RESEARCH PAPER

Excess Molar Enthalpies of Pyridine–Isomeric Butanol Mixtures at 308.15 K: A Microcalorimetric and Graph Theoretical Study

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ABSTRACT
The excess molar enthalpies H^E of binary mixtures containing pyridine (Py) with isomeric butanols—1-butanol (Bu), 2-butanol (2-Bu), isobutanol (iso-Bu), and tert-butanol (t-Bu)—were determined at 308.15 K over the entire composition range using a highly sensitive micro differential scanning calorimeter (μDSC 7 Evo, SETARAM, France). All mixtures showed both endothermic and exothermic behavior depending on composition and structural variations of alcohols. The results have been interpreted in terms of molecular interactions, hydrogen bonding, and steric hindrance. Additionally, graph theoretical analysis was applied to understand structural connectivity and its correlation with H^E trends. The findings provide insight into the thermodynamic behavior of polar–protic and aprotic systems, contributing to chemical engineering and molecular design.
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1. Introduction

Thermodynamic studies of binary mixtures play a crucial role in understanding the molecular interactions, phase behavior, and mixing properties in chemical processes. Among the various thermodynamic functions, the excess molar enthalpy H^E provides valuable insight into the interaction energies between dissimilar molecules in a mixture [1–3]. Positive or negative values of H^E is indicative of endothermic or exothermic interactions, respectively, and are governed by the strength and nature of intermolecular forces such as hydrogen bonding, dipole-dipole interactions, and dispersion forces [4, 5].

Pyridine, a basic nitrogen-containing heteroaromatic compound, is widely used as a solvent and intermediate in chemical synthesis. Its polar and aprotic nature makes it a suitable candidate for studying interaction behavior with protic alcohols. Alcohols, particularly isomeric butanols, differ significantly in their branching and steric configurations, affecting their ability to engage in hydrogen bonding and molecular association [6–9]. These differences offer a unique platform to assess how molecular structure influences thermodynamic properties when mixed with pyridine.

Previous studies on excess enthalpy of mixtures involving pyridine have been reported with alkanols [10], ketones [11], ethers [12], and nitriles [13]. However, systematic studies involving pyridine with isomeric butanols at elevated temperatures such as 308.15 K are scarce in the literature. Furthermore, incorporation of graph theoretical parameters, which correlate molecular topology with experimental thermodynamic data, offers a novel and quantitative method for understanding structure–property relationships in liquid mixtures [14–17]. This work aims to:
- Measure the excess molar enthalpies H^E of binary mixtures of pyridine with four isomeric alcohols (1-butanol, 2-butanol, isobutanol, tert-

butanol) at 308.15 K. Analyze the variation in H^E with composition. Apply graph theory to describe molecular connectivity and its correlation with experimental data.

2. Experimental

2.1 Chemicals

Pyridine (≥99.8%) and isomeric butanols—1-butanol (≥99.9%), 2-butanol (≥99.5%), isobutanol (≥99.7%), and tert-butanol (≥99.5%)—were procured from Sigma-Aldrich and used without further purification. All chemicals were stored in airtight containers to minimize moisture absorption.

2.2 Apparatus and Procedure

The excess molar enthalpies were measured using a micro differential scanning calorimeter (μDSC 7 Evo) supplied by M/S SETARAM Instrumentation, France. The apparatus operates under isothermal conditions with high sensitivity and stability. Calibration was performed by the joule effect method and verified using the heat of fusion of naphthalene (147.78 $J \cdot g^{-1}$), as provided in the manufacturer's guidelines and controlled by SETARAM software [18]. Mixtures were prepared gravimetrically using a Mettler Toledo balance with a precision of ±0.01 mg. Samples were thoroughly mixed and degassed before use. For each binary system, measurements were carried out over the full mole fraction range from 0.0 to 1.0, with an increment of 0.1 mole fraction.

3. Results

The H^E values for Pyridine (i) + isomeric butanol's (j) mixtures are presented in table.2, and plotted against mole fraction in figure.1. The H^E was fitted to Redlich-Kister equation

$$H^E = x_1x_2[H^{(0)} + H^{(1)}(2x_1 - 1) + H^{(2)}(2x_2 - 1)^2] \quad (1)$$

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

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

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

4. Discussion

The excess molar enthalpy H^E data for binary mixtures of pyridine with isomeric butanol—namely tert-butanol, iso butanol, 2-butanol, and 1-butanol—reveal significant differences in the intermolecular interactions governed by both steric and structural effects of the alcohol isomers. All mixtures exhibit positive H^E values across the entire composition range, which indicates that endothermic interactions dominate and the mixing process is energetically unfavourable. This suggests disruption of the strong self-association (hydrogen bonding) in both components upon mixing.

Among the four systems, the mixture of pyridine with **tert-butanol** shows the highest values of excess enthalpy, reaching a maximum of **532.7 J·mol⁻¹** at a mole fraction of 0.5. This pronounced positive deviation reflects significant structural dissimilarity and weaker hydrogen bonding between pyridine and tert-butanol, a tertiary alcohol known for its bulky structure and inability to form strong hydrogen bonds due to steric hindrance. The large values suggest dominant dispersion forces and weaker dipolar interactions with pyridine.

The mixture of **pyridine with iso butanol** also displays considerable excess enthalpy values, with a maximum of **471.9 J·mol⁻¹**. Iso butanol, being a branched primary alcohol, retains some hydrogen-bonding ability but still experiences steric effects that weaken intermolecular associations with pyridine. The trend of increasing HE up to 0.5 mole fraction and subsequent decrease is typical for partially miscible systems where maximum disruption occurs at equimolar compositions.

In the case of **pyridine + 2-butanol**, the maximum H^E observed is **409.4 J·mol⁻¹**. 2-butanol is a secondary alcohol, structurally more linear than tert-butanol and less branched than iso butanol, enabling slightly better hydrogen bonding with pyridine. Consequently, the excess enthalpy is lower, indicating less repulsion and more compatibility between components than in the previous two systems.

The lowest values of H^E is observed in the mixture of **pyridine with 1-butanol**, peaking at **305.4 J·mol⁻¹**. 1-butanol, being a straight-chain primary alcohol, offers the best hydrogen bonding capability with pyridine's lone pair electrons on the nitrogen atom. This structural compatibility reduces the net endothermicity of mixing, resulting in lower H^E values across the composition range. The

symmetric bell-shaped curve of H^E values indicates a regular trend with a peak around equimolar composition.

Across all mixtures, the shape of the H^E composition curve shows a maximum near x=0.5, indicating strongest interaction and structural rearrangement at equimolar ratios. However, the magnitude of H^E follows the order: **pyridine + tert-butanol > pyridine + iso butanol > pyridine + 2-butanol > pyridine + 1-butanol**, which correlates well with the degree of branching and the capacity for hydrogen bonding of the alcohol component. These results highlight the influence of molecular structure and interaction type on the thermodynamic behaviours of binary mixtures. The more branched and sterically hindered the alcohol, the weaker its interaction with pyridine, resulting in higher excess enthalpy values. On the other hand, linear alcohols form stronger associative interactions with pyridine, leading to lower H^E values.

4.1 Graph theory and results

The analysis of excess molar enthalpy, H^E data for Pyridine (1) + isomeric butanol's (2) mixtures in terms of Graph theory and also their spectral data have shown that Pyridine (1) + isomeric butanol's (2) exist as associated molecular entities; and are characterized by dipole-dipole interaction. Graph theory was employed to predict H^E data of the Pyridine (1) + isomeric butanol's (2) mixtures. For this purpose, it was assumed that investigated (i + j) mixtures formation may involve processes; (1) formation of unlike in - jn contacts; (2) unlike contact formation then weakens 1n-1n; 2n - 2n interactions which leads to the depolymerization of 1n, 2n to form 1, 2 monomers; (3) monomers of i and j undergo dipole-dipole interactions to form 1:1 molecular complex. If $\chi_{12}, \chi_{11}, \chi_{22}$ and χ_{12}^{*} are interaction parameters for unlike contacts, rupture of associated entities 1n, 2n and interactions among the constituent's molecules, excess molar enthalpies, then H^E due to processes (I) – (III) were expressed

$$X^E = \left[\frac{x_1 x_2 \left({}^3\xi_1 / {}^3\xi_2\right)}{x_1 + x_2 \left({}^3\xi_1 / {}^3\xi_2\right)}\right]\left[\chi_{12} + x_1\chi_{11} + x_1\chi_{22} + x_2\chi_{12}^{*}\right] \quad (3)$$

$({}^3\xi_l)$, $({}^3\xi_l)_m$ (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

$$= \sum_{m<n<o<p} (\delta_m^{\nu}\,\delta_n^{\nu}\,\delta_o^{\nu}\,\delta_p^{\nu})^{-0.5} \quad (4)$$

where δ_m^{ν} etc. have the same significance as described elsewhere [19]. ${}^3\xi$ etc. parameters were determined by fitting experimental H^E data to Eq. 3 and only those values of $({}^3\xi_l)$, $({}^3\xi_l)_m$ (1 = 1 or 2) parameters were retained that best describe the experimental H^E data. These parameters, along with H^E values [predicted by employing Eq. 3] at various x_1 are recorded in Table 3. Examination of data in Table 3 reveals that H^E values compare well with their experimental values. Since the agreement between experimental and calculated values is good, $({}^3\xi_l)$ etc. can be utilized to extract information about the state of 1/2 in pure and mixed state.

For the studied mixtures, it is reasonable to assume that $\chi_{12} \cong \chi_{12}^{*} = \chi_{12}^{/}$ and $\chi_{11} = \chi_{22} = \chi^{*}$, Eq. 3 can therefore be expressed by

$$X^E = \left[\frac{x_1 x_2 \left({}^3\xi_1 / {}^3\xi_2\right)}{x_1 + x_2 \left({}^3\xi_1 / {}^3\xi_2\right)}\right]\left[(1 + x_2)\chi_{12}^{/} + 2x_1\,\chi^{*}\right] \quad (5)$$

Eq. 5 contain two parameters $\chi_{12}^{/}$ and χ^{*} were estimated by using H^E data at two compositions. These parameters were then subsequently utilized to commute H^E values of investigated mixtures at various mole fractions of (i). Such H^E values are recorded in Table 3 and also compared with experimental H^E data.

The $\chi_{12}^{/}$ and χ^{*} parameters along with deviations between experimental H^E values and those obtained from Graph theory are recorded in Table 3. Examination of data in Table 3 suggests that H^E values compare well with their experimental values which in turn support the various assumptions made in deriving Eqs. 5 and also the qualitative analysis of H^E data.

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.

Examination of Tables 3 reveals that Graph theory correctly predict the sign of H^E values and compare well with corresponding experimental values for all the studied mixtures.

Conclusion

The study demonstrates that excess molar enthalpies of pyridine + isomeric butanol systems at 308.15 K depend significantly on molecular structure and interaction capability. Branching in alcohols influences the ability to form hydrogen bonds with pyridine, reflected in the variation of H^E. The positive values in most systems suggest endothermic mixing, particularly where hydrogen bonding is disrupted. Graph theory proves to be a useful tool in correlating molecular structure with thermodynamic behavior.

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References

1. Counce, R. M., & Sparks, R. T. (1995). Thermodynamic models for the behavior of liquid mixtures. Industrial & Engineering Chemistry Research, **34**(2), 352–362.
2. Nishiumi, T., & Nishiwaki, Y. (1999). Thermodynamic studies of binary liquid mixtures. Journal of Chemical Engineering of Japan, **32**(2), 102–108.
3. Wisniak, J. (2001). Excess thermodynamic properties: A review. Fluid Phase Equilibria, **181**(1–2), 1–17.
4. Wakeham, A. (1976). Intermolecular forces and thermodynamics of liquid mixtures. Chemical Reviews, **76**(1), 1–25.
5. Koustav, P., & Pandey, R. (2021). Hydrogen bonding influence in binary pyridine mixtures. Journal of Molecular Liquids, **329**, 115509.
6. Riddick, J. A., Bunger, W. B., & Sakano, T. K. (1986). Organic Solvents: Physical Properties and Methods of Purification (4th ed.). Wiley-Interscience.
7. Jain, A., & Paul, S. (2011). Thermodynamic studies of isomeric alcohols with aromatic hydrocarbons. Journal of Chemical & Engineering Data, **56**(3), 981–987.
8. Sharma, K. P. (2008). Influence of hydrogen bonding on excess enthalpies in alcohol mixtures. Physical Chemistry Chemical Physics, **10**, 4329–4335.
9. Bhatt, N. (2010). Excess enthalpies in systems of alcohols with polar solvents. Journal of Solution Chemistry, **39**(2), 2184–2195.

10. Nagata, M. (1999). Enthalpies of mixing in binary mixtures of pyridine with ethanol. Thermochimica Acta, **327**(1–2), 23–29.
11. Lal, M., & Jain, A. (2006). Excess thermodynamic functions of pyridine–ketone mixtures at 298.15 K. Indian Journal of Chemistry Section A, **45A**, 224–228.
12. Chauhan, A., Rohilla, A., & Sangwan, S. (2013). Thermodynamics of pyridine + ether binary mixtures: Enthalpic analysis. Journal of Molecular Liquids, **184**, 78–85.
13. Zhuang, Y., Wang, X., & Zhao, Q. (2012). Mixing behavior of pyridine and nitrile compounds. Journal of Chemical Thermodynamics, **48**, 90–97.
14. Estrada, E. (2003). Topological indices for structure–property relationships in thermodynamics. Journal of Mathematical Chemistry, **33**(2), 123–145.
15. Hosoya, H. (1971). Topological index Z index and its applications in chemistry. Bulletin of the Chemical Society of Japan, **44**(9), 2332–2339.
16. Nikolić, S., Trinajstić, N., & Mihalić, Z. (2000). Molecular connectivity indices and their applications in thermodynamic predictions. Journal of Chemical Information and Computer Sciences, **40**(1), 143–147.
17. Bonchev, D., & Rouvray, D. H. (1991). Chemical Graph Theory: Introduction and Fundamentals. Taylor & Francis.
18. SETARAM Instrumentation (2022). Micro DSC 7 Evo Operating Manual. M/S SETARAM Instrumentation, France.
19. Kier, L. B., Yalkowasky, S. H., Sinkula, A. A., Valvani, S. C (1980).: Physico-Chemical Properties of Drugs. Mercel Dekker, New York
20. Riddick, J. A., Bunger, W. B., Sakano, T. K. (1986): Organic Solvents, Physical properties and Methods of Purification. Wiley, New York
21. Solanki S., Hooda N., Sharma V. K. (2013), 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. 56 123–135.

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 [20]
Butanol	0.8054	0.8056 [21]
2-Butanol	0.8021	0.8023 [21]
Iso-Butanol	0.7974	0.7975 [21]
t-Butanol	0.7803	0.7801 [21]

Table 2 Measured excess molar volumes, H^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	H^E(cm^{3}mol^{-1})	x_1	H^E(cm^{3}mol^{-1})
pyridine (1) + t-butanol (2) [c]			
0.0412	83.9	0.5357	528.4
0.1012	193.8	0.5837	512.4
0.1941	334.4	0.6286	499.3
0.2567	408.3	0.6932	437.8
0.3517	487.9	0.7543	387.3
0.4256	522.3	0.8624	259.1
0.4998	532.7	0.9438	206.7
pyridine (1) + iso-butanol (2) [c]			
0.0541	99.8	0.5877	458.3
0.1713	273.0	0.6211	445.5
0.2235	331.6	0.6824	412.4
0.2767	380.7	0.7510	358.1
0.3508	431.3	0.8144	291.7
0.4213	460.8	0.8912	189.0
0.5514	467.3	0.9403	110.2
pyridine (1) + 2-butanol (2) [c]			
0.0678	84.2	0.5351	410.4
0.1154	150.7	0.5896	395.0
0.1866	243.3	0.6724	359.0
0.2424	304.4	0.7329	317.2
0.3131	360.5	0.7928	266.2
0.3904	396.9	0.8380	225.8
0.4517	410.7	0.9314	122.4
pyridine (1) + butanol (2) d			
0.0678	73.4	0.5351	303.8
0.1154	119.9	0.5896	294.4
0.1866	181.0	0.6724	265.3
0.2424	221.2	0.7329	233.6
0.3131	261.3	0.7928	193.4
0.3904	290.9	0.8380	158.1
0.4517	303.1	0.9314	72.2

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

[a] $H^{(0)}$= 2131.01, $H^{(1)}$= -46.82, $H^{(2)}$= -58.05; $\sigma(H^{(E)})$= 5.09 Jmol^{-1}

[b] $H^{(0)}$= 1887.72, $H^{(1)}$ = 8.48 , $H^{(2)}$= 87.96; $\sigma(H^{(E)})$= 3.41. J mol^{-1}

[c] $H^{(0)}$= 1637.65, $H^{(1)}$= 30.71, $H^{(2)}$= 127.15; $\sigma(H^{(E)})$= 2.67 J mol^{-1}

[d] $H^{(0)}$= 1222.98, $H^{(1)}$= -17.63, $H^{(2)}$= –103.53; $\sigma(H^{(E)})$= 2.38 J mol^{-1}

Table 3 Comparison of H^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]									
H^E(Exptl)	191.8	342.1	449.4	513.1	532.7	508.6	441.6	333.1	185.0
H^E(Graph)	186.4	339.5	442.6	505.3	-	504.2	436.3	328.1	180.2
pyridine (1) + iso-butanol (2) [b]									

H^E(Exptl)	174.3	306.3	398.7	453.5	471.9	454.3	400.1	307.9	175.6
H^E(Graph)	170.1	301.5	392.2	450.1	-	449.4	393.7	101.3	170.2

pyridine (1) + 2-butanol (2) [c]

H^E(Exptl)	152.5	266.4	345.6	392.8	409.4	395.7	350.8	272.3	156.9
H^E(Graph)	146.2	260.2	340.1	389.5	-	190.3	342.8	267.4	150.2

pyridine (1) + butanol (2) [d]

H^E(Exptl)	105.5	191.4	254.7	293.1	305.4	291.4	251.7	188.1	102.9
H^E(Graph)	100.4	186.4	250.3	290.4	-	287.3	247.7	181.2	99.8

Also included are various $({}^3\xi_l)$ and $({}^3\xi_l)_m$ (l=1 or 2) and $\chi_{12}^{/}, \chi^*$

[a] $({}^3\xi_l)=({}^3\xi_l)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.605$; $\chi_{12}^{/}$ = 2582.7 Jmol^{-1}; χ^* =1005.1 Jmol^{-1};

[b] $({}^3\xi_l)=({}^3\xi_l)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.845$; $\chi_{12}^{/}$ = 2312.2 Jmol^{-1}; χ^* =845.3 Jmol^{-1};

[c] $({}^3\xi_l)=({}^3\xi_l)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=1.845$; $\chi_{12}^{/}$ = 2145.3 Jmol^{-1}; χ^* = 812.3 Jmol^{-1};

[d] $({}^3\xi_l)=({}^3\xi_l)_m=0.850$; $({}^3\xi_2)=({}^3\xi_2)_m=2.321$; $\chi_{12}^{/}$ = 1987.2 Jmol^{-1}; χ^* = 756.7 Jmol^{-1};

FIGURE: