RESEARCH PAPER

Topological and Thermodynamic studies for binary mixtures of pyridine with isomeric butanaol at 308.15 K

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ABSTRACT

Excess molar volumes of pyridine (1) and isomeric butanol (2) binary mixtures have been measured as a function of composition at 308.15 K. The V^E data have been estimated by (i) Graph theory and (ii) Prigogine-Flory-Patterson theory (PFP). It has been observed that V^E values predicted by Graph theory compare well in comparison to PFP theory with their corresponding experimental values.

Keywords: Excess molar volumes V^E, connectivity parameters $^3\xi$ and interaction parameter, χ.
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1. Introduction

Thermodynamic data for multicomponent liquid mixtures are crucial for the engineering design of separation processes and unit operations. The mixing of different compounds typically results in mixtures exhibiting non-ideal behaviour. Deviations from ideality can be characterized using thermodynamic properties such as excess molar volumes (V^E), excess molar enthalpies (H^E), changes in isentropic compressibility upon mixing, and excess Gibbs free energy (G^E). These properties provide insight into the behaviour of components in both pure and mixed states, as well as the molecular interactions between them.

Chemical graph theory offers a structural perspective by representing chemical compounds as molecular graphs, where vertices correspond to atoms and edges to chemical bonds [1]. The foundational idea in chemistry—those molecular properties stem from molecular structure—dates back to the mid-19th century, when the first structure–property models were introduced [2,3]. Structure–activity relationships (SAR) aim to quantify this structure–property connection [4]. Topological indices are commonly employed in SAR studies to encode molecular structure [5–7]. Despite the existence of hundreds of topological indices, their interpretability has received comparatively limited attention [8,9].

Past studies [10–14] have demonstrated that the third-degree connectivity index, which is inherently linked to molecular topology, can effectively predict thermodynamic properties such as excess molar volumes, excess molar enthalpies, and changes in isentropic compressibility for binary and ternary mixtures. In the present work, an effort is made to evaluate the excess Gibbs free energy (G^E) of binary mixtures by utilizing the topological features of their constituent molecules.

Alcohols represent a class of simple yet significant amphiphilic substances that remain in the liquid phase, primarily due to hydrogen bonding involving their hydroxyl (–OH) groups. These compounds are characterized by their polar

nature and the ability to form self-associated structures. When alcohols are combined with aromatic hydrocarbons, their dipolar associations tend to weaken, which can be attributed to specific intermolecular interactions occurring between the alcohol and the aromatic component [15,16]. Primary alcohols possess both hydrogen-donating and hydrogen-accepting sites, facilitating extensive hydrogen bonding. This leads to notable self-association in their pure form, while in binary mixtures, both self- and cross-association phenomena are likely to occur. [17,18]

2. Experimental

Pyridine (Py) (AR Grade, 99 mol %), Butanol (Bu) (Fulka, 99 mol %), 2-Butanol (2-Bu) (Fluka, 98 mol %), iso-Butanol (iso-Bu) (Fluka, 99 mol %) and t-Butanol (t-Bu) (Fluka, 99 mol %) were purified by standard methods [19]. The purities of the purified liquids were checked by measuring their densities [recorded in Table 1] using Anton Parr DSA 5000 at 298.15±0.01K and these agreed to within $\pm 2.10^{-3}$ kg.m^{-3} with their literature values [20-21].

Densities of the pure liquids and their binary mixtures were measured using a commercial density and sound analyzer apparatus (Anton Parr DSA 5000). Before each series of measurements, the calibration of the apparatus was carried out with the double distilled, deionized water. The mole fraction of each mixture was obtained with uncertainty of $1*10^{-4}$ from the measured apparent masses of the components. All the measurements were performed on an electric balance. The uncertainty in the density is $\pm 2.10^{-3}$ kg.m^{-3}.

3. Results

The experimental excess molar volumes, V^E of Py (1) + Bu or 2-Bu or iso-Bu or t-Bu (2) binary mixture over entire composition range at 308.15K are presented in Tables 2.

The densities, ρ_{12} of binary mixtures were evaluated from their excess molar volumes data by employing Eq. 1

$$V^E = \sum_{i=1}^{2} x_1 M_1 (\rho_{12})^{-1} - \sum_{1=1}^{2} x_1 M_1 (\rho_1)^{-1} \quad (1)$$

where x_1, M_1 and ρ_1 are the mole fraction, molar mass and density of component (1) of (1+2) binary mixture.

where φ_1 is the volume fraction of component (1) in the mixed state $\kappa_{S,1}$, V_1, a_1 and $C_{p,1}$ are isentropic compressibility, molar volume, thermal expansion coefficient and molar heat capacity respectively of the pure component (1).

The values of a_1 and $C_{p,1}$ were taken from literature [22]. a_1 for Py was evaluated in the same manner as described elsewhere [23]. The dependence of V^E values on mole fraction of Py for the studied (1 + 2) mixtures are graphically represented in Fig respectively, and were fitted to Redlich-Kister equation

$$V^E = x_1 x_2 [V^{(0)} + V^{(1)} (2x_1 - 1) + V^{(2)} (2x_2 - 1)^2] \quad (2)$$

Where $V^{(n)}$ (n = 0 – 2) etc. are the parameters characteristic of (1 + 2) mixtures. These parameters were evaluated by fitting X^E ($X = V$) data to Eq. 2 by least squares method and are recorded along with standard deviations, $\sigma(X^E)(X = V)$ defined by Eq. 3

$$\sigma(X^E) = [\sum (X^E_{exptl} - X^E_{calcEq.5})^2 / (m - n)]^{0.5} \quad (3)$$

[where m is the number of data points and n is the number of adjustable parameters in Eq. 3] in Tables 2.

4. Discussion

We are unaware of any V^E data of Py (1) + Bu or 2-Bu or iso-Bu or t-Bu (2) mixtures with which to compare our results. V^E data of these mixtures are negative over range of composition. V^E data for an equimolar mixture vary in the order t-Bu > iso-Bu > 2-Bu > Bu respectively. The value show decreasing from t-Bu to Bu which reflects: (i) decreasing branching and steric hindrance (ii) increasing Hydrogen bonding ability with pyridines nitrogen.

At the qualitative level the observed V^E data of various (1+2) mixtures can be explained, if it be assumed that (i) Py (1) + Bu or 2-Bu or iso-Bu or t-Bu (2) are associated molecular entities; (ii) there is interaction between nitrogen atom of Py and hydrogen atom of Bu or 2-Bu or iso-Bu or t-Bu (2);

V^E for various (1+2) mixtures are the commutative effect of several contributions; (i) interaction between hydrogen atom of Bu or 2-Bu or iso-Bu or t-Bu (2) with nitrogen atom of Py; (ii) closer molecular arrangement; and (iii) depolymerization of Py or Bu or 2-Bu or iso-Bu or t-Bu. The negative values of V^E suggest that contribution to V^E due to factors (i) and (ii) far outweigh the contribution from factor (iii). Thus, the addition of Py or Bu or 2-Bu or iso-Bu or t-Bu results in not enhancing of the structure in Py+ Bu or 2-Bu or iso-Bu or t-Bu mixtures and is more

pronounced in Py + Bu as compared to 2-Bu or iso-Bu or t-Bu mixtures.

4.1 Graph theory and results

4.1.1 Excess molar volumes. Excess molar volumes, V^E is a packing effect and influenced by the change in topology of the constituents in mixed state. Thus, it was worthwhile to analyze V^E data of the studied mixtures in terms of Graph theory to extract information about the state of components in pure and mixed state and molecular entities existing in these mixtures. According to this theory [24], V^E is given by

$$V^E = \alpha_{12}\{[\sum x_1({}^3\xi_1)_m]^{-1} - [\sum x_1({}^3\xi_1)]^{-1}\} \quad (4)$$

where α_{ij} is a constant characteristic of (1+2) mixture. $({}^3\xi_1)$, $({}^3\xi_1)_m$ (1 = 1 or 2) etc are the connectivity parameters of the third degree of components (1) and (2) in pure and mixed state and are defined by

$${}^3\xi = \sum_{m<n<o<p} (\delta^v_m \delta^v_n \delta^v_o \delta^v_p)^{-0.5} \quad (5)$$

where δ^v_m etc. have the same significance as described elsewhere [25]. ${}^3\xi$ etc. parameters were determined by fitting experimental V^E data to Eq. 4 and only those values of $({}^3\xi_1)$, $({}^3\xi_1)_m$ (1 = 1 or 2) parameters were retained that best describe the experimental V^E data. These parameters, along with V^E values [predicted by employing Eq. 4] at various x_1 are recorded in Table 3. Examination of data in Table 3 reveals that V^E values compare well with their experimental values. Since the agreement between experimental and calculated values is good, $({}^3\xi_1)$ etc. can be utilized to extract information about the state of 1/2 in pure and mixed state.

A number of structures were then assumed for (1) and (2) components in pure and mixed state and their ${}^3\xi'$ values were evaluated from their structural consideration (via Eq. 5). These ${}^3\xi'$ values were then compared with ${}^3\xi$ values (obtained via Eq. 4). Any structure or combination of structures which provided ${}^3\xi'$ values comparing with ${}^3\xi$ value was taken to be representative structure of that component. Such an analysis revealed that Py (molecular entities I-II, ${}^3\xi'$ =0.516, 0.706) exist as a mixture of monomer and dimmers; Bu (molecular entities III-IV, ${}^3\xi'$ = 0.707, 1.614); 2-Bu (molecular entities V-VI, ${}^3\xi'$ =0.690, 1.560); iso-Bu (molecular entities VII-VIII, ${}^3\xi'$ =0.675, 1.510) t-Bu (molecular entities IX-X, ${}^3\xi'$ =0.554, 1.440) exists as an associated molecular entity.

$({}^3\xi'_2)_m$ values were then calculated to extract information about the state of Bu or 2-Bu or iso-Bu or t-Bu (2) in Py (1). It was assumed that Py (1) + Bu (2); Py (1) + 2-Bu (2); Py (1) + iso-Bu (2) and Py (1) + t-Bu (2) contain molecules entities XI-XIV respectively and are characterized by interactions between hydrogen atom of Bu or 2-Bu or iso-Bu or t-Bu and nitrogen atom of Py. $({}^3\xi'_2)_m$ values for molecular entities XI-XIV were then calculated to be 1.674, 1.951, 1.951 and 2.635. $({}^3\xi_2)_m$ values of 1.605, 1.845, 1.845 and 2.321 (Table 3) suggest the presence of molecular entities IX-XI in these mixtures. The existence of these molecular entities then suggests that addition of Bu or 2-Bu or iso-Bu or t-Bu to Py should have influenced the C=N stretching in pyridine and –O-H stretching in Bu or 2-Bu or iso-Bu or t-Bu of Py. In view of this, we analyzed IR spectra of pure Py or Bu or 2-Bu or iso-Bu or t-Bu and their equimolar Py (1) + Bu or 2-Bu or iso-Bu or t-Bu (2) mixtures. It was observed that Py, Bu, 2-Bu, iso-Bu and t-Bu in their pure state show characteristic absorption at 1595 cm^{-1} (C=N stretching) and 3300, 3320, 3340 and 3550 cm^{-1} (O-H stretch). On the other hand, IR spectra of equimolar Py (1) + Bu, 2-Bu, iso-Bu and t-Bu (2) mixtures show characteristic absorption at1580, 1582, 1583 and 1588 cm^{-1} (C=N stretch) and 3250, 3260, 3270 and 3350 cm^{-1} (O-H stretch) respectively. The IR spectral data of the investigated mixtures thus suggest that addition of (2) to (1) does influence the C=N stretching of Py and O-H stretching vibrations of Bu, 2-Bu, iso-Bu and t-Bu and thus support the existence of molecular entities XI-XIV.

4.2 Prigogine-Flory-Patterson theory

4.2.1 Excess molar volumes. According to PFP theory [26] excess molar volumes, V^E is considered to be comprised of three contributions, (i) interaction contribution; (ii) free volume contribution; (iii) the contribution that depends on the difference in both internal pressure and reduced volumes of two components constituting binary mixtures. V^E in terms of these three contributions is expressed by

$$V^E = V^E_{interaction} + V^E_{free\ volume} + V^E_{P^* effect} \quad (6)$$

where

$$\frac{V^E_{interaction}}{\sum x_1 v^*_1} = \frac{[(\tilde{v}^{1/3} - 1)\tilde{v}\psi_1\theta_2\chi'_{12}]}{[(4/3)\tilde{v}^{-1/3} - 1]\tilde{v}}$$

$$\frac{V^E_{free\ volume}}{\sum x_1 v_1^*} = \left[(\tilde{v}_1 - \tilde{v}_2)^2\left\{(14/9)\tilde{v}^{-1/3} - 1\right\}\right]\frac{\psi_i\psi_j}{\left[(4/3)\tilde{v}^{-1/3} - 1\right]\tilde{v}} \quad (7)$$

(8)

$$\frac{V^E_{P^* effict}}{\sum x_1 v_1^*} = \frac{(\tilde{v}_1 - \tilde{v}_2)(P_1^* - P_2^*)\psi_1\psi_2}{(P_1^*\psi_2 - P_2^*\psi_1)} \quad (9)$$

where all the terms in Eqs. 6-9 have the same significance as described elsewhere [27-28].

Evaluation of V^E using Eqs. 6 to 9 requires knowledge of the interactional energy parameter, $\chi_{12}^{//}$ in addition to the Flory's parameters $\bar{v}, v^*, T^*, C^*_{p,i}$ etc. for pure components. The various parameters for pure components were determined using isothermal compressibility reported in literature [22]. The κ_T values for those liquids that were not available were determined by using their ΔH_v values in the manner suggested by Hilderbrand [23]. Such values of V^E predicted by employing Eqs. 6-9 are recorded in Table 3, where they are also compared with their corresponding experimental values.

Examination of Tables 3 reveals that PFP theory correctly predict the sign of V^E values for all the studied mixtures, However V^E calculated by Graph theory compare well in comparison to values predicted by PFP theory with their corresponding experimental values.

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References

[1] Trinajstic, N.: Chemical graph theory. CRC Press, Boca Raton, Florida (1983)

[2] Turro, N. J.: Geometric and topological thinking in organic chemistry. Angew Chem. 28, 882-901 (1986)

[3] Mihalic, Z., Trinajstic, N.: A graph theoretical approach to structure-property relationships. J. Chem. Educ. 69, 701-713 (1992)

[4] Balaban, A. T., Motoc, I., Bonchev, D., Mekenyan, O.: Topological indices for structure activity correlations. Charton, M., Motoc, I. (eds) Top. Curr. Chem., pp. 21-55. Springer, Heidelberg (1983)

[5] Rouvary, D. H.: Chemical applications of topology and graph theory. King, R. B. (ed) Elsevier, Amsterdam (1983)

[6] Hansen, P. J., Jurs, P. C.: Chemical applications of graph theory. Part 1. Fundamentals and topological indices. J. Chem. Educ. 65, 574-580 (1988)

[7] Randic, M.: The nature of chemical structure. J. Math. Chem. 4, 157-184 (1990)

[8] Randic, M., Zupan, J.: On interpretation of well-known topological indices. J. Chem. Inf. Comput. Sci. 41, 550-560 (2001)

[9] Randic, M., Balaban, A. T., Basak, S. C.: On Structural interpretation of several distance related topological indices: J. Chem. Inf. Comput. Sci. 41, 593-601 (2001)

[10] Sharma, V. K., Romi, Kumar, S.: Topological investigation of binary and ternary mixtures: excess isentropic compressibilities. Thermochim. Acta 417, 91-97 (2004)

[11] Dimple, Yadav, J. S., Singh, K. C., Sharma V. K.: Molecular interaction in binary mixtures containing 2-methylaniline. Thermochim. Acta 468, 108-115 (2008)

[12] Sharma, D., Yadav, J. S., Singh, K. C., Sharma, V. K.: Molar excess volume and excess isentropic compressibilities of ternary mixtures containing 2-methylaniline. J. Solution Chem. 37, 1099-1112 (2008)

[13] Yadav, J. S., Sharma, D., Sharma, V. K.: Topological investigation of thermodynamic properties of binary mixtures containing 2-pyrrolidinone. Thermochim. Acta 489, 45-52 (2009)

[14] Yadav, J. S., Sharma, D., Sharma, V. K.: Molar excess volume and excess isentropic compressibilities of 2-pyrrolidinone at 308.15 K. Thermochim. Acta 496, 166-172 (2009)

[15] Patil S. S., Mirgane. S. R.: Volumetric and Viscometric Properties of Binary Liquid Mixtures of Acrylic Esters with Heptane2ol at 298.15 and 308.15 K Temperatures J. Chem. 445-451, 4(2) (2011).

[16] Bhatia S. C., Rani R., Bhatia R.: Volumetric and viscometric behavior of binary mixtures of tetrahydrofuran with methanol, ethanol, propan-1-ol and butan-1-ol at 298.15 K. J. Mol. Liq. 132, 159-164 (2011).

[17] Fedeles, Ciocirlan O., Iulian O. Experimental Viscosity and Density Data for Binary Liquid Mixtures. U. P. B. Sci. Bull. B 99-106, 71(4) (2009).
[18] Oswal S. L., Desai H. S.: Volumetric and Viscosity Studies of Binary Mixtures Containing N,N- Dimethylformamide at 303.15 K. Fluid Phase Equilib. 191, 161-172 (1999).
[19] Riddick, J. A., Bunger, W. B., Sakano, T. K.: Organic Solvents, Physical properties and Methods of Purification. Wiley, New York (1986)
[20] Solanki S., Hooda N., Sharma V. K., Thermodynamic study of interactions in binary mixtures containing dimethyl sulfoxide with alcohols at 298.15 K, 303.15 K, and 308.15 K. J. Chem. Thermodyn. 56 (2013) 123–135.
[21] Dakua V. K., Sinha B. and Roy M. N.: Thermophysical properties of binary mixtures of N,N-dimethylformamide with isomeric butanols at 298.15, 308.15 and 318.15 K. J. Indian Chern. Soc., 37-45, 84 (2007).
[22] Weast, R. C. (ed): CRC Handbook of Chemistry and Physics, 68th ed. CRC Hand Press, Boca Raton, FL (1987)
[23] Hilderbrand, J. H., Prausnitz, J. M., Scot, R. L.: Regular and Related Solutions: the solubility of Gases, Liquids, and Solids. Van Nonstand-Reinhelds, New York (1971)
[24] Singh, P.P., Sharma, V.K., Sharma, S.P.: Topological studies of the molecular species that characterize lower alkanol + methylene bromide mixtures: molar excess volumes and molar excess enthalpies. Thermochim. Acta 106, 293-307 (1986)
[25] Kier, L. B., Yalkowasky, S. H., Sinkula, A. A., Valvani, S. C.: Physico-Chemical Properties of Drugs. Mercel Dekker, New York (1980)
[26] Van, H. T., Patterson, D.: Volume of Mixing and the P* Effect: Part 1. Hexane isomers with normal and branched hexadecane. J. Sol. Chem. 11,793-805 (1982)
[27] Flory, P. J.: The Statistical thermodynamics of liquid mixtures. J. Am. Chem. Soc. 87, 1833-1838 (1965)
[28] Flory, P. J.: The thermodynamic properties of mixtures of small non-polar molecules. J. Am. Chem. Soc. 87, 1838-1846 (1965)

Table 1 Comparison of pure liquids with their literature values at 298.15 K.

Liquids	ρ (gcm^{-3})	
	Exp.	Lit.
Pyridine	0.9781	0.9782 [19]
Butanol	0.8054	0.8056 [20]
2-Butanol	0.8021	0.8023 [20]
Iso-Butanol	0.7974	0.7975 [20]
t-Butanol	0.7803	0.7801 [20]

Table 2 Measured excess molar volumes, V^E data for the various (1+2) mixtures as a function of mole fraction, x_1, of component (1) at 308.15 K.

x_1	V^E(cm^{3}mol^{-1})	x_1	V^E(cm^{3}mol^{-1})
pyridine (1) + t-butanol (2) [c]			
0.0412	-0.2674	0.5357	-0.8284
0.1012	-0.5485	0.5837	-0.8063
0.1941	-0.7916	0.6286	-0.7841
0.2567	-0.8639	0.6932	-0.7452
0.3517	-0.8902	0.7543	-0.6924
0.4256	-0.8735	0.8624	-0.5189
0.4998	-0.8442	0.9438	-0.2675
pyridine (1) + iso-butanol (2) [c]			
0.0541	–0.4111	0.5877	–1.0469
0.1713	–0.9267	0.6211	–1.0251
0.2235	–1.0383	0.6824	–0.9758
0.2767	–1.1020	0.7510	–0.8962
0.3508	–1.1332	0.8144	–0.7827
0.4213	–1.1252	0.8912	–0.5622
0.5514	–1.0681	0.9403	–0.3526
pyridine (1) + 2-butanol (2) [c]			
0.0678	-0.5770	0.5351	-1.2174
0.1154	-0.8468	0.5896	-1.2034
0.1866	-1.0955	0.6724	-1.1726
0.2424	-1.1966	0.7329	-1.1264

0.3131	-1.2490	0.7928	-1.0391
0.3904	-1.2527	0.8380	-0.9303
0.4517	-1.2393	0.9314	-0.5242

pyridine (1) + butanol (2) d			
0.0678	-0.5890	0.5351	-1.2381
0.1154	-0.8624	0.5896	-1.2294
0.1866	-1.1121	0.6724	-1.2076
0.2424	-1.2121	0.7329	-1.1670
0.3131	-1.2628	0.7928	-1.0827
0.3904	-1.2661	0.8380	-0.9731
0.4517	-1.2544	0.9314	-0.5519

Also included are various $V^{(n)}$ (n=0-2) parameters along with standard deviations, $\sigma(V^E)$

[a] $V^{(0)}$= -3.3764, $V^{(1)}$= 0.8636, $V^{(2)}$= -3.0882; $\sigma(V^{(E)})$= 0.005 cm^3mol^{-1}

[b] $V^{(0)}$= –4.3784, $V^{(1)}$= -0.9485, $V^{(2)}$= –0.3519; $\sigma(V^{(E)})$= 0.001 cm^3mol^{-1}

[c] $V^{(0)}$= –4.9058, $V^{(1)}$= 0.5278, $V^{(2)}$= –5.0417; $\sigma(V^{(E)})$= 0.004 cm^3mol^{-1}

[d] $V^{(0)}$= –4.9782, $V^{(1)}$= 0.3861, $V^{(2)}$= –5.3642; $\sigma(V^{(E)})$= 0.004 cm^3mol^{-1}

Table 3 Comparison of V^E values calculated from eq (4) with their corresponding experimental values at 308.15K for the various (1+2) mixtures as a function of x_1, mole fraction of component (1).

Property	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
pyridine (1) + t-butanol (2) [a]									
V^E(Exptl)	-0.5567	-0.7791	-0.8686	-0.8828	-0.8737	-0.7799	-0.7319	-0.6191	-0.4442
V^E(Graph)	-0.5012	-0.7128	-0.8222	-0.8854		-0.7732	-0.7110	-0.6012	-0.4222
V^E(PFP)	-0.0882	-0.1769	-0.2695	-0.2955	-0.3556	-0.3588	-0.2886	-0.2695	-0.1566
pyridine (1) + iso-butanol (2) [b]									
V^E(Exptl)	-0.6896	-0.9776	-1.0881	-1.1572	-1.1512	-1.0552	-0.9211	-0.7844	-0.5844
V^E(Graph)	-0.6622	-0.9341	-1.0111	-1.1122		-1.0101	-0.9013	-0.7322	-0.5111
V^E(PFP)	-0.1044	-0.1883	-0.2539	-0.2997	-0.3171	-0.3313	-0.2881	-0.2200	-0.1288
pyridine (1) + 2-butanol (2) [c]									
V^E(Exptl)	-0.8007	-1.0985	-1.2054	-1.2872	-1.2522	-1.2121	-1.1252	-0.9772	-0.7711
V^E(Graph)	-0.7889	-1.0219	-1.1832	-1.2039		-1.2001	-1.1004	-0.9432	-0.7333
V^E(PFP)	-0.1157	-0.1546	-0.1668	-0.2268	-0.2292	-0.2379	-0.2121	-0.1525	-0.1111
pyridine (1) + butanol (2) [d]									
V^E(Exptl)	-0.8233	-1.1215	-1.2295	-1.2954	-1.2722	-1.2443	-1.1616	-1.0155	-0.8055
V^E(Graph)	-0.8032	-1.1002	-1.2200	-1.2707		-1.2202	-1.1022	-1.0001	-0.7665
V^E(PFP)	-0.1177	-0.1786	-0.2468	-0.2786	-0.2970	-0.2861	-0.2541	-0.1853	-0.0998

Also included are various $({}^3\xi_1)$ and $({}^3\xi_1)_m$ (1=1 or 2) and α_{12}

[a] $({}^3\xi_1)=({}^3\xi_1)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.605$; $\alpha_{1\,2}$ $=6.467\ cm^3mol^{-1}$

[b] $({}^3\xi_1)=({}^3\xi_1)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.845$; α_{12} $=5.236\ cm^3mol^{-1}$

[c] $({}^3\xi_1)=({}^3\xi_1)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.845$; α_{12} $=8.436\ cm^3mol^{-1}$

[d] $({}^3\xi_1)=({}^3\xi_1)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=2.321$; α_{12} $=7.433\ cm^3mol^{-1}$

FIGURE: