i=1}^{2} x_i V_i}{\sum_{i=1}^{2} x_i R_i}\right)^3, \tag{8}$$

Table 8. Root mean square deviations for estimation of density with respect to corresponding experimental data for the binary mixtures at different temperatures.

T (K)	σ (Rackett)	σ (Hankinson)
Methanol + chlorobenzene		
293	0.00069	0.00091
303	0.00062	0.00084
313	0.00058	0.00079
Methanol + bromobenzene		
293	0.06117	0.04272
303	0.06129	0.09922
313	0.06122	0.09183

$$\kappa_\mathrm{s} = \left(\frac{1}{\rho^3}\right)\left(\frac{M}{u_\infty \sum_{i=1}^{2} x_i S_i \sum_{i=1}^{2} x_i B_i}\right)^2, \tag{9}$$

where R, M, and ρ represent molar sound velocity, molecular weight and density of mixtures, respectively. The collision factor (S) and the characteristic molecular volumes (B) of the pure component used in the CFT calculations were estimated by using the molar volumes. In equation (9) u_∞ is taken as $1600\,\mathrm{m\,s^{-1}}$.

The standard root mean square deviation for predicting isentropic compressibility using CFT theory has been found to be in the range of 0.3727–1.014 for both the mixtures as given in Table 6. However, Nomoto relation is found to be more suitable in the case of methanol + bromobenzene mixture.

In order to analyse how accurate densities are predicted, consideration was given to the Rackett equation of state and Hankinson method. According to Racket technique [14], the density will be described as:

$$\rho = \left(\frac{MP_\mathrm{c}}{RT_\mathrm{c}}\right) Z_\mathrm{RA}^{-\{1+(1-T_\mathrm{r})^{2/7}\}}, \tag{10}$$

where T_r is the reduced temperature, T_c and P_c are the pseudo critical properties of mixture, M the average molecular weight in mixture and Z_RA the acentric factor dependent parameter.

The Hankinson equation of state [15] for density could be described as

$$\rho = \frac{M}{V^* V_\mathrm{R}^{(\mathrm{o})}\left[1 - \omega_{\mathrm{sR}k} V_\mathrm{R}^{(\delta)}\right]}, \tag{11}$$

where

$$V_\mathrm{R}^{(\mathrm{o})} = 1 + a(1-T_\mathrm{r})^{1/3} + b(1-T_\mathrm{r})^{2/3} + c(1-T_\mathrm{r}) + d(1-T_\mathrm{r})^{4/3} \quad 0.25 < T_\mathrm{r} < 0.95$$

and

$$V_\mathrm{R}^{(\delta)} = \frac{(e + fT_\mathrm{r} + gT_\mathrm{r}^2 + hT_\mathrm{r}^3)}{T_\mathrm{r} - 1.00001} \quad 0.25 < T_\mathrm{r} < 0.95,$$

where

$$a = -1.52816, \quad b = 1.43907, \quad c = -0.81446,$$
$$d = 0.190454, \quad e = -0.296123, \quad f = 0.386914,$$
$$g = -0.04273, \quad h = -0.04806.$$

In order to predict density, critical values required for each compound are given in Table 7. The correlation with these equations showed the suitability of Rackett and Hankinson relation for representing the mixing densities of the two binary mixtures.

5. Conclusion

The negative values of the ΔR_m and $\Delta \kappa_s$ can be interpreted in terms of the intermolecular interaction through hydrogen bonding between unlike molecules. Due to the strong dependence of the adequate industrial design on computation and simulation, an estimation of physical properties were made by different theoretical procedures. The results obtained show the practical application of the simple models used.

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