Academic Sciences

International Journal of Chemistry Research

ISSN- 0976-5689 Vol 3, Issue 1, 2012

Research Article

TOPOLOGICAL INVESTIGATION OF SOME ALKANOL + WATER BINARY MIXTURES: MOLAR EXCESS VOLUME AT 298.15 AND 308.15 K.

DAYA NAND, VIJAY SINGH YADAV

Department of Chemistry, M.I.T.R.C. Engg. College, Alwar 301001, Department of Chemistry, Raj Rishi Govt. (P.G) College, Alwar 301001

Received: 7 Oct 2011, Revised and Accepted: 11 Nov 2011

ABSTRACT

The excess molar volume V^E { x(CH_3OH or CH_3CH_2OH or $CH_3CH_2CH_2OH$ or $CH_3CH(OH)CH_3$ or $CH_3CH_2CH_2CH_2OH$ or $CH_3CH(OH)CH_2CH_3$ + water } have been calculated from measured values of density over the whole composition range at the temperature 298.15K and 308.15k in order to investigate OH….O specific interactions. The results are explained in term of the strong self association of the alkanols, the specific interaction between the alkanol and water and packing effects up on mixing. The experimental V^E results presented here has been analyzed in term of the Graph theory which in turn deals with topology of the constituents of mixtures. It has been observed that V^E values predicted by the graph theory compare well with their corresponding experimental values.

Keywords: Alkanols (Methanol, Ethanol, Propan-1-ol, Propan-2ol, Butan-1-ol, Butan-2-ol), Excess molar volume, Binary mixture, Hydrogen bond.

INTRODUCTION

Industry demand reliable and accessible reference data on the thermodynamic properties (excess molar volumes) of wide variety of liquid mixtures. These properties not only provide reliable data and empirical rules for science and technology, but also enhance the understanding of the behavior of liquid mixtures. We have determined the V^E for {x (CH_3OH or CH_3CH_2OH or $CH_3CH_2CH_2$-OH or CH_3CH (OH)-CH_3 or CH_3CH_2-CH_2-CH_2-OH or CH_3-CH (OH)-CH_2-CH_3+ Water} Alcohols are known to be self associated through hydrogen bonded linear chains to variable degrees of polymerization [1-5]. The degree and strength of polymerization decrease with increasing hydrocarbon chain length and also with position of the hydroxyl group in the molecule. Binary solution of alkanols with non-polar solvents generally breaks the three-dimensional hydrogen-bonded network of pure alkanols and gives positive excess molar volumes in mixtures [6], Treszczanowicz and Benson [7] determined the V^E at 298.15 K for (methanol or ethanol or n- propanol and heptanol) and found that the excess volume is positive over the whole mole fraction range. similar results were observed by Zielkiewicz [8] for mixtures of (propane-2-ol and heptanes) at 333.15 K.These results were attributed to the dissociation of the hydrogen bonds in the alcohol molecule.Treszczanowicz [9] has reported positive excess molar volumes for mixtures of (methyl butyl ether or di-iso propyl and heptane) at 298.15 K with V^E 0.5=0.239 cm^3 mol^{-1} for the (di-iso propyl ether and heptanes) system. Arm and Bankay[1] have reported volume changes up on mixing for (methanol+ diethyl ether) which are negative over the whole composition range with V^E (0.5) =0.80cm^3 mol^{-1}.They have discussed the results in terms of the dominance of the association between the component molecules. The V^E results for the mixtures (methanol or ethanol or 2-propanol + IPE or MTBE) [10-12] have been reported in the literature. As far as we know the V^E results for the other mixtures discussed hare have not been reported.

MATERIALS AND METHODS

Methanol, Ethanol,Propan-1-ol,Propan-2-ol,Butan-1-ol,Butan-2-ol (AR Grade) were purified by standard methods [13].The purities of the compound were checked by measuring their densities by pycnometer at 298.15 ±0.01k and these agreed to within ± $5x10^{-5}$ gcm-3 with their literature values [13,14]. Molar excess volumes,V^E for binary mixtures were measured in a V-shaped dilatometer in the manner described elsewhere[15]. The change in liquid level of the dilatometer capillary was measured with a cathetometer that could read to ± 0.001 cm. The uncertainly in the measured V^E values is 0.5%.

RESULTS AND DISCUSSION

The measured X^E (X=V) data for the studied i+j binary mixtures recorded in table 1 at 298.15 and 308.15 K were expressed as.

$$X^E (X = V) = x_i x_j [X^{(0)} + X^{(1)}(2x_i\text{-}1) + X^{(2)} (2x_i\text{-}1)^2] \quad (1)$$

Table 1: Measured molar excess volumes, V^E values for the various (i+j) binary mixtures as function of x_i, the mole fraction of component (i) at298.15 K and 308.15 K.

x_i V^E (cm^3mol^{-1}	x_i V^E (cm^3 mol^{-1})			x_i V^E(cm^3mol^{-1}	x_i V^E(cm^3 mol^{-1})		
Water (i) + Methanol (j) T= 298.15 K				Water (i) + Methanol (j) T= 308.15 K			
0.1092	-0.192	0.5526	-0.462	0.1102	-0.094	0.5221	-0.275
0.1962	-0.312	0.6209	-0.424	0.1920	-0.154	0.5820	-0.273
0.2964	-0.412	0.6965	-0.365	0.2302	-0.178	0.6421	-0.262
0.3820	-0.460	0.7365	-0.329	0.2806	-0.205	0.6902	-0.249
0.4565	-0.476	0.7720	-0.290	0.3323	-0.230	0.7129	-0.240
0.4926	-0.474	0.8624	-0.183	0.3612	-0.240	0.7616	-0.215
0.5169	-0.470	0.9201	-0.109	0.4102	-0.257	0.8820	-0.128
				0.4426	-0.265	0.9126	-0.099
Water (i) + Ethanol (j) T= 298.15 K				Water (i) + Ethanol (j) T= 308.15 K			
0.1117	-0.176	0.4680	-0.362	0.0901	-0.098	0.5601	-0.266
0.1669	-0.247	0.5294	-0.351	0.1695	-0.158	0.6801	-0.255
0.1901	-0.273	0.6171	-0.315	0.2601	-0.204	0.7220	-0.245
0.2447	-0.322	0.7112	-0.256	0.2857	-0.214	0.7802	-0.222
0.2713	-0.337	0.7814	-0.208	0.3890	-0.245	0.8106	-0.205
0.3315	-0.356	0.8299	-0.168	0.4010	-0.248	0.8920	-0.142
0.3917	-0.361	0.9713	-0.035	0.4601	-0.258	0.9201	-0.112

0.4120	-0.363	0.9820	-0.021	0.4811	-0.260	0.9621	-0.059
Water (i) + Propan-1-ol (j) T= 298.15 K				Water (i) + Propan-1-ol (j) T= 308.15 K			
0.1235	-0.150	0.5298	-0.285	0.1559	-0.115	0.6510	-0.216
0.1927	-0.208	0.5926	-0.273	0.1926	-0.140	0.6802	-0.206
0.2644	-0.252	0.6327	-0.261	0.2996	-0.200	0.7020	-0.197
0.3251	-0.272	0.6809	-0.242	0.3202	-0.206	0.7328	-0.184
0.3965	-0.288	0.7260	-0.220	0.4005	-0.228	0.7910	-0.154
0.4262	-0.292	0.7926	-0.180	0.5010	-0.238	0.8102	-0.142
0.4869	-0.293	0.9699	-0.034	0.5912	-0.232	0.8620	-0.109
				0.6106	-0.227	0.9001	-0.082
Water (i) + Propan-2-ol (j) T= 298.15 K				Water (i) + Propan-2-ol (j) T= 308.15 K			
0.1019	-0.035	0.4735	-0.117	0.0971	-0.042	0.3910	-0.102
0.1395	-0.047	0.5334	-0.120	0.1120	-0.047	0.4321	-0.104
0.1721	-0.057	0.5615	-0.119	0.1723	-0.065	0.4713	-0.105
0.2303	-0.073	0.5910	-0.118	0.2103	-0.075	0.5315	-0.106
0.2915	-0.088	0.6916	-0.108	0.2557	-0.084	0.5880	-0.103
0.3150	-0.093	0.7365	-0.100	0.2923	-0.091	0.6313	-0.100
0.3616	-0.102	0.7990	-0.084	0.3247	-0.096	0.7515	-0.082
0.4139	-0.110	0.8916	-0.052	0.3715	-0.101	0.8735	-0.052
Water (i) + Butan-1-ol (j) T= 298.15 K				Water (i) + Butan-1-ol (j) T= 308.15 K			
0.1260	-0.056	0.5202	-0.148	0.0500	-0.030	0.4502	-0.143
0.1802	-0.076	0.5706	-0.150	0.1010	-0.054	0.4721	-0.144
0.2506	-0.099	0.6280	-0.146	0.1802	-0.086	0.5010	-0.145
0.2908	-0.110	0.7020	-0.136	0.2201	-0.100	0.6301	-0.138
0.3246	-0.119	0.7926	-0.112	0.2501	-0.109	0.7010	-0.128
0.4504	-0.142	0.8503	-0.090	0.2802	-0.118	0.7520	-0.115
0.4802	-0.146	0.9501	-0.036	0.3201	-0.126	0.8210	-0.089
				0.4201	-0.141	0.9510	-0.030
Water (i) + Butan-2-ol (j) T= 298.15 K				Water (i) + Butan-2-ol (j) T= 308.15 K			
0.1210	-0.029	0.4525	-0.085	0.0991	-0.030	0.4459	-0.070
0.1517	-0.035	0.4815	-0.087	0.1192	-0.032	0.4710	-0.071
0.1913	-0.044	0.5419	-0.088	0.1339	-0.036	0.5315	-0.072
0.2317	-0.053	0.6712	-0.080	0.1791	-0.044	0.6295	-0.069
0.2901	-0.065	0.6985	-0.076	0.1989	-0.047	0.7313	-0.060
0.3310	-0.072	0.7619	-0.065	0.2185	-0.050	0.8215	-0.047
0.3715	-0.078	0.8250	-0.052	0.2595	-0.057	0.8516	-0.042
0.3995	-0.081	0.9101	-0.031	0.3199	-0.062	0.9095	-0.028

Table II: Values of parameters V^n (n= 0 – 2) along with standard deviation, σ (V^E) of the molar excess volumes ,V^E for the various (i+j) binary mixtures at 298.15 K and 308.15 k

Mixture	Temperature	$V^{(0)}$	$V^{(1)}$	$V^{(2)}$	σ $V^{(E)}$
				$cm^3\ mol^{-1}$	
Water (i) +Methanol (j)	298.15 K	-1. 879	-0. 303	-0. 286	0.004
	308.15 K	-1.084	-0. 174	-0. 023	0.003
Water (i) +Ethanol (j)	298.15 K	-1. 417	-0. 568	-0. 086	0.003
	308.15 K	-1. 043	-0. 186	-0. 418	0.002
Water (i) +Propan-1-ol (j)	298.15 K	-1.149	-0. 179	-0. 124	0.003
	308.15 K	-0.961	-0.0 45	-0.041	0.002
Water (i) +Propan-2-ol (j)	29815 K	-0.469	-0.103	-0.031	0.001
	308.15 K	-0.418	-0.010	-0.094	0.001
Water (i) +Butan-1-ol (j)	298.15 K	-0. 584	-0. 341	-1.445	0.001
	308.15 K	-0. 686	-0. 217	-0.033	0.002
Water (i) +Butan-2-ol (j)	298.15 K	-0. 427	-0.055	-0.031	0.001
	308.15 K	-0. 281	-0.022	-0.050	0.001

Where x_i is the mole fraction of component i and x(n) (n=0-2) are adjustable parameters were evaluated by fitting the V^E data of various mixture to Eq.(1) by the least square method and are recorded along with standard deviation σ(X^E ,X=V) defined by Eq.(2):

$$\sigma(X^E), = [\Sigma(X^E_{exptl} - X^E_{calc.eq.\ (1)})^2/(m-p)]^{0.5} \qquad (2)$$

Where m is number of data points and p-is the number of adjustable parameters of equation (1) in table 1 our V^E values at Xi= 0.5 for water + butan-1-ol are 0.05 $cm^3\ mol^{-1}$ higher than value at 298.15 k reported in literature [16] .There are no literature values of V^E for other mixtures with which to compare our results.

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

Graph theory and results

Molar excess volumes, V^E are a packing effect 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 [17-19].Consequently, if δ^v_l , δ^v_m 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 [20] by

$$^{3}\xi = \sum_{1<m<n<o} (\delta_1^{v}\delta_m^{v}\delta_n^{v}\delta_o^{v})^{-0.5} \quad (3)$$

Where δ^{v}_{1} , etc. values explicitly reflect the valency of the atoms forming the bond and is expressed(20) as $\delta^{v} = Z_m - h$, where Z_m is the maximum valency of atom and h is the number of hydrogen atoms attached to it. Consequently, for carbon in CH_3 (δ^{v}_{c}= 4-3=1 and for carbon in CH_2 (δ^{v}_{c}= 4-2=2). The addition of i and 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 data of the studied mixtures in terms of graph theoretical approach that takes in to 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 [21, 22].

$$V^E = a_{ij}\left[\sum\left\{x_i\left(^{3}\xi_i\right)_m^{-1}\right\} - \Sigma x_i\left(^{3}\xi_i\right)^{-1}\right] \quad (4)$$

Where x_i is the mole fraction of component i and $^{3}\xi_i$ and $(^{3}\xi_i)_m$ .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.

Table lll: Comparison of V^E values calculated with their corresponding experimental values along with various $(^{3}\xi_i)$,$(^{3}\xi_i)_m$ (i=i or j) ,α_{ij} parameters for the various (i+j) binary mixtures as functions of X_i the mole fraction of component (i) at 298.15 K and 308.15 K.

Property	Mole Fraction (X_i)								
	0.1	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**0.9**
Water (i) + Methanol (j) T=298.15 K									
V^E_{Exptl}	-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
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.601, $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.952, α_{ij}= 9.767									
Water (i) + Methanol (j) T=308.15 K									
V^E_{Exptl}	-0.083	-0.155	-0.212	-0.251	-	-0.268	-0.242	-0.190	-0.108
V^E_{Graph}	-0.090	-0.163	-0.216	-0.252	-	-0.265	-0.236	-0.183	-0.105
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.601 , $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.952 , α_{ij}= 24.423									
Water (i) + Ethanol (j) T=298.15 K									
V^E_{Exptl}	-0.94	-0.163	-0.197	-0.225	-	-0.243	-0.218	-0.198	-0.120
V^E_{Graph}	-0.076	-0.138	-0.190	-0.224	-	-0.232	-0.204	-0.252	-0.81
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.750, $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.902 , α_{ij}= 3.008									
Water (i) + Ethanol (j) T=308.15 K									
V^E_{Exptl}	-0.104	-0.173	-0.217	-0.245	-	-0.263	-0.248	-0.208	-0.130
V^E_{Graph}	-0.086	-0.158	-0.210	-0.244	-	-0.252	-0.224	-0.272	-0.101
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.750, $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.902 , α_{ij}= 5.608									
Water (i) + Propan-1-ol (j) T=298.15K									
V^E_{Exptl}	-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
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.650 , $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.901, α_{ij}= 8.348									
Water (i) + Propan-1-ol (j) T=308.15 K									
V^E_{Exptl}	-0.087	-0.155	-0.204	-0.232	-	-0.227	-0.196	-0.147	-0.080
V^E_{Graph}	-0.050	-0.147	-0.198	-0.234	-	-0.224	-0.177	-0.177	-0.103
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.650, $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.901 , α_{ij}= 9.304									
Water (i) + Butan-1-ol (j) T=298.15K									
V^E_{Exptl}	-0.044	-0.082	-0.112	-0.133	-	-0.145	-0.135	-0.109	-0.064
V^E_{Graph}	-0.047	-0.86	-0.117	-0.137	-	-0.147	-0.133	-0.105	-0.061
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.541 , $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.701 , α_{ij}= 3.107									
Water (i) + Butan-1-ol (j) T=308.15K									
V^E_{Exptl}	-0.051	-0.091	-0.119	-0.136	-	-0.138	-0.122	-0.094	-0.054
V^E_{Graph}	-0.054	-0.099	-0.126	-0.141	-	-0.138	-0.121	-0.089	-0.052
$(^{3}\xi_i) = (^{3}\xi_i)_m$ = 0.541, $(^{3}\xi_j) = (^{3}\xi_j)_m$= 0.701 , α_{ij} = 4.667									

α_{ij} are in cm^3mol^{-1}

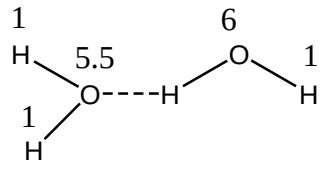
As the degree of association of i and j is not know with certainty, $(^{3}\xi_i)$ (i=i or j), etc. parameters were regarded as adjustable parameters. These parameters were determined by fitting V^E data to Eq. (4) and only those $^{3}\xi_i$ and $(^{3}\xi_i)_m$ (i=i or j) were retained that best reproduced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

A number of structures were assumed for components in pure and mixture state and their $^{3}\xi'$ values were calculated from their structural considerations via Eq. (3). Only those structure or combination of structures that yielded $^{3}\xi'$ [calculated via Eq. (3)]

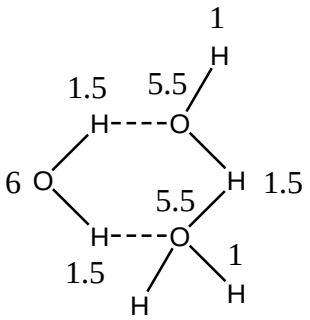
which compare well with ${}^3\xi$ values (determined from eqn. (4) were taken to be good representative structures of that component. for W(i) + methanol or ethanol or propan-1-ol or butan1-ol (j) binary mixtures, its was assumed that W, methanol, ethanol, propan-1-ol, butan-1-ol exist as molecular entities I-II, III-IV, V-VI, VII-VIII and IX-X (Scheme-1) respectively. ${}^3\xi'$ values for these molecular entities were then calculated to be 0.426, 1.379, 0.447, 1.587, 0.663, 1.326, 0.721, 2.063, 1.032 and 2.194 respectively. ${}^3\xi$ values of 0.952, 0.902, 0.901 and 0.701 (Table lll) of methanol, ethanol, propan-1-ol and butan-1-ol suggest that methanol, ethanol and propan-1-ol exist as a mixture of monomer and dimer $({}^3\xi' = 1.032, 0.908, 0.877)$; butan-1-ol exist as monomer (${}^3\xi'$ =1.010) Further, ${}^3\xi$ values of 0.601, 0.750, 0.650 and 0.541 for W(i) in these mixtures suggest that W(i) exist as molecular entities XI-XIV. $({}^3\xi')_m$ values were evaluated (via Eq. 3) to understand the state in which various alkanols exist in W(i). It was assumed that studied (i + j) mixture may contain molecular entities XI-XIV (Scheme-I) respectively and characterized by interaction between hydrogen/oxygen atom of W(i) and oxygen / Hydrogen atom of alcoholic group of alkanols. In calculating $({}^3\xi'_j)_m$ values for these molecular entities, it was assumed further that only O-H edge of alkanol is involved in hydrogen bond interaction with oxygen atom of W (i). The $({}^3\xi')_m$ values for molecular entities XI-XIV were then calculated to be 1.159; $({}^3\xi'_j)_m$ values of 0.952, 0.902, 0.901 and 0.701 (Table-lll) suggest the presence of molecular entities XI-XIV in the studied mixtures.

CONCLUSIONS

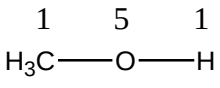
Molar excess volumes of Methanol,Ethanol,Propan-1-ol,Propan-2-ol,Butan-1-ol,Butan-2-ol (A) with Water(B) measured with V-shaped dilatometer at 298.15 K. data were interpreted in terms of specific interactions of electron donor-acceptor type between oxygen/hydrogen atom of water and hydrogen/oxygen atom of alkanols.



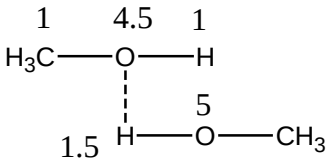
(I) ${}^3\xi' = 0.426$



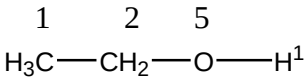
(II) ${}^3\xi' = 1.379$



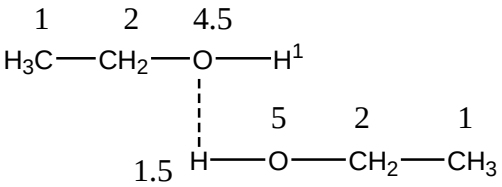
(III) ${}^3\xi' = 0.447$



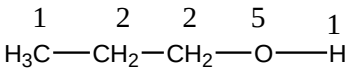
(IV) ${}^3\xi' = 1.587$



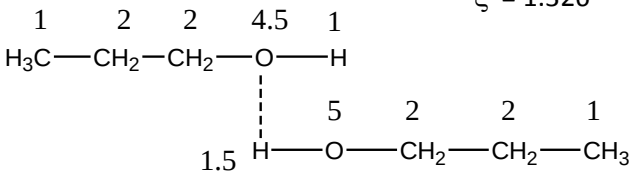
(V) ${}^3\xi' = 0.633$



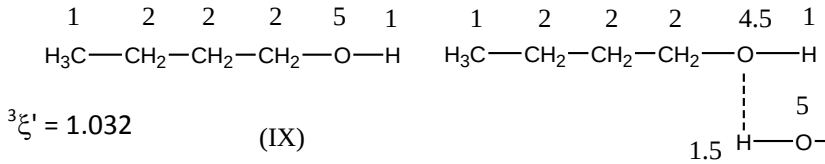
(VI) ${}^3\xi' = 1.326$



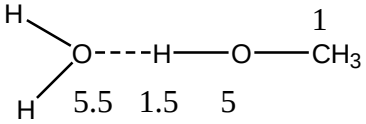
(VII) ${}^3\xi' = 0.721$



(VIII) ${}^3\xi' = 2.063$

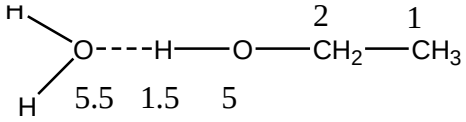


$^3\xi'$ = 1.032 (IX) (X) $^3\xi'$ = 2.194



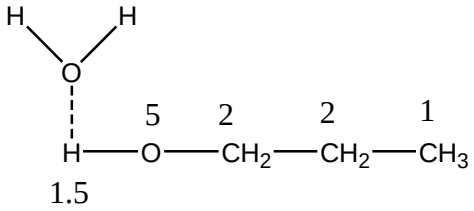
XI

$^3\xi'$ = 1.159



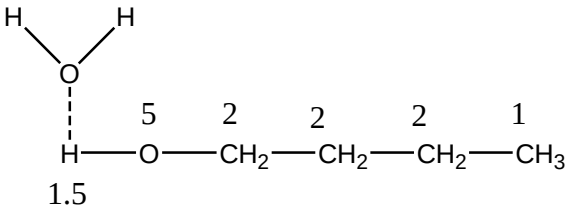
XII

$^3\xi'$ = 1.159



XIII

$^3\xi'$ = 1.159



XIV

$^3\xi'$ = 1.159

Scheme I: Connectivity parameters of various molecular entities I -XIV

REFERENCES

1. H. Arm, F.Bankay, Helv. Chim. Acta 51 (1968) 1243.
2. J.S. Rowlinson, Liquids and Liquid mixtures, Second edn. Butter worth, London 1969.
3. A.J. Treszczanowicz, B.C.Y. Lu, Bull. Acad. Pol. Sci. 29 (5-6) (1981) 285.
4. G.N. Swani, G.K.Ravan, Can. J. Chem. 58 (1980) 229-230.
5. C. Panaytiou, J. Chem. Soc., Faraday Trans. 280 (1984) 1435-1449.
6. J.R. Goates, R.L. Show, J.B. Ott, J.Phys. Chem. 66 (1962) 1301-1304.
7. A.J.Treszczanowicz, G.C. Benson, J.Chem. Thermodyn. 9 (1977) 1189-1197.
8. J. Zielkiewicz, J. Chem. Thermodyn. 26 (1994) 959.
9. A.J. Treszczanowicz, Thermochim.Acta 160 (1990) 253.
10. S.F. Blanco, J.M. Embid, S. Otin, J Chem. Thermodyn. 26 (1994) 23-28.
11. K.Nakashini, K.Naka Sato, R. Toba, H. Shirai, J. Chem. Eng. Data 12 (1967) 440-442.

12. I.Farkova, Fluid Phase Equilibria 109 (1995) 53-65.
13. J.A. Riddick, W.B. Bunger, T.K. Sakana, Organic solvents: Physical Properties and Methods of Purification, Fourth ed., Wiley, New York, 1986.
14. R. Francesconi, F. comelli, J.Chem. Engg.Data 40 (1995) 31.
15. P.P Singh, S.P. Sharma, J.Chem. Engg.Data 30 (1985) 477.
16. R. Bravo, E.Caivo, A. Pineiro, P.Brocos, A. Amigo, J. Chem. Engg.Data 14 (1999) 1341.
17. D.H. rouvary, Ric Rev. 4 (1971) 173.
18. A.T. Balaban, Chemical Applications of Graph Theory, Academic Press, London, 1976.
19. C.A. Coulson, Proc. Camb.Phil.Soc. 46 (1950) 202.
20. L.B.Kier, S.H.Yalkowasky, A.A.Sinkula, S.C.Valvani, Physico-Chemical Properties of Drugs, Marcel Dekker, New York, 1980, p. 297.
21. P.P.Singh, R.k. Nigam, K.C. Singh, V.K. Sharma, Thermochim. Acta 46 (1981) 175.
22. P.P.Singh, V.K. Sharma, S.P. Sharma, Thermochim. Acta 106 (1986) 293.