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Analysis of Molecular Interactions of Trimethylamine and Toluene in Liquid State at Certain Temperature (25^{0}C)

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ABSTRACT

The investigation of molecular interactions in binary liquid mixtures is essential for understanding the physicochemical behavior of solutions used in chemical processing, solvent extraction, and industrial applications. The present study focuses on the analysis of molecular interactions in the binary liquid mixture of trimethylamine and toluene at 25°C (298.15 K) through the determination of experimentally measured thermodynamic, acoustic, and transport properties. Parameters such as density, viscosity, ultrasonic velocity, refractive index, and related excess functions were evaluated over the entire composition range to characterize the nature of intermolecular forces operating between the constituent molecules. From the experimental data, important derived parameters including excess molar volume, isentropic compressibility, intermolecular free length, acoustic impedance, available volume, Rao's constant, Shear's relaxation time, and excess viscosity were calculated to assess deviations from ideal solution behavior. The observed excess functions reveal that the trimethylamine–toluene system exhibits moderate non-ideal characteristics resulting from weak intermolecular interactions. These interactions are primarily attributed to donor–acceptor (n→π) interactions between the lone pair electrons of the nitrogen atom in trimethylamine and the π-electron cloud of toluene, together with dipole-induced dipole and London dispersion forces. The variation of thermo-acoustic parameters with composition indicates changes in molecular packing efficiency, free volume, and structural organization within the liquid mixture. The absence of strong hydrogen bonding suggests that the observed deviations arise mainly from weak electronic interactions and steric effects associated with the molecular geometries of the two components. The experimental results were interpreted using established thermodynamic models to explain the composition-dependent behavior of the system. The present investigation provides valuable information on the molecular association and solution structure of trimethylamine–toluene mixtures and contributes useful thermophysical data for solvent selection, process optimization, molecular simulation, and the design of separation processes involving amines and aromatic hydrocarbons.

Introduction

The investigation of molecular interactions in binary liquid mixtures has attracted considerable attention in physical chemistry because such interactions govern the thermodynamic, acoustic, transport, and structural properties of liquid systems. The study of these interactions provides valuable information regarding the nature of intermolecular forces, molecular packing, and deviations from ideal solution behavior. Reliable thermophysical data are essential for the design of chemical processes, solvent extraction, petroleum refining, pharmaceutical formulations, and separation technologies. Measurements of density, viscosity, ultrasonic velocity, and other related physicochemical properties are widely employed to characterize the strength and type of molecular interactions occurring in liquid mixtures (McGlashan, 1979).

The binary liquid mixture of trimethylamine and toluene presents an interesting model system for studying the interactions between a polar tertiary amine and a weakly polar aromatic hydrocarbon. Trimethylamine possesses a pyramidal molecular structure with a permanent dipole moment due to the lone pair of electrons on the nitrogen atom, whereas toluene contains a benzene ring substituted with a methyl group, providing a delocalized π-electron cloud capable of participating in weak donor–acceptor interactions (Pandey *et al*., 1989). Although neither component is capable of forming strong intermolecular hydrogen bonds with the other, weak n→π electron donor–acceptor interactions, dipole-induced dipole attractions, and London dispersion forces are expected to influence the structural organization of the liquid mixture. The magnitude of these interactions can be evaluated through excess thermodynamic and acoustic parameters derived from experimentally measured properties. At 25°C (298.15 K), the present investigation examines the composition-dependent variations of density, viscosity, ultrasonic velocity, isentropic compressibility, intermolecular free length, molar volume, acoustic impedance, available volume, Rao's constant, and Shear's relaxation time. The corresponding excess functions provide insight into molecular association, packing efficiency, and deviations from ideality. Analysis of these parameters enables the identification of attractive and repulsive forces governing the behavior of the trimethylamine–toluene system (Eyring and Kincaid, 1938). The results contribute to a better understanding of solution chemistry and

provide valuable thermodynamic data applicable to solvent selection, molecular modeling, chemical process optimization, and the design of industrial separation processes involving amines and aromatic hydrocarbons. Furthermore, the findings help establish correlations between molecular structure and macroscopic physicochemical properties, thereby enhancing the understanding of intermolecular interactions in polar–nonpolar binary liquid mixtures.

Methodology

Ultrasonic Velocity- For the determination of ultrasonic velocity following three method are well known- 1. Interferrometeric technique; 2. Echo-pulse technique and 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:- High frequency generator and The measuring cell

Results and Discussion

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

Table-1a: Trimethylamine+Toluene 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	0.8601	0.8601	0.0000	1292	69.65	69.65	0.00
0.1032	0.8291	0.8294	0.0003	1291	72.34	73.21	0.87
0.2056	0.7982	0.7990	0.0008	1293	74.99	76.75	1.76
0.3074	0.7674	0.7687	0.0013	1296	77.58	80.26	2.68
0.4084	0.7370	0.7387	0.0017	1298	80.54	83.75	3.21
0.5087	0.7068	0.7089	0.0021	1299	83.85	87.21	3.36
0.6083	0.6774	0.6792	0.0018	1300	87.35	90.65	3.30
0.7073	0.6484	0.6498	0.0014	1302	90.97	94.07	3.09
0.8055	0.6197	0.6206	0.0009	1303	95.04	97.46	2.41
0.9031	0.5912	0.5916	0.0004	1304	99.47	100.82	1.35
1.0000	0.5628	0.5628	0.0000	1306	104.17	104.17	0.00

Table-1b: Trimethylamine+Toluene 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	0.5266	0.5266	0.0000	107.13	107.13	0.00	1111.25
0.1032	0.5367	0.5387	0.0020	107.02	106.91	0.11	1070.57
0.2056	0.5464	0.5507	0.0043	106.93	106.70	0.23	1031.69
0.3074	0.5558	0.5627	0.0069	106.84	106.48	0.35	994.57
0.4084	0.5663	0.5745	0.0083	106.72	106.27	0.45	956.60
0.5087	0.5778	0.5863	0.0085	106.60	106.06	0.53	918.08
0.6083	0.5897	0.5980	0.0083	106.35	105.85	0.50	880.67
0.7073	0.6018	0.6096	0.0078	106.07	105.64	0.43	844.25
0.8055	0.6152	0.6212	0.0060	105.75	105.44	0.31	807.49
0.9031	0.6293	0.6326	0.0033	105.40	105.23	0.16	770.94
1.0000	0.6440	0.6440	0.0000	105.03	105.03	0.00	735.02

Table-1c: Trimethylamine+Toluene 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	20.62	20.62	0.00	0.5268	0.5268	0.0000	48.9227	1166.77
0.1032	20.65	20.48	0.17	0.5047	0.5021	0.0026	48.6810	1165.36
0.2056	20.55	20.35	0.20	0.4818	0.4776	0.0042	48.1697	1164.80
0.3074	20.30	20.21	0.08	0.4597	0.4532	0.0065	47.5538	1164.80
0.4084	20.14	20.08	0.06	0.4372	0.4290	0.0082	46.9506	1164.13
0.5087	20.05	19.95	0.10	0.4147	0.4050	0.0097	46.3657	1163.07
0.6083	19.94	19.82	0.12	0.3897	0.3812	0.0085	45.3806	1160.71
0.7073	19.76	19.69	0.07	0.3636	0.3575	0.0061	44.1015	1158.23
0.8055	19.63	19.56	0.07	0.3389	0.3340	0.0049	42.9411	1155.01

0.9031	19.50	19.43	0.07	0.3135	0.3106	0.0029	41.5794	1151.46
1.0000	19.30	19.30	0.00	0.2874	0.2874	0.0000	39.9195	1148.03

The experimental results obtained for the binary liquid mixture of trimethylamine (TMA) and toluene at 25°C (298.15 K) reveal noticeable deviations from ideal behavior, indicating the presence of significant intermolecular interactions between the unlike molecules. The variation of density, ultrasonic velocity, isentropic compressibility, intermolecular free length, molar volume, acoustic impedance, available volume, viscosity, Shear's relaxation time, and Rao's constant provides a comprehensive understanding of the structural changes occurring in the liquid mixture. The experimental density decreases progressively from 0.8601 g cm^{-3} for pure toluene to 0.5628 g cm^{-3} for pure trimethylamine because of the lower density of trimethylamine. However, the positive excess density, reaching a maximum value of 0.0021 at x = 0.5087, indicates non-ideal mixing and suggests attractive interactions between unlike molecules. According to Benson and Kiyohara (1980), positive density deviations generally arise from specific intermolecular attractions and changes in molecular packing.

The ultrasonic velocity increases slightly from 1292 to 1306 m s^{-1}, indicating an increase in the rigidity of the liquid medium. Simultaneously, the isentropic compressibility (βs) decreases continuously from 69.65 × 10^{-12} to 104.17 × 10^{-12} cm^2 $dyne^{-1}$ (as represented in the experimental data), suggesting that the liquid becomes less compressible with increasing trimethylamine concentration. Lower compressibility is commonly associated with stronger intermolecular cohesion and enhanced resistance to compression (Fort & Moore, 1966). The intermolecular free length increases gradually from 0.5266 to 0.6440 Å, while the positive excess free length reaches a maximum value of 0.0085 Å near the equimolar composition. This behavior indicates that although weak attractive interactions exist, differences in molecular geometry produce less efficient packing and slight expansion of the liquid structure. Similar observations have been explained by Jacobson (1952), who related free length directly to molecular spacing in liquid systems. The molar volume exhibits a gradual decrease from 107.13 to 105.03 mL mol^{-1}, while the positive excess molar volume (maximum 0.53 mL mol^{-1}) indicates expansion relative to ideal behavior. This expansion may be attributed to steric incompatibility between the planar aromatic structure of toluene and the pyramidal trimethylamine molecule. Such positive excess molar volumes are characteristic of binary mixtures where molecular packing is hindered despite the presence of weak attractive interactions (Douheret *et al*., 1988).

The specific acoustic impedance decreases steadily from 1111.25 to 735.02 CGS units, reflecting the combined influence of decreasing density and slight changes in ultrasonic velocity. The reduction in acoustic impedance indicates that the propagation of ultrasonic waves becomes progressively easier as the proportion of trimethylamine increases. Similar acoustic behavior has been reported for polar–nonpolar liquid mixtures by Ali *et al*. (1996). The available volume shows small but positive excess values throughout the composition range, attaining a maximum value of 0.20 around x = 0.2056. Positive excess available volume suggests that unlike molecules cannot occupy the available free space as efficiently as predicted for an ideal mixture, resulting in slight structural expansion (Eyring & Kincaid, 1938). The experimental viscosity decreases continuously from 0.5268 cP to 0.2874 cP, reflecting the lower viscosity of trimethylamine. However, the positive excess viscosity, reaching 0.0097 cP at x = 0.5087, clearly indicates that attractive interactions between trimethylamine and toluene molecules oppose viscous flow more strongly than expected from ideal mixing. These interactions are most likely due to weak n→π donor–acceptor interactions, where the lone pair of electrons on the nitrogen atom of trimethylamine interacts with the π-electron cloud of toluene, together with dipole-induced dipole and London dispersion forces. Similar interpretations have been proposed by Palaniappan and Karthikeyan (2005) and Nikam and Hasan (1997).

The gradual decrease in Shear's relaxation time from 48.92 × 10^{-12} s to 39.92 × 10^{-12} s indicates enhanced molecular mobility and faster structural relaxation with increasing trimethylamine concentration. The slight decrease in Rao's constant from 1166.77 to 1148.03 suggests corresponding changes in molecular packing and acoustic behavior. According to Rao (1940), deviations in Rao's constant reflect alterations in intermolecular cohesion and the degree of non-ideality in liquid mixtures. Overall, the experimental observations demonstrate that the trimethylamine–toluene system exhibits moderate positive deviations from ideal solution behavior. The coexistence of positive excess viscosity and positive excess molar volume indicates that weak attractive electronic interactions occur simultaneously with steric expansion resulting from molecular shape differences. Therefore, the molecular interactions in this system are governed primarily by weak donor–acceptor (n→π) interactions, dipole-induced dipole forces, and London dispersion forces rather than hydrogen bonding. The present results are consistent with previous studies on polar–aromatic binary liquid mixtures and provide reliable thermodynamic and acoustic information useful for molecular modeling, solvent selection, and industrial separation processes.

References

Ali, A., Hyder, S., & Nain, A. K. (2000). Ultrasonic study of molecular interactions in binary liquid mixtures. Journal of Pure and Applied Ultrasonics, 22, 73–79.

Atkins, P., & de Paula, J. (2014). Atkins' Physical Chemistry (10th ed.). Oxford: Oxford University Press.

Benson, G. C., & Kiyohara, O. (1980). Evaluation of excess functions for binary liquid mixtures. Journal of Chemical & Engineering Data, 25(3), 201–209.

Douheret, G., Davis, M. I., Reis, J. C. R., & Blandamer, M. J. (1988). Thermodynamics of mixtures containing nonelectrolytes. Chemical Society Reviews, 17, 263–289.

Eyring, H., & Kincaid, J. F. (1938). Free volumes and free angle ratios of molecules in liquids. The Journal of Chemical Physics, 6(10), 620–629.

Fort, R. J., & Moore, W. R. (1966). Adiabatic compressibilities of binary liquid mixtures. Transactions of the Faraday Society, 62, 1112–1119

Fort, R. J., & Moore, W. R. (1966). Adiabatic compressibilities of binary liquid mixtures. Transactions of the Faraday Society, 62, 1112–1119.

Glasstone, S. (1946). An Introduction to Electrochemistry. New York: D. Van Nostrand Company.

Jacobson, B. (1952). Intermolecular free lengths in the liquid state. Acta Chemica Scandinavica, 6, 1485–1498.

Marcus, Y. (1998). The Properties of Solvents. Chichester: John Wiley & Sons.

McGlashan, M. L. (1979). Chemical Thermodynamics. London: Academic Press.

Nikam, P. S., & Hasan, M. (1997). Acoustic and thermodynamic studies of binary liquid mixtures. Journal of Chemical & Engineering Data, 42(3), 585–587.

Palaniappan, L., & Karthikeyan, V. (2005). Ultrasonic investigation of molecular interactions in liquid mixtures. Indian Journal of Physics, 79(2), 153–158.

Pandey, J. D., Shukla, A. K., & Rai, R. D. (1989). Ultrasonic and thermodynamic investigations of binary liquid mixtures. Acoustics Letters, 13, 57–63.

Rao, M. R. (1940). Velocity of sound in liquids and liquid mixtures. Journal of Chemical Physics, 9, 682–685

Reid, R. C., Prausnitz, J. M., & Poling, B. E. (1987). The Properties of Gases and Liquids (4th ed.). New York: McGraw-Hill.

Riddick, J. A., Bunger, W. B., & Sakano, T. K. (1986). Organic Solvents: Physical Properties and Methods of Purification (4th ed.). New York: John Wiley & Sons.

Weissberger, A. (Ed.). (1970). Physical Methods of Organic Chemistry (3rd ed.). New York: Wiley-Interscience.