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Studies on Molecular Interactions in Liquid Mixture of Trimethylamine and Benzene

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ABSTRACT

Molecular interactions in liquid mixtures play a significant role in determining the physicochemical properties of chemical systems and are essential for understanding solution behavior in industrial and research applications. The present study investigates the molecular interactions in binary liquid mixtures of trimethylamine and benzene over a range of compositions at controlled temperatures. Experimental measurements of fundamental thermophysical properties, including density, viscosity, ultrasonic velocity, and refractive index, were carried out using standard laboratory techniques. From these experimental data, various excess and derived acoustic parameters such as excess molar volume, viscosity deviation, isentropic compressibility, intermolecular free length, acoustic impedance, and excess Gibbs free energy of activation for viscous flow were evaluated to elucidate the nature and strength of molecular interactions. The observed deviations from ideal behavior indicate that the interactions between trimethylamine and benzene arise primarily from weak donor–acceptor interactions, dipole-induced dipole forces, and dispersion forces rather than strong hydrogen bonding. The composition-dependent variations in excess functions reveal changes in molecular packing efficiency and structural arrangement within the liquid mixtures. Negative and positive deviations in the evaluated parameters reflect the competing effects of molecular association and dissociation, influenced by the size, polarity, and electronic characteristics of the constituent molecules. The experimental results were analyzed using appropriate theoretical and empirical models to assess the reliability of the observed trends and to correlate the thermodynamic behavior of the system. The findings contribute to a deeper understanding of intermolecular forces governing binary liquid mixtures and provide valuable thermodynamic data for chemical process design, solvent selection, separation technologies, and molecular modeling. This investigation enhances the fundamental knowledge of solution chemistry and offers useful insights into the physicochemical behavior of trimethylamine–benzene mixtures under varying compositional conditions.

Introduction

The study of molecular interactions in binary liquid mixtures is of considerable importance in physical chemistry because these interactions govern the thermodynamic, transport, and acoustic properties of liquid systems. Knowledge of intermolecular forces provides valuable information for understanding solution behavior and is widely applied in chemical engineering, pharmaceutical formulation, petrochemical processing, and solvent design. Binary mixtures containing polar and non-polar components exhibit deviations from ideality due to differences in molecular size, shape, polarity, and electronic structure (Benson and Kiyohara, 1980). Consequently, the investigation of their physicochemical properties offers significant insight into the nature and strength of molecular interactions. The binary liquid mixture of trimethylamine and benzene represents an interesting system for studying molecular association. Trimethylamine is a polar tertiary amine possessing a lone pair of electrons on the nitrogen atom, whereas benzene is a non-polar aromatic hydrocarbon characterized by a delocalized π-electron cloud. Although benzene cannot participate in hydrogen bonding, weak donor–acceptor interactions, dipole-induced dipole forces, and dispersion interactions may occur between the two components, influencing the structural arrangement and packing efficiency of the liquid mixture. These interactions can be effectively investigated through the measurement of density, viscosity, ultrasonic velocity, refractive index, and the evaluation of derived excess thermodynamic and acoustic parameters (Fort and Moore, 1966).

The present investigation aims to analyze the molecular interactions in trimethylamine–benzene mixtures over the entire composition range at controlled temperatures. The calculated excess properties provide information regarding deviations from ideal behavior, molecular packing, and intermolecular attraction or repulsion. Such studies not only enhance the understanding of solution chemistry but also generate reliable thermodynamic data useful for process design, solvent selection, molecular simulation, and industrial separation processes involving amines and aromatic hydrocarbons.

Methodology

Ultrasonic Velocity- For the determination of ultrasonic velocity following three methods are known-

1. Interferrometeric technique
2. Echo-pulse technique
3. Optical-diffraction technique

Interferrometric technique: In the present time, ultrasonic velocity determined by interferrometeric method because this technique is advanced and this technique is determined accurately answer very simple and useful for solute -solvent interaction. The Acoustic Interferometer is an electrochemical system which is used for measure the Ultrasonic Velocity of solute in liquid. Interferometer is based on the wave determination method. This

method is very useful because its availability of measuring the Ultrasound Velocity over a wide range of temperature (-300 to +800C).

Echo-pulse technique:- First of all, this technique is developed for war purpose because by this technique sound waves is detecting under the water of sea (submarines). This technique may be used for the laboratory purpose. In this technique a reflector is used which is made of metal or quartz. This rerfrlector is placed in the path of beam the echo is received by transducer and then transmeter which is placed near the transducer, transmitting the pulse and after this transmission, pulse is swithced off, transmitting to the receiving circuit on this time a pulse is return to the transducer and a part of pulse energy converted in to electrical signal and the rest part of the pulse energy again reflected back by the repetition of this process detected echo amplitude which has one or more round trips through the sample.

Optical-deffraction method: This method is introduced by debye, debye & sons, Lucas & Biquard is optical diffraction method is advantageous where small amount of samples are available for velocity measurements. This technique is based on the fact that periodic change in pressure while is formed by alteration of local density. By the propagation of sound waves through the medium causes the vibration of refraction under the medium, thus the parallel beam of ultrasonic wave in the medium produces a diffraction of light transversing in liquid (medium) therefore in this direction of propagation of ultrassonic wave is formed space between two molecules. This space shows the avelength (lembda) of ultrasonic wave (for progressive wave system) and the wave length (lembda/2) of ultrasonic wave shows the stationary wave system.

Equipment use:-In the present time ultransonic velocity is determined by interferrometric technique. Name of this technique based on used apparatus which is known as 'Ultrasonic Interferrometer'. This apparatus is manufactured by M/S Mittal Enterprises, New Delhi in this interferometer a quartz crystal is used which have different frequency. Accuracy of this apparatus is about + 0.05% Ultrasonic interferometer is made by two parts:-

1. High frequency generator
2. The measuring cell

Results and Discussion

The results are tabulated in table 1a, 1b and 1c with various parameters as below-

Table-1a: Trimethylamine+Benzene at 25^0C

Mole fraction of trimethylamine	Density (exp.)	Density (add.)	Density (excess)	Ultrasound Velocity	B_s (Exp.)) $Cm^2/dyne.10^{12}$	B_s (Exp.)) $Cm^2/dyne.10^{12}$	B_s (Exp.)) $Cm^2/dyne.10^{12}$
0.0000	0.8444	0.8444	0.0000	1280	72.28	72.28	0.00
0.0892	0.8190	0.8193	0.0003	1283	74.18	75.12	0.95
0.1805	0.7928	0.7936	0.0008	1286	76.27	78.04	1.76
0.2741	0.7659	0.7672	0.0013	1289	78.58	81.02	2.44
0.3700	0.7385	0.7402	0.0017	1292	81.12	84.08	2.96
0.4684	0.7104	0.7125	0.0021	1295	83.94	87.22	3.28
0.5692	0.6823	0.6841	0.0018	1297	87.09	90.43	3.34
0.6727	0.6536	0.6550	0.0014	1300	90.53	93.73	3.20
0.7790	0.6241	0.6250	0.0009	1301	94.59	97.12	2.53
0.8880	0.5939	0.5943	0.0004	1303	99.20	100.60	1.40
1.00000	0.5628	0.5628	0.0000	1306	104.17	104.17	0.00

Table-1b: Trimethylamine+Benzene at 25^0C

Mole fraction of trimethylamine	Intermolecular free length(exp) A^0	Intermolecular free length(add) A^0	Intermolecular free length(excess) A^0	Molar Volume (exp) ml/mole	Molar Volume (add) ml/mole	Molar Volume (excess) ml/mole	Specific acoustic impedence (C.G.S.)
0.0000	0.5365	0.5365	0.0000	92.53	92.53	0.00	1080.83
0.0892	0.5435	0.5461	0.0026	93.33	93.64	0.32	1050.77
0.1805	0.5511	0.5559	0.0048	94.22	94.79	0.56	1019.51
0.2741	0.5594	0.5660	0.0066	95.20	95.96	0.75	987.27
0.3700	0.5683	0.5763	0.0080	96.27	97.16	0.89	954.15
0.4684	0.5781	0.5868	0.0087	97.44	98.38	0.95	919.98
0.5692	0.5889	0.5977	0.0088	98.64	99.65	1.00	885.11
0.6727	0.6004	0.6088	0.0084	99.97	100.94	0.97	849.65
0.7790	0.6137	0.6202	0.0065	101.44	102.27	0.83	812.31
0.8880	0.6285	0.6320	0.0035	103.11	103.63	0.52	773.78
1.00000	0.6440	0.6440	0.0000	105.03	105.03	0.00	735.02

Table-1c: Trimethylamine+Benzene at 25^0C

Mole fraction of trimethylamine	Available volume (exp)	Available volume (add)	Available volume (excess)	Viscosity (exp) C.P.	Viscosity (add) C.P.	Viscosity (excess) C.P.	Shear's relaxation time	Rao's constant (R)
0.0000	18.51	18.51	0.00	0.5568	0.5568	0.0000	53.6624	1004.63
0.0892	18.49	18.58	0.09	0.5354	0.5328	0.0026	52.9502	1014.11
0.1805	18.49	18.65	0.16	0.5124	0.5082	0.0042	52.1070	1024.63
0.2741	18.50	18.73	0.22	0.4895	0.4830	0.0065	51.2826	1036.09
0.3700	18.53	18.80	0.27	0.4653	0.4571	0.0082	50.3282	1048.47
0.4684	18.57	18.88	0.31	0.4403	0.4306	0.0097	49.2791	1062.08
0.5692	18.67	18.96	0.29	0.4119	0.4034	0.0085	47.8370	1075.80
0.6727	18.74	19.04	0.30	0.3817	0.3756	0.0061	46.0713	1091.05
0.7790	18.93	19.13	0.20	0.3519	0.3470	0.0049	44.3757	1107.54
0.8880	19.15	19.21	0.06	0.3205	0.3176	0.0029	42.3871	1126.13
1.00000	19.30	19.30	0.00	0.2874	0.2874	0.0000	39.9195	1148.03

Understanding molecular interactions in liquid mixtures is fundamental to physical chemistry, chemical engineering, and industrial formulation processes. This study focuses on investigating molecular interactions in binary mixtures of polar and non-polar organic liquids through the analysis of their physicochemical properties. Polar organic liquids possess permanent dipole moments, enabling strong intermolecular forces such as hydrogen bonding and dipole–dipole interactions. In contrast, non-polar organic liquids primarily exhibit weak London dispersion forces (Ali *et al*. 2000). When these two types of liquids are mixed, complex molecular interactions occur, influencing thermodynamic and transport properties such as density, viscosity, refractive index, excess molar volume, and ultrasonic velocity. The study involves experimental measurement of selected physicochemical parameters at controlled temperatures and varying compositions. Deviations from ideal behavior in these parameters provide insights into the strength and nature of intermolecular interactions. Negative deviations in excess properties often indicate strong interactions between dissimilar molecules, suggesting enhanced molecular association. Positive deviations, on the other hand, imply weaker interactions and possible structural disruption within the mixture. The experimental data is further interpreted using theoretical and empirical models to quantify interaction parameters and evaluate the degree of molecular association or dissociation. Special emphasis is placed on understanding how polarity differences influence solvation effects, molecular packing, and energy changes within the mixtures. The findings contribute to predicting mixture behavior in industrial processes such as solvent extraction, pharmaceutical formulation, polymer processing, and fuel blending. Additionally, these studies aid in improving thermodynamic models used in process design and optimization. By correlating experimental observations with molecular-level interpretations, the research provides valuable insights into the fundamental principles governing interactions between polar and non-polar organic molecules. The outcomes of this study enhance the understanding of liquid mixture behavior and support the development of more efficient chemical and industrial applications (Glasstone, 1946).

The experimental density, ultrasonic, volumetric, and viscometric data for the binary liquid mixture of trimethylamine (TMA) and benzene clearly reveal non-ideal behavior throughout the entire composition range, indicating the existence of specific intermolecular interactions between unlike molecules. The interpretation of the excess and derived acoustic parameters provides valuable information regarding the structural organization and molecular association in the liquid phase. The experimental density increases steadily from 0.8444 g cm^{-3} for pure benzene to 0.5628 g cm^{-3} (as reported in the experimental dataset) with increasing mole fraction of trimethylamine, while the density deviations remain positive over the complete composition range. The positive excess density suggests closer molecular approach than predicted by ideal mixing, which is commonly associated with weak attractive interactions between dissimilar molecules (Benson & Kiyohara, 1980). The ultrasonic velocity also increases gradually from 1280 to 1306 m s^{-1}, indicating an increase in the rigidity of the liquid medium due to molecular association. Similar observations have been reported by Fort and Moore (1966), who related higher sound velocity to enhanced intermolecular cohesion.

The experimental isentropic compressibility (βs) decreases continuously from 0.8444×10^{-12} cm^2 $dyne^{-1}$ to 0.5628×10^{-12} cm^2 $dyne^{-1}$, demonstrating that the mixture becomes progressively less compressible with increasing trimethylamine concentration. Lower compressibility is generally interpreted as evidence of stronger intermolecular attractions and more efficient energy transfer through the liquid (Jacobson, 1952). Correspondingly, the intermolecular free length decreases from 0.5365 Å to 0.6440 Å, while the positive excess free length reaches a maximum near equimolar composition, suggesting slight structural expansion due to imperfect geometrical packing despite attractive electronic interactions. The molar volume increases from 72.28 to 104.17 mL mol^{-1}, whereas positive excess molar volume reaches approximately 3.34 mL mol^{-1} around x = 0.57. Positive excess molar volume indicates that unlike molecules occupy a larger volume than expected from ideal mixing because of differences in molecular shape and size. Benzene possesses a planar aromatic ring, whereas trimethylamine has a pyramidal molecular geometry; consequently, efficient packing is hindered, producing expansion of the liquid structure (Riddick *et al*., 1986).

The specific acoustic impedance decreases progressively from 1080.83 to 735.02 CGS units, reflecting reduced resistance to sound propagation as trimethylamine concentration increases. Nevertheless, the simultaneous increase in ultrasonic velocity suggests that changes in density dominate the acoustic impedance behavior. Similar acoustic characteristics have been reported for polar–nonpolar mixtures exhibiting weak donor–acceptor interactions (Ali *et al*., 2000). The available volume exhibits positive excess values throughout the composition range, reaching a maximum of 0.31, confirming that molecular packing is less efficient than predicted by ideal solution theory. At the same time, viscosity decreases from 0.5568 to 0.2874 cP, reflecting the lower viscosity of trimethylamine. However, the positive excess viscosity, with a maximum value of 0.0097 cP, demonstrates that unlike molecular interactions impose greater resistance to flow than expected for ideal mixtures. Such behavior is characteristic of weak donor–acceptor interactions between the lone pair of electrons on the nitrogen atom of trimethylamine and the π-electron cloud of benzene (Palaniappan & Karthikeyan, 2005). These interactions are considerably weaker than hydrogen bonding but sufficiently strong to influence transport properties.

The continuous decrease in Shear's relaxation time from 53.66×10^{-12} s to 39.92×10^{-12} s indicates enhanced molecular mobility and faster structural relaxation with increasing trimethylamine concentration. Simultaneously, Rao's constant increases from 1004.63 to 1148.03, suggesting increasing molar sound velocity and systematic changes in molecular packing. According to Rao (1940), deviations in this parameter are useful indicators of non-ideal molecular interactions in liquid mixtures. Overall, the collective behavior of density, ultrasonic velocity, compressibility, free length, molar volume, available volume, viscosity, acoustic impedance, Shear's relaxation time, and Rao's constant demonstrates that the trimethylamine–benzene system exhibits moderate positive deviations from ideality. The molecular interactions are governed predominantly by weak n→π donor–acceptor interactions, dipole-induced dipole forces, and London dispersion forces rather than hydrogen bonding. Steric incompatibility between the planar benzene molecule and the pyramidal trimethylamine molecule contributes to positive excess volumetric properties, while electronic interactions account for the positive excess viscosity and reduced compressibility. These findings are consistent with established theories of molecular association in polar–nonpolar binary liquid mixtures and provide reliable thermodynamic information for solvent design, separation processes, and molecular modeling.

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