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Topological investigations of molecular interactions in mixtures containing alkanols: molar excess volumes and molar excess enthalpies

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Abstract

Molar excess volumes, V^E and molar excess enthalpies, H^E of 1,3-dioxolane (D) (i) + propan-1-ol, 1,3-dioxolane (i) + butan-1-ol and 1,3-dioxolane (i) + butan-2-ol (j) binary mixtures have been measured as a function of composition at 308.15 K. The analysis of V^E data by graph, theoretical approach reveals that while propan-1-ol, butan-1-ol exist as associated entities in the pure state; 1,3-dioxolane and butanol exist as monomers in their pure state. These ($i + j$) binary mixtures are characterized by interactions between ethereal oxygen atom of D(i) and hydrogen atom of alkanols. The IR studies lend additional support to the proposed structure of molecular entitles in these mixtures. The energetics of the mixtures have also been studied.

Keywords: Alkanols; Molar excess volumes; Molar excess enthalpies; Molar interaction energy

1. Introduction

One of the general problems of graph theory is, how to relate molecular structure reflected in the molecular graph with measurable physico-chemical and other properties of chemical compounds. One of the current tendencies in chemical and biological investigations is the prediction of physico-chemical and biological properties of chemical compounds and drugs from their structures [1–4]. The concept of connectivity parameters of third degree of the constituents of binary as well as ternary mixtures have been successfully employed to determine molar excess volumes and molar excess enthalpies of binary and ternary mixtures of non-electrolytes [5–8]. In the present study, an attempt has been made to evaluate molar excess volumes and molar excess enthalpies of binary mixtures containing cyclic ether and alkanol by employing connectivity parameters of third degree of the components of binary mixture.

2. Experimental

1,3-Dioxolane (D) (Fluka), propan-1-ol, propan-2-ol, and butan-2-ol (AR Grade) were purified by standard methods [9]. The purities of the compounds were checked by measuring their densities by pycnometer at 298.15 ± 0.01 K and these agreed to within $\pm 5 \times 10^{-5}$ g cm^{-3} with their literature values [9,10]. Molar excess volumes, V^E, for binary mixtures were measured in a V-shaped dilatometer in the manner described elsewhere [11]. The change in liquid level of the dilotometer capillary was measured with a cathetometer that could read to ±0.001 cm. The uncertainty in the measured V^E values is 0.5%.

Molar excess enthalpies, H^E for the studied mixtures were measured as a function of composition at 308.15 in a flow calorimeter (LKB, Sweden) that has been described elsewhere [12]. The uncertainty in the measured H^E values is ±1%.

Samples for IR were prepared by mixing i and j components in 1:1 (w/w) ratio and their IR spectra were recorded on a Beckman spectrophotomer (Model 4200) using sodium chloride optics.

3. Results and discussion

The measured X^E ($X = V$ or H) data for the studied $i + j$ binary mixtures recorded in Tables 1 and 2 at 308.15 K were expressed as

$$X^E\ (X = V \text{ or } H) = x_i x_j \sum_{n=0}^{2} X^{(n)} (2x_i - 1)^n \tag{1}$$

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Table 1
Measured V^E values at 308.15 K for the various $i+j$ mixtures as function of x_i, the mole fraction of component i; also included are various $V^{(n)}$ ($n = 0$–2) parameters along with standard deviation $\sigma(V^E)$

x_i	V^E (cm^3 mol^{-1})	x_i	V^E (cm^3 mol^{-1})
1,3-Dioxolane (i) + propan-1-ol (j)[a]			
0.1260	0.056	0.5202	0.148
0.1802	0.076	0.5706	0.150
0.2506	0.097	0.6280	0.146
0.2908	0.110	0.7620	0.120
0.3246	0.119	0.7926	0.112
0.4504	0.142	0.8503	0.090
0.4802	0.146	0.9501	0.036
1,3-Dioxolane (i) + butan-1-ol (j)[b]			
0.1235	0.150	0.5298	0.285
0.1920	0.205	0.5926	0.273
0.2640	0.240	0.6327	0.261
0.3250	0.272	0.6809	0.242
0.3960	0.288	0.7260	0.220
0.4262	0.292	0.7926	0.180
0.4869	0.293	0.9699	0.034
1,3-Dioxolane (i) + butan-2-ol (j)[c]			
0.1092	0.192	0.5526	0.462
0.1962	0.312	0.6209	0.424
0.2964	0.412	0.6960	0.365
0.3820	0.460	0.7365	0.329
0.4565	0.476	0.7720	0.290
0.4926	0.474	0.8620	0.183
0.5169	0.470	0.9201	0.109

$V^{(n)}$ ($n = 0$–2) and $\sigma(V^E)$ are in cm^3 mol^{-1}.

[a] $V^{(0)} = 0.5841$; $V^{(1)} = 0.3405$; $V^{(2)} = 1.4453$; $\sigma(V^E) = 0.001$.

[b] $V^{(0)} = 1.1494$; $V^{(1)} = -0.1794$; $V^{(2)} = 0.1244$; $\sigma(V^E) = 0.003$.

[c] $V^{(0)} = 1.8790$; $V^{(1)} = -0.3027$; $V^{(2)} = -0.2855$; $\sigma(V^E) = 0.004$.

Table 2
Measured H^E values at 308.15 K for the various $i+j$ mixtures as function of x_i, the mole fraction of component i; also included are various $H^{(n)}$ ($n = 0$–2) parameters along with standard deviation $\sigma(H^E)$

x_i	H^E (J mol^{-1})	x_i	H^E (J mol^{-1})
1,3-Dioxolane (i) + propan-1-ol (j)[a]			
0.0962	662	0.5026	1883
0.1120	753	0.5620	1876
0.1640	1029	0.5960	1856
0.1920	1159	0.6102	1840
0.2660	1450	0.6826	1720
0.2920	1536	0.7260	1604
0.3426	1660	0.8026	1315
0.4590	1856	0.9010	780
1,3-Dioxolane (i) + butan-1-ol (j)[b]			
0.0620	466	0.4826	2044
0.1262	877	0.5320	2052
0.1926	1236	0.5911	2025
0.2107	1321	0.6326	1962
0.2911	1648	0.6990	1820
0.3502	1826	0.7860	1496
0.3901	1910	0.8702	1038
0.4102	1950	0.9106	760
1,3-Dioxolane (i) + butan-2-ol (j)[c]			
0.0922	820	0.4960	2372
0.1026	900	0.5820	2308
0.2162	1630	0.6102	2250
0.3301	2106	0.7603	1738
0.3620	2206	0.8102	1470
0.3760	2230	0.8960	890
0.4106	2306	0.9810	184
0.4620	2360		

$H^{(n)}$ ($n = 0$–2) and $\sigma(H^E)$ are in J mol^{-1}.

[a] $H^{(0)} = 7524.97$; $H^{(1)} = 706.29$; $H^{(2)} = 984.2$; $\sigma(H^E) = 3.7$.

[b] $H^{(0)} = 8200.03$; $H^{(1)} = 824.65$; $H^{(2)} = 618.52$; $\sigma(H^E) = 4.4$.

[c] $H^{(0)} = 9483.8$; $H^{(1)} = -75.84$; $H^{(2)} = 311.27$; $\sigma(H^E) = 4.7$.

where x_i is the mole fraction of component i and $x^{(n)}$ ($n =$ 0–2) are adjustable parameters. These parameters were evaluated by fitting the V^E and H^E data of various mixtures to Eq. (1) by the least square method and are recorded alongwith standard deviation σ ($x^E, x = V$ or H) defined by Eq. (2):

$$\sigma(X)^E = \left[\sum \frac{(X^E_{\text{expt1}} - X^E_{\text{calc. Eq. (1)}})^2}{m-p}\right]^{0.5} \tag{2}$$

where m is number of data points and p is the number of adjustable parameters of Eq. (1) in Tables 1 and 2.

The H^E data for D(i) + butan-1-ol, D(i) + butan-2-ol (j), mixtures at 298.15 and 313.15 K have been reported in the literature [13]. Our H^E values lie within the values reported at 298.15 and 308.15 K and the general shape of the curves are same. For D(i) + butan-2-ol (j) mixture our H^E values $x_1 = 0.5$ are 66 J mol^{-1} higher than values at 298.15 K reported in literature [14]. Our V^E values at $x_1 = 0.5$ for D(i) + butan-1-ol are 0.05 cm^3 mol^{-1} higher than values at 298.15 K reported in literature [14]. There are no literature values of V^E for other mixtures with which to compare our results.

V^E and H^E data, for the studied $i + j$ mixtures, are positive over the whole composition range and for an equimolar composition vary in the order: butan-2-ol > butan-1-ol > propan-1-ol.

The observed H^E data for these mixtures can be explained qualitatively, if it be assumed that (i) alkanols exist as associated molecular entities; (ii) there is interaction between ethereal oxygen atoms of D(i) and hydrogen atom of alkanols; (iii) interaction between alkanol and ether molecules then leads to depolymerization of alkanols; (iv) monomers of D(i) and alkanols (j) then undergoes interaction to form i:j molecular entity; and (v) there is steric repulsion between D(i) and butan-2-ol (j) due to the presence of bulky –CH$_3$ group. H^E data for D(i) + propan-1-ol suggests that contributions due to factors (iii) far outweigh the contribution due to factors (ii) and (iv), so that overall H^E for this mixture are positive. Higher values for D(i) + butan-1-ol and butan-2-ol mixture than D(i) + propan-1-ol may be due to the presence of long carbon chain which leads to decrease in alkanol–alkanol interaction and bulky –CH$_3$ group which restrict the approach of D(i) to form i:j molecular complex. Consequently, H^E values for D(i) + butan-1-ol and butan-2-ol (j) mixtures should be more positive than that for D(i) + propan-1-ol mixture. This is indeed true.

4. Graph theory and results

Molar excess volumes, V^{E} is a packing effect and molar excess enthalpies, H^{E} are due to the replacement of *i*–*i* and *j*–*j* contacts in pure state by *i*–*j* contacts in mixture state. The replacement of *i*–*i* and *j*–*j* contacts by *i*–*j* may then lead to change in topology of *i*/*j* components of $i + j$ mixtures. According to mathematical discipline of graph theory, if the atoms in a structural formula of a molecule are represented by letters and bonds joining them by lines then the resulting graph describes the total information contained in that molecule [15–17]. Consequently, if δ^{v}_{m}, δ^{v}_{n}, etc. represent the degree of *m* and *n*, etc. vertices of the graph of a molecule, then connectivity parameter of third degree, ${}^{3}\xi$ is defined [18] by

$$
{}^{3}\xi = \sum_{m<n<o<p} (\delta^{\mathrm{v}}_{m}\delta^{\mathrm{v}}_{n}\delta^{\mathrm{v}}_{o}\delta^{\mathrm{v}}_{p})^{-0.5} \tag{3}
$$

where δ^{v}_{m}, etc. values explicitly reflect the valency of the atoms forming the bond and is expressed [18] as $\delta^{\mathrm{v}} = Z_{\mathrm{m}} - h$, where Z_{m} is the maximum valency of atom and *h* is the number of hydrogen atoms attached to it. Consequently, for carbon in $\mathrm{CH_3}$ $\delta^{\mathrm{v}}_{(\mathrm{C})} = 4 - 3 = 1$ and for carbon in $\mathrm{CH_2}$ $\delta^{\mathrm{v}}_{(\mathrm{C})} = 4 - 2 = 2$.

The addition of *i* to *j* causes structural changes in the topology of *i* or *j* in $i + j$ mixture, so it would be of interest to analyze V^{E} and H^{E} data of the studied mixtures in terms of graph theoretical approach that takes into consideration the connectivity of parameters of third degree of the constituents of mixture (which describes the topology of molecule). According to this theory, V^{E} is given by [5,19]

$$
V^{\mathrm{E}} = \alpha_{ij} \left[\sum x_i ({}^{3}\xi_i)^{-1}_{\mathrm{m}} - \sum x_i ({}^{3}\xi_i)^{-1} \right] \tag{4}
$$

where x_i is the mole fraction of component *i* and ${}^{3}\xi_i$ and $({}^{3}\xi_i)_{\mathrm{m}}$, etc. ($i = i$ or *j*) represent ${}^{3}\xi_i$ values of *i* in pure and mixture state and α_{ij} is a constant characteristic of $i + j$ mixture.

As the degree of association of *i* and *j* is not known with certainty, ${}^{3}\xi_i$ ($i = i$ or *j*), etc. parameters were regarded as adjustable parameters. These parameters were determined by fitting V^{E} data to Eq. (4) and only those ${}^{3}\xi_i$ and $({}^{3}\xi_i)_{\mathrm{m}}$ ($i = i$ or *j*) were retained that best reproduced the experimental V^{E} values. These parameters calculated via Eq. (4) alongwith V^{E} are recorded in Table 3 and V^{E} values are also compared with their corresponding experimental values. Examination of Table 3, reveals that V^{E} values compare reasonably well with their corresponding values and thus ${}^{3}\xi_i$ and $({}^{3}\xi_i)_{\mathrm{m}}$ ($i = i$ or *j*) values can be relied upon to extract information about the state of components in pure as well in mixture state.

A number of structures were assumed for propan-1-ol, butan-1-ol, and butan-2-ol (Scheme 1) and their ${}^{3}\xi'$ values were calculated from their structural considerations. Only those structure or combination of structures that yielded ${}^{3}\xi'$ (determined via Eq. (3)) values which compare well with ${}^{3}\xi$ values (evaluated from Eq. (4)) were taken be good representative structures of that components. For this purpose, it was assumed that propan-1-ol, butan-1-ol, and butan-2-ol exist as molecular entities I–II, III–IV, and V–VI, respectively. ${}^{3}\xi'$ values for these molecular entities were then calculated to be 0.447, 1.526, 0.721, 2.063, 1.031, and 2.194, respectively. ${}^{3}\xi_1$ values of 0.702, 0.901, 0.952 for propan-1-ol, butan-1-ol, and butan-2-ol (Table 3) suggest that while propan-1-ol and butan-1-ol exist as mixture of monomer and dimer; butan-2-ol exist as monomer (${}^{3}\xi' = 1.013$). Further ${}^{3}\xi$ values of 0.541, 0.650, 0.601 (Table 3) suggest that D(*i*) exist as monomer molecular entity VII (${}^{3}\xi' = 0.534$).

Table 3

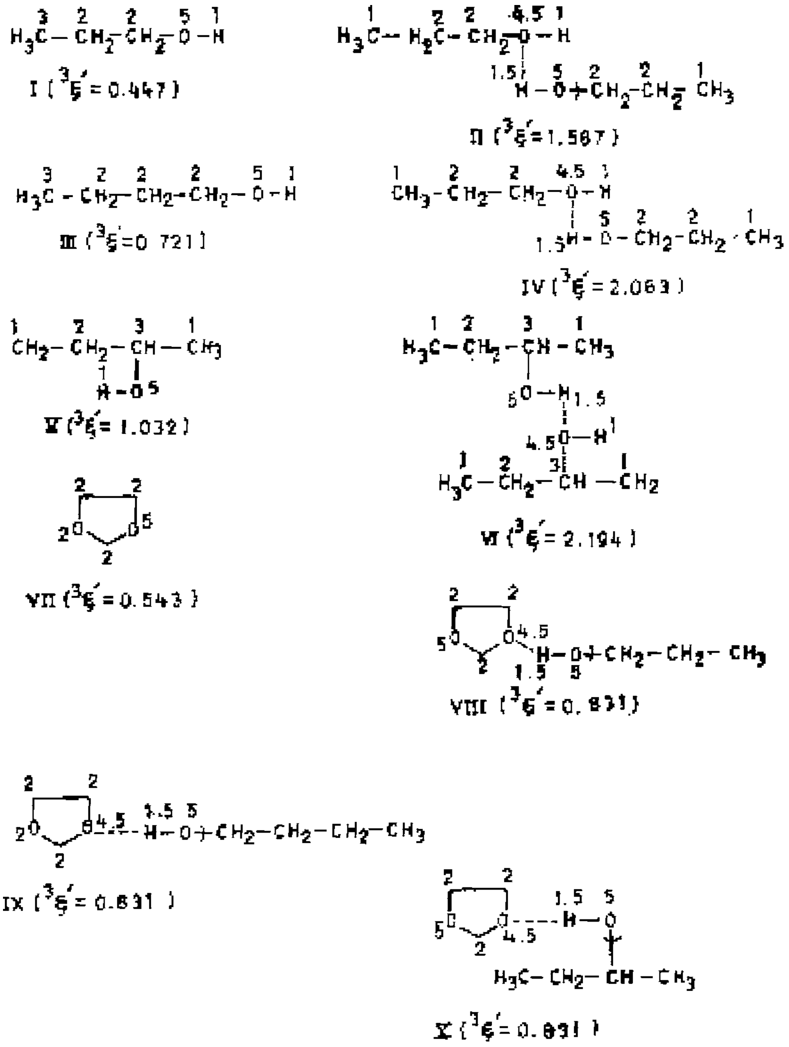
Comparison of V^{E} and H^{E} values calculated from appropriate equation with the corresponding experimental values at 308.15 K for the various $i + j$ mixtures as a function of x_i, mole fraction of *i*; also included are the various interaction energies χ_{ii}, χ_{jj}, etc. parameter

	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
1,3-Dioxolane (*i*) + propan-1-ol (*j*)[a]									
V^{E} (experimental)	0.044	0.082	0.112	0.133	–	0.145	0.135	0.109	10.064
V^{E} (graph)	0.047	0.086	0.117	0.137	–	0.147	0.133	0.105	0.061
H^{E} (experimental)	683	1192	1553	–	–	1849	1672	1328	784
H^{E} (graph)	617	1135	1536	–	–	1894	1693	1356	753
1,3-Dioxolane (*i*) + butan-1-ol (*j*)[b]									
V^{E} (experimental)	0.123	0.210	0.260	0.285	–	0.268	0.230	0.173	0.099
V^{E} (graph)	0.091	0.167	0.227	0.268	–	0.285	0.258	0.204	0.119
H^{E} (experimental)	714	1268	1673	–	–	2013	1812	1426	833
H^{E} (graph)	704	1008	1684	–	–	1946	1752	1346	763
1,3-Dioxolane (*i*) + butan-2-ol (*j*)[c]									
V^{E} (experimental)	0.174	0.313	0.410	0.462	–	0.433	0.359	0.255	0.130
V^{E} (graph)	0.143	0.265	0.361	0.431	–	0.472	0.434	0.347	0.206
H^{E} (experimental)	876	1542	2008	–	–	2275	1995	1528	866
H^{E} (graph)	876	1567	2067	–	–	2392	2100	1606	906

[a] ${}^{3}\xi_i = {}^{3}\xi_j = 0.541$; ${}^{3}\xi_j = {}^{3}\xi_j = 0.701$; $\alpha_{ij} = -3.1071\,\mathrm{cm^3\,mol^{-1}}$; $\xi'_{ij} = 645.9\,\mathrm{J\,mol^{-1}}$; $\xi'_{jj} = 5954.6\,\mathrm{J\,mol^{-1}}$.

[b] ${}^{3}\xi_j = ({}^{3}\xi_j)_{\mathrm{m}} = 0.650$; ${}^{3}\xi_j = ({}^{3}\xi_j)_{\mathrm{m}} = 0.901$; $\alpha_{ij} = -8.3485\,\mathrm{cm^3\,mol^{-1}}$; $\chi'_{ij} = 1794.4\,\mathrm{J\,mol^{-1}}$; $\chi'_{jj} = 5913.7\,\mathrm{J\,mol^{-1}}$.

[c] ${}^{3}\xi_j = ({}^{3}\xi_j)_{\mathrm{m}} = 0.601$; ${}^{3}\xi_j = ({}^{3}\xi_j)_{\mathrm{m}} = 0.952$; $\alpha_{ij} = -6.7677\,\mathrm{cm^3\,mol^{-1}}$; $\chi_{ij} = 15977.9\,\mathrm{J\,mol^{-1}}$; $\chi_{12} = -6307.8\,\mathrm{J\,mol^{-1}}$.



Scheme 1. Connectivity parameter for various molecular entaties.

$(^3\xi'_j)_m$ values were then calculated and utilized to understand the state in which propan-1-ol, butan-1-ol, and butan-2-ol exist in D(*i*). For this purpose, we assumed that D(*i*) exists in alkanols (*j*) as molecular entities VIII–X and $(^3\xi'_j)_m$ value calculated for these molecular entities was 0.831. In evaluating $(^3\xi'_j)_m$ values, it was assumed that these molecular entities are characterized by interactions between hydrogen atom of alkanols and oxygen atom of D(*i*). The $(^3\xi'_j)_m$ values of 0.701, 0.901, 0.952 for Table 3 suggest that D(*i*) + alkanol (*j*) mixtures are characterized by the presence of molecular entities VIII–X.

The postulation of the existence of molecular entities VIII–X in D(*i*) + propan-1-ol, D(*i*) + butan-1-ol and D(*i*) + butan-2-ol mixtures then suggest that there must be changes in O–H stretching vibrations of alkanols and cyclic ether oxygen vibration in D(*i*). In view of this, we analyzed the IR spectral data of pure D(*i*), propan-1-ol, and their equimolar mixture. It was observed that D(*i*) and propan-1-ol in pure state show characteristic absorption (C–O stretching vibrations and O–H stretching band [20]) at 1145 and 3370 cm^{-1}, respectively. The IR spectra of equimolar mixture of D(*i*) + propan-1-ol show characteristics vibrations at 1162 and 3385 cm^{-1}, respectively. Further, it has been observed, there is widening of various bands in D(*i*) + propan-1-ol (*j*) mixture as compared to their bands in pure state, which suggest interactions between the components of the mixture [20]. The IR spectra, thus clearly indicate that addition of *j* and *i* does influence the O–H vibrations of propan-1-ol and also the cyclic ether (C–O) vibrations in D(*i*). The IR studies, thus lend additional support to the presence of molecular entities VIII–X in these mixtures.

In order to understand the energetic of molecular interactions operating between the components of these mixtures, we assumed that if propan-1-ol and butan-1-ol exist as associated molecular entity then D(*i*) + propan-1-ol and D(*i*) + butan-1-ol (*j*) mixtures formation involves (a) the establishment of unlike contact between D(*i*) and propan-1-ol or butan-1-ol (*j*); (b) the establishment of unlike contact formation then leads to depolymerization of *j* to give their monomers; (c) the monomers of D(i) then undergo specific interactions with monomers of propan-1-ol or butan-1-ol (j) to give i:j molecular complex. If χ_{ij}, χ_{jj}, and χ_{12} are molar interaction energies for i–j, j–j contacts and specific interactions, then enthalpy changes for processes (a)–(c) are given [21–23] by

$$\Delta H_1 = \frac{x_i x_j \chi_{ij} V_j}{\sum x_i V_i} \tag{5}$$

$$\Delta H_2 = \frac{x_i^2 x_j \chi_{jj} V_j}{\sum x_i V_i} \tag{6}$$

$$\Delta H_3 = \frac{x_i x_j^2 \chi_{12} V_j}{\sum x_i V_i} \tag{7}$$

where x_i, V_j are mole fraction and molar volume of the ith and jth components, respectively.

The net enthalpy change accompanying $i + j$ mixture formation can then be expressed by

$$\Delta H = \sum_{i=1}^{3} \Delta H_1 = \left[\frac{x_i x_j V_j}{\sum x_i V_i}\right] [\chi_{ij} + x_i \chi_{jj} + x_j \chi_{12}] \tag{8}$$

Since V_j/V_i has been taken [5] equal to $^3\xi_i/^3\xi_j$, then Eq. (8) reduces to

$$H^{\mathrm{E}} = \frac{x_i x_j \left(^3\xi_i/^3\xi_j\right)}{x_i + x_j \left(^3\xi_i/^3\xi_j\right)} [\chi_{ij} + x_i \chi_{jj} + x_j \chi_{12}] \tag{9}$$

For the studied mixture, if it be assumed that $\chi_{ij} \approx \chi_{jj} \approx \chi'_{ij}$ then Eq. (9) is expressed as

$$H^{\mathrm{E}} = \frac{x_i x_j \left(^3\xi_i/^3\xi_j\right)}{x_i + x_j \left(^3\xi_i/^3\xi_j\right)} [(1 + x_i)\chi'_{ij} + x_j \chi_{12}] \tag{10}$$

D(i) + butan-2-ol mixture formation would involves only processes (a) and (c), i.e. $\chi_{jj} = 0$, and so that Eq. (10) for this mixture reduces to

$$H^{\mathrm{E}} = \frac{x_i x_j \left(^3\xi_i/^3\xi_j\right)}{x_i + x_j \left(^3\xi_i/^3\xi_j\right)} [\chi'_{ij} + x_j \chi_{12}] \tag{11}$$

Eqs. (10) and (11) contain two unknown parameters χ'_{ij} and χ_{12}, etc. and for the present study, we evaluated these parameters, by employing H^{E} data at two arbitrary compositions ($x_i = 0.4$ and 0.5). The calculated parameters were then subsequently employed to evaluate H^{E} data for the respective $i + j$ mixtures as functions of x_i. Such H^{E} values (along with χ'_{ij} and χ_{12} parameter) are recorded in Table 3 and are also compared with their corresponding experimental values. Examination of Table 3 reveals that H^{E} values compare reasonably well with the corresponding experimental values. This lends additional support to the assumptions made in deriving Eqs. (10) and (11) and also to the validity of assumption $V_j/V_i =^3 \xi_i/^3\xi_j$.

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