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Studies acoustic behaviour of the binary mixture of 1-Butyl-3-methylimidazolium hexafluorophosphate with 1-hexanol at 298.15 K

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Abstract
Densities and speeds of sound and their excess properties for 1-butyl-3- methylimidazolium Hexafluorophosphate [Bmim] [PF_6] with 1-Hexanol over the entire range of mole fraction are reported at temperature 298.15 K and atmospheric pressure. Isentropic and excess isentropic compressibility for ionic liquid with 1-Hexanol were calculated from the experimental results. The excess values are fitted to the Redlich−Kister polynomial equation to estimate the binary coefficients and standard error between the experimental and calculated values. The measured speeds of sound were compared to the values obtained from Schaaffs' collision factor theory, Jacobson's intermolecular free length theory of solutions and Nomoto's relation. The theoretical results obtained from these relations fairly agrees within the experimental precision. Further, the molecular interactions involved in IL binary mixture system were studied.

Keywords: Binary mixture, density, isentropic compressibility, ionic liquid, speed of sound

Introduction
The measurement of density, velocity, refractive index and related excess properties are included in the investigation of the physico-chemical behavior of liquid systems and provides useful information regarding the intermolecular interactions in liquids and their mixtures. This experimental data is useful for industrial objectives, for the oretical and applied thermodynamics. The nature and strength of molecular interactions can be known by studying the variation of thermo physical properties with several parameters which enables to determine the deviation and excess properties of mixtures [1-2]. Ionic liquids (ILs) have recently emerged as environment friendly solvents for their use in the industrial manufacture of chemicals. In the past decade, ILs have been increasingly used for diverse applications such as organic synthesis, catalysis, electrochemical devices, and solvent extraction of a variety of compounds [3-6]. The interest in ILs was initiated because of their advantageous physico−chemical properties. ILs are composed of cations and anions having a low melting point. The physico−chemical properties of the ILs can be tuned by changing the cation or the anion. Thus, novel solvents can be formed and can be used for a specific application which cannot be done with the use of conventional organic solvents. The information regarding the thermo- physical properties of pure ILs as well as their mixtures with other compounds is essential for the design and development of equipment for commercial applications. [Bmim] [PF_6] is most efficient in the removal of di- benzothiophene (DBT) containing liquid fuels [7]. 1-Hexanol is produced industrially by the oligomerization of ethylene using triethylaluminium followed by oxidation of the alkylaluminium products. It also is partly responsible for the fragrance of strawberries. Similar study has been carried out by us [8-10] and many other workers for nonionic liquids, particularly hydro carbons, cyclic compound, to validate these theoretical models and also the solvent - solvent interactions present in liquid mixture.
The present work is aimed at studying the molecular interactions in the binary mixture of the IL 1-Butyl-3-methylimidazolium Hexafluorophosphate [Bmim] [PF_6] with 1-Hexanol. Isentropic and excess isentropic compressibility's for ionic liquids with 1–Hexanol were calculated from the experimental results. Excess and deviation properties were further correlated using the Redlich-Kister polynomial eqation [11].
The measured speeds of sound were compared to the values obtained from Schaaffs' collision factor theory (CFT) [12], Jacobson's intermolecular free length theory (FLT) [13-14] of solutions and Nomoto's relation (NR) [15].

Experimental values and excess thermodynamic properties of IL systems allow researchers to draw information on the corresponding excess molar volume and excess isentropic compressibility and coefficients of thermal expansion were calculated. Furthermore, the Redlich and Kister (R–K) polynomial was used to obtain the coefficients and to estimate the standard deviations for the calculated excess and deviation properties. Moreover, the effect of the alkyl chain in ILs, chain length of 1–Hexanol and the temperature on the excess and deviation properties are investigated.

Experimental

Materials

[Bmim] [PF_6] (Mass fraction, 0.99) is procured from Merck, Germany, and is used without further purification. 1-Hexanol (mass fraction 0.97) is procured from Sigma-Aldrich, USA, and is purified by the fractional distillation method under reduced pressure. The water content is checked by conductometric titration with platinum electrode. The purity of the chemicals was ascertained by comparing the experimental values of density and speed of sound at temperatures T = 298.15 K with the literature value [16-18].

Apparatus and Procedure

The binary mixture is prepared by weighing appropriate amounts of pure liquids on a digital electronic balance model Shimadzuax-200 with an uncertainty of ± $1 \cdot 10^{-4}$kg. Before each series of experiments, I calibrated the instrument at atmospheric pressure with doubly distilled water. The average uncertainty in the composition of the mixtures was estimated to be less than ±0.0001. A crystal controlled variable path ultrasonic interferometer supplied by M/s Mittal enterprises (model-05F), New Delhi (India), operating at a frequency of 2 MHz was used in the ultrasonic measurements. The reported uncertainty is less than ± 3% which is the highest uncertainty found from all the data points. The purity of chemicals used was confirmed by comparing the densities and ultrasonic speeds with those reported in the literature as shown in Table 1. The uncertainty in the density measurement was within ± 0.7 $kg.m^{-3}$ (about 0.06%). The densities of the pure components and their mixture were measured with the bi-capillary pyknometer. The liquid mixture was prepared by mass in an air tight stopped bottle using an electronic balance model Shimadzuax-200 accurate to within ±0.1 mg. Isentropic compressibility, k_s, were calculated from the relation,

$$k_s = u^{-2}\rho^{-1} \quad (1)$$

Where
ρ is the density and u is the ultrasonic velocity.

Results and Calculations

The experimental density and speed of sound for binary systems of 1 Butyl-3-methylimidazolium Hexafluorophosphate with 1- Hexanol are reported at 298.15 K and atmospheric pressure are listed in Table 2. The excess volume, V^E and excess isentropic compressibility values

$$V^E = \sum_i^n{}_1 \frac{XiMi}{\rho} - \sum_i^n{}_1 \frac{XiMi}{\rho i} \quad (2)$$

$$K_s^E = K_s - K_s^{idl} \quad (3)$$

$$K_s^{idl} = K_s\, x_1 + K_s\, x_2 \quad (4)$$

and volume fractions, ∅ were calculated from the relation;

$$\emptyset = \frac{Xi\ V1}{\sum_{i=1}^{n} Xi\ Vi} \quad (5)$$

The dependency of V^E on composition is shown in figure 1 where all V^E values are negative for the systems under study and this is due to the interstitial accommodation of ILs into 1-Hexanol structure [7]. The negative V^E trend reflects the formation of hydrogen bonded hetero associations and the issociation of 1- Hexanol structure as the chain length increases. This is conformed from the previously reported studies [4, 5, 7]. In addition as expected, V^E becomes less negative as the temperature increases for ILs with 1-Hexanol. The excess isentropic compressibility values k^E were calculated from relations by Benson *et al.* [19] where K_s^{idl} is the isentropic compressibility of the ideal solution, K_s is the isentropic compressibility and it is calculated using the Laplace–Newton $V = 1/u^2\rho$ where the relation is judged to be valid and therefore the speed of sound may be regarded as a thermodynamic quantity. The excess isentropic compressibility are negative for the system under study and exhibited a similar trend as the excess volume (see fig.2) while K^E becomes more negative as the temperature increases as shown in Table 2. Which suggest the dominance of interstitial of accommodation of the components effect over the dissociation effect. The calculated excess properties were fitted to the Redlich-Kister (R–K) polynomial equation, Schaaff's Collision Factor Theory (CFT), Jacobson's Free Length Theory (FLT) and Nomoto's relation (NR) [11-15] were used to predict the speed of sound (u_m) for 1-Butyl- 3-methylimidazolium Hexafluorophosphate + 1- Hexanol binary systems. The critical temperature for the pure ILs were predicted using available data since they are needed for CFT,

$$u = u_\infty \sum_i^n{}_1 \frac{(XiSi)(\sum_i^{\mu}{}_1 Xi\ Bi)}{V} \quad (6)$$

Where
u_∞ = 1600 $m \cdot s^{-1}$, S_i and B_i are the space filling factor and the actual volume of the molecule per mole of pure component i in the mixture. Jacobson's Free Length Theory (FLT) can be expressed as;

$$u = \frac{K}{L_f\, \rho_{1/2}} \quad (7)$$

$$u = \left(\frac{\sum_i^n{}_1 Xi\ ui}{\sum_i^n{}_1 Xi\ Vi} \right) 3 \quad (8)$$

The comparison shows that Nomoto's relation for predicting speed of sound is the best among the relations used in the case of + 1-Hexanol while both Nomoto's and Schaaff's Collision Factor Theory are also comparable.

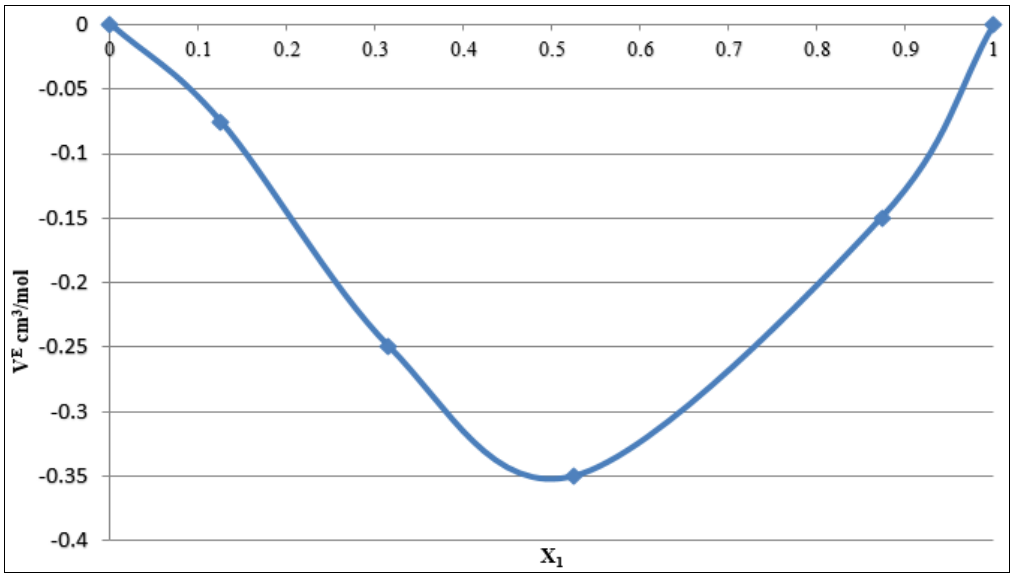

Fig 1: Excess molar volumes V^E, as a function of x_1 for {x [Bmim] [PF_6] + (1 − x) Hexanol} binary mixtures at 298.15 K

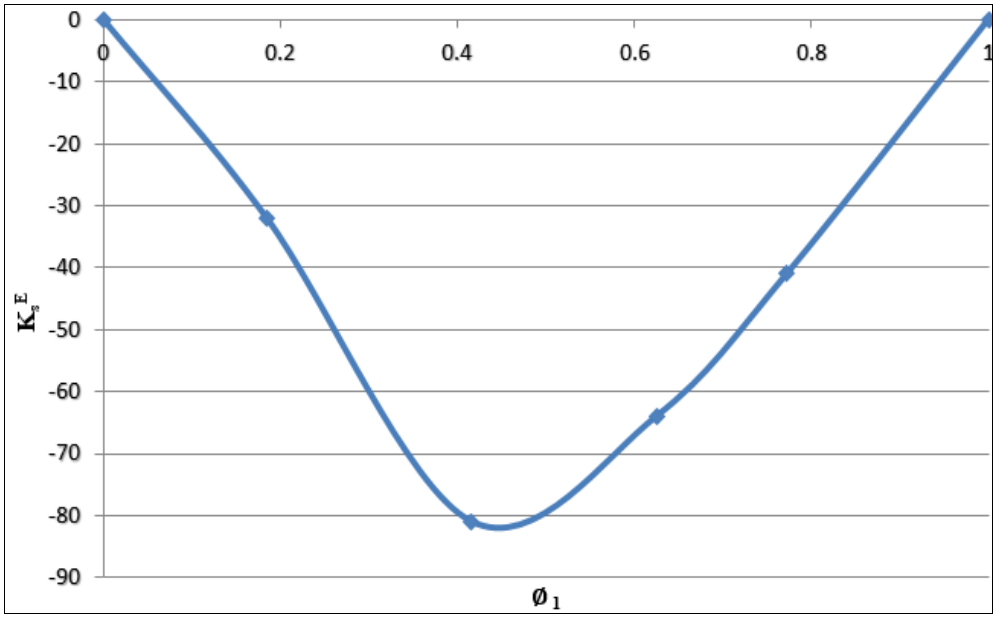

Fig 2: Excess isentropic compressibility k_s^E, as a function of $\emptyset_1$for {x [Bmim] [PF_6] + (1 − x) Hexanol }binary mixtures, at 298.15K

Table 1: Comparison of Experimental Density (ρ_{exp}), Speed of Sound (u_{exp}) of Pure Components with Literature (lit) Values at Temperatures from T = 298.15 K

Components	ρ/kg·m^{-3}		u/m·sec^{-1}	
	ρexp	ρlit	u exp	u lit
1-Butyl-3-methylimidazolium Hexafluorophosphate	1368.3	1367.88	1442.58	1442.80
1-Hexanol	816.10	816.20	1303.7	1303.0

Table 2: Experimental Density (ρ_{exp}), Speed of Sound (u_{exp}) and values obtained from theoretical models (u_{Sch}, u_{Nom} and u_{Jacob}) and Isentropic Compressibility (k_s) of Binary Liquid Mixtures of 1-Butyl-3-methylimidazolium Hexafluorophosphate + 1-Hexanol at 298.15 K

x_1	ρ_{exp}/kg· m−3	u_{exp}/m· sec^{-1}	u_{Sch}/m ·sec^{-}	u_{Nom}/m· sec^{-}	u_{Jacob}/m ·sec^{-}	k_s TPa^{-1}
0.1025	0891.45	1311.45	1312.3	1384.4	1310.3	652.22
0.2124	0934.29	1342.39	1341.2	1334.0	1338.1	593.96
0.3148	0975.06	1368.15	1371.3	1365.6	1369.5	547.89
0.4206	1002.35	1389.04	1390.6	1384.1	1390.3	517.07
0.5021	1016.48	1418.35	1419.3	1411.7	1418.5	489.02
0.6158	1029.59	1447.62	1448.2	1435.2	1449.2	463.47
0.7241	1054.79	1470.18	1471.5	1458.3	1471.4	438.62
0.8021	1078.42	1498.87	1499.8	1483.1	1499.0	412.74
0.9087	1094.62	1528.07	1528.8	1525.8	1529.2	391.24

Conclusion

Density, speed of sound and their excess or deviation properties of IL with 1– Hexanol binary mixture have been reported at 298.15 K temperature and atmospheric pressure. Although IL show stronger hydrogen bonding 1-Butyl-3-ethylimidazolium Hexafluorophosphate with 1–Hexanol than conventional solvents. Prediction of the speed of sound can be obtained using Nomoto's relation and Schaaff's Collision Factor Theory mixing rules for systems containing ionic liquids. In addition, the calculations showed a systematic dependence of excess and deviation properties on the chain length for investigated mixture.

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Conflict of Interest

Not available

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Not available

References

1. Harris KR, Woolf LA, Kanakubo M. Temperature and pressure dependence of the viscosity of the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate. J Chem Eng Data. 2005;50:1777-1782.
2. Murthy NB, Rangacharyulu M, Krishna JSR. Acoustic and Thermodynamic Properties of Binary Mixtures of Ionic Liquid [Bmim] [PF6] and 2- Pyrrolidone fromT = (298.15to 323.15) K. International Journal of Science and Research. 2017;6(11):124-134.
3. Shekaari H, Sedighehnaz SM. Volumetric properties of ionic liquid 1, 3-dimethyl imidazolium methyl sulfate + molecular solvents at T = (298.15–328.15) K. Fluid Phase Equilib. 2010;291:201-207.
4. Wang JY, Zhao FY, Liu YM, Wang XL, Hu Y-Q. Thermo physical properties of pure 1-ethyl-3-methylimidazolium methyl sulphate and its binary mixtures with alcohols. Fluid Phase Equilib. 2011;305:114-120.
5. Requejo PF, Gonzalez EJ, Macedo EA, Dominguez AJ. Effect of the temperature on the physical properties of the pure ionic liquid 1-ethyl-3-methylimidazolium methyl sulfate and characterization of its binary mixtures with alcohols. Chem. Thermodyn. 2014;74:193-200.
6. Pereiro AB, Rodiguez A. Thermodynamic Properties of Ionic Liquids in Organic Solvents from (293.15 to 303.15) K. J Chem. Eng. Data. 2007;52:600-608.
7. Domanska U, Pobudkowska A, Wisniewska A. Solubility and Excess Molar Properties of 1,3- Di methylimidazolium Methyl sulfate, or 1-Butyl-3-Methylimidazolium Methyl sulfate, or 1-Butyl-3-Methylimidazolium Octylsulfate Ionic Liquids with n-Alkanes and Alcohols: Analysis in Terms of the PFP and FBT Models1. J Solution Chem. 2006;35:311-334.
8. Shukla RK, Gangwar VS, Singh SK. Effect of Molecular Structure of Lubricating Oil on Sound Velocity and Bulk Modulus. J Pure Appl. Ultrason. 2018;40(4):111-115.
9. Shukla RK, Gangwar VS, Pundhir VK. Density and speed of sound of binary liquid systems in temperature range 288.15 to 318.15 K. J Pure Appl. Ultrason, 2017;39:18-22.
10. Shukla RK, Gupta GK, Pramanik SK, Sharma AK, Singh B. Comparative Study of Speed of Sound and Isentropic Compressibility of Chlorobenzene + Benzene Binary Mixture from Various Models at Temperature Range 298.15 to 313.15 K. J Pure Appl Ultrason. 2013;35:80-86.
11. Redlich O, Kister AT. Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. Ind. Eng. Chem. 1948;40:345-348.
12. Schaffs W. Molecular Acoustics / Molekularakustik Springer-Verlag Berlin; c1963. (Chapters. XI and XII).
13. Jacobson B. Intermolecular Free Length in the Liquid State. Adiabatic and Isothermal Compressibilities. Acta Chem Scand. 1952;8:1485-1498.
14. Jacobson B. Ultrasonic Velocity in Liquids and Liquid Mixtures. J Chem Phys. 1952;20:927-928.
15. Nomoto O. Empirical Formula for Sound Velocity in Liquid Mixtures. J Phys Soc Jpn. 1958;13:1528-1532.
16. Timmermans J. Physico- Chemical Constants of Pure Organic Compounds. 8th Ed., Elsevier Pub Corp Inc New York; c1950.
17. Riddick JA, Bunger WS, Sakano T. Organic Solvents, Physical Properties and Methods of Purification. 4th ed John wiley and Sons Press New York; c1986.
18. Letcher TM, Domanska U, Mwenesongole E. The excess molar volumes and enthalpies of (N- methyl-2-pyrrolidinone + an alcohol) at T = 298.15 K and the application of the ERAS theory. Fluid Phase Equilib. 1998;149:323-337.
19. Benson GC, Kiyohara O. Evaluation of excess isentropic compressibilities and isochoric heat capacities. J Chem Thermodyn. 1979;11: 1061-1064

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