ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Theoretical Investigation of Ultrasonic Studies and Molecular Interactions in Binary Liquid Mixtures

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ABSTRACT

The ultrasonic velocity can be measured using a single crystal variable path interferometer with 2MHZ by standard procedure. Using the ultrasonic velocity, various acoustical parameters such as adiabatic compressibility(β_a), free length(L_f), acoustic impedance(Z), free volume(V_f), molar volume(V), internal pressure($\prod_i$), relaxation time(τ), Rao's constant(R), Enthalpy(H), Wada's constant(W), apparent molar volume(ϕ_v), apparent molar compressibility(ϕ_k) can be calculated. Using the experimental and computed data excess parameters such as excess adiabatic compressibility (β^E), excess acoustic impedance (Z^E), excess intermolecular free length (L_f^E), excess volume(Δv), excess viscosity($\Delta\eta$), can be computed. The density and viscosity for the binary liquid mixtures can be measured by using the specific gravity bottle method and Ostwald viscometer respectively. This papers investigates the theoretical aspects for the ultrasonic and molecular interactions in binary liquids.
Keywords: ultrasonic velocity, density, viscosity, acoustical parameter, excess parameter.

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INTRODUCTION

Ultrasonic investigations finds extensive applications in characterising aspects of thermodynamic and physico-chemical behaviour of binary and ternary liquid mixtures.In recent years, the measurements of ultrasonic velocity have been adequately employed in understanding the nature of molecular interactions in liquid mixtures. Ultrasonic propagation parameters results with valuable information regarding the behaviour of binary liquid systems because of intramolecular and intermolecular association, dipolar interactions, complex formation and related structural changes affect the compressibility of the system which inturn produces corresponding variations in the ultrasonic velocity[1].The ultrasonic velocity measurements are highly sensitive to molecular interaction and can be used to provide qualitative information about the physical nature and strength of molecular interaction in the liquid mixture [2-4].Ultrasonic velocity of a liquid is fundamentally related to the binding forces between the atoms or the molecules. Ultrasonic velocities of the liquid mixtures may consist of polar and non-polar components are of considerable importance in understanding intermolecular interaction between component molecules and find applications in several industrial and technological processes [5-9]. Ultrasonic velocity measurements are helpful to interpret solute-solvent, ion-solvent and solvent-solvent interaction in aqueous and non-aqueous medium [10,11].The ultrasonic velocities were measured by using single crystal ultrasonic pulse echo interferometer. It consists of a high frequency generator and a measuring cellwith capacity of about 12ml [12]. The variation of ultrasonic velocity and related parameters throw much light upon the structural changes associated with the liquid mixtures having weak and strong interacting components[13,14]. Ultrasonic velocity (u), density (ρ) and the viscosity (η) for various volume fractioncan be measured at a particular frequency (say 2MHZ or 3MHZ or 5MHZ) with or without variation in temperature. The various acoustical parameters such as adiabatic compressibility(β_a), free length(L_f), acoustic impedance(Z), free volume(V_f), molar volume(V), internal pressure($\prod_i$), relaxation time(τ), Rao's constant(R), Enthalpy(H), Wada's constant(W), apparent molar volume(ϕ_v), apparent molar compressibility(ϕ_k) can be calculated. Using these experimental and computed data excess parameters such as excess adiabatic compressibility(β^E), excess acoustic impedance(Z^E), excess intermolecular free length(L_f^E), excess volume(Δv), excess viscosity(Δη), can be computed [15-18]. The present works discuss about the possible theoretical approach for the determination of ultrasonic parameters and molecular interactions of any binary or ternary liquids.

Theoretical Details

Ultrasonic Velocity (u):

The ultrasonic (u) can be measured using ultrasonic interferometer at the frequency 2MHZ [19].

$$u = \lambda f \, m/sec$$

Where, λ is the wave length and f is the frequency of interferometer

Density (ρ):

The densities were measured by using specific gravity bottle and electronic balance. The density (ρ), is given by,

$$\rho_2 = \frac{W_2}{W_1}\rho_1 \text{ kgm}^{-3}$$

Where, W_1 is the weight of the distilled water, W_2 is the weight of the experimental liquid
ρ_1 is the density of the water, ρ_2 is the density of the experimental liquid

Viscosity (η):

Viscosities were measured at the desired temperature using Ostwald's viscometer. The flow time can be measured for the solution taken. The flow measurements were made an electronic stop watch with a precision of 0.01s.The viscosity (η) is given by,

$$\eta_2 = \eta_1 \frac{t_2}{t_1}\frac{\rho_2}{\rho_1} \text{ N s m}^{-2}$$

Where, η_1 is the viscosity of water, η_2 is the viscosity of the experimental liquid
t_1 is the time of flow of water, t_2 is the time of flow of the experimental liquid
ρ_1 is the density of water, ρ_2 is the density of the experimental liquid

Acoustic Impedance (Z):

Acoustic impedance (Z) is found to be almost inversely to the adiabatic compressibility. The relation is given by [20].

$$Z = u\rho \text{ m}^{-2}\text{s}^{-1}$$

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

Adiabatic Compressibility (β_a):

Adiabatic compressibility can be calculated from the speed of sound(u), and the density of the medium(ρ).The relation is given by[21].

$$\beta_a = \frac{1}{u^2\rho} \text{ ms}^2\text{kg}^{-1}$$

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

Intermolecular Free Length (L_f):

The adiabatic compressibility of a liquid can be expressed interms of the intermolecular free length which is the distance between the surfaces of the neighbouring molecules and is given by [22].

$$L_f = K\beta^{1/2} m$$

Where, K = 1.98 × 10^{-6} Jacobson constant (K values for different temperatures were taken from the work of Jacobson) [23].

Free Volume (V_f):

The free volume (v_f), is the effective volume (M_{eff}), in which particular molecular liquid and ultrasonic velocity(u), and viscosity of the liquid(η), as[24].

$$V = \left(\frac{M_{eff}\, u}{K}\right)^{3/2}$$

Where, K = 4.28 × 10^9, M_{eff} is the effective molecular weight= $X_1M_1 + X_2M_2$
M_1, M_2 is the molecular weight of the component, X_1,$X_2$is the mole fraction of the individual component, u is the ultrasonic velocity and η is the viscosity

Molar Volume (V):

The molar volume of the liquid is given by [25].

$$V = \frac{M_{eff}}{\rho}$$

Where,M_{eff} is the effective molecular weight= $X_1M_1+X_2M_2$
M_1, M_2 is the molecular weight of the components, X_1,X_2 is themole fraction of components
ρis the density

Internal Pressure ($\prod_i$):

The measurements of internal pressure are important in the study of the thermodynamic properties of liquids [26] and is given by.

$$\prod_i = \{bRT/(V^2V_f)^{1/2}\}\ Nm^{-2}$$

Where, b is the packing factor, R is the gas constant, $V_f$is the free volume, T is the temperature

Viscosity Relaxation Time (τ):

The relaxation time is given by [27].

$$\tau = \frac{4}{3\rho u^2}$$

Where, ρ is the density and η is theviscosity

Apparent Volar Volume (ϕ_v):

The apparent molar volume (ϕ_v), is given by [28].

$$\phi_v=[10^3(\rho_0-\rho)/m\rho\rho_0]+(M/\rho_0)$$

Where, m is the molarity of the solution, Mis the relative molar mass of the solute and ρ_0,$\rho$is the densities

Apparent Molar Compressibility (ϕ_k):

The apparent molar compressibility (ϕ_k), is given by [28].

$$\Phi_k= [10^3(K_s\rho_0-\rho)/m\rho\rho_0]+(K_sM/\rho_0)$$

Where, m is the molarity of the solution, M is the relative molar mass of the solute and ρ_0,$\rho$is the densities

Rao's Constant (R):

The Rao's constant(R), is given by,

$$R = u^{1/3} V$$

Where, u is the ultrasonic velocity and V is the molar volume

Enthalpy (H):

The enthalpy (H), is given by,

$$H = \prod_i V$$

Where, $\prod_i$ is the internal pressure and V is the molar volume

Wada's Constant (W):

The Wada's constant is given by [29].

$$W = \beta_a^{1/7}V$$

Where, β_a is the adiabatic compressibility and V is the molar volume

Gibb's Free Energy (ΔG):

Gibb's free energy is calculated from the relation [30].

$$\Delta G = kT\ln[k T \square \quad \not\square h]$$

Where is the viscous relaxation time, k the Boltzmaan's constant (1.23 × 10–23 JK–1), T the absolute temperature and h is the Planck's constant (6.6 × 10–34 Js).

Relative Association (RA):

The relative association RA has been determined using the standard formula [31].

$$R_A = \left(\frac{\rho}{\rho}\right)\left(\frac{U}{U}\right)^{1/3}$$

Where $\rho_\circ$ and ρ are the densities and U_0 and U, the ultrasonic velocities of the solvent and the solution, respectively.

Excess Parameters

Excess Value (A^E):

Excess value (A^E) of the interaction parameter can be calculated by[32],

$$A^E = A_{exp} - A_{id}$$

Where, $A_{id} = \sum_{i=1}^{n} A_i x_i$

A_i is the acoustical parameter and x_i is the mole fraction of liquid components

CONCLUSION

The ultrasonic studies of liquid is a non-destructive investigation used for probing the nature of the acoustical and molecular interaction in liquids. Ultrasonic velocity measurements can be employed to detect and assess weak and strong molecular interactions present in binary and ternary liquid mixtures. This can be employed to all types of liquid mixtures (binary, ternary, oils etc). The various acoustical parameters, excess parameters and thermodynamic parameters describe in this paper can be calculated for the liquid mixtures from ultrasonic velocity, density and viscosity of the binary liquid mixtures.

REFERENCES

[1] B Sathyanarayana, T SavithaJyostna, N Satyanarayana. Indian J Pure Appl Physics 2006;44:587-591.

[2] Kincaid JF, Eyring H. J Chem Physics 1937;5:587.

[3] Mahta SK, Chauhan RK. J Solution Chem1996;26:295.

[4] Dewan RK, Mehta SK, Parashar R, Bala K. J Chem Soc Faraday Trans1991;87:1561.

[5] Rama Rao GV, Sarma AV,Rambabu C. Indian J Pure Appl Phys 2004;42: 820.

[6] Pal A , Kumar H. J Chem Thermodyn 2004;36:173.

[7] Rao TS, Veeraiah N , Rambabu C. Indian J Pure Appl Phys 2002;40: 850.
[8] Valen A, Lopez MC, Urieta JS, Royo FM , Lafuente C. J Mol Liquids 2002;95:157.
[9] Nikkam PS, Jagdale BS, Sawant AB, Mehdi Hasan. Indian J Pure Appl Phys2001;39:433.
[10] Tabhane VA. Acoust Lett (G.B) 1983;6:120.
[11] Balaja S, Oza S. 2012; 200:11-18.
[12] FakruddinSrinivasu Ch, Sarma NT, Narendra kola. Journal of chemical Biological and physical science 2012;2.
[13] Thirumaran S, Sathish K. Bull Pure Appl Sci 2008;27(2):239-248.
[14] Thirumaran S, Karthikeyan N. Int J Chem Res 2011;3:83-98.
[15] Kanhekar SR 2012;2(3):71-85.
[16] Rita Mehra , Meenakshipancholi. Indian J Pure Appl Phys 45:580-590.
[17] Nomoto O, J Phys Soc Jpn 1958; 13:1528.
[18] Kalidoss S , Saivasamoorthy T. J Pure Appl 1997;19:9.
[19] Rajathi K, Askar Ali SJ, and Rajendran A. J Chem Pharm Res 3(5):348-358.
[20] Sangita Sharma, Jasmine Bhalodia, Jayesh Ramani, Rigneshpatel. Intl J Phys Sci 2012;7(8):1205-1214.
[21] Fakruddin SK, Srinivasuch, Narendra Kolla. J Chem Pharm Res 2012;4(7):3606-3609.
[22] Nath G, Sahu S, Paikaray R. Indian J Physics2009;83(4):429-436.
[23] Jacobson B. J Chem Phys1952;29: 927.
[24] Ramteke JN. Adv App Sci Res 2012;3(3):1832-1835.
[25] Santhi N, Sabarathinam PL, Alamelumangai G, Madhumitha J, Emayavaramban M. 2012;5:59-71.
[26] Ubagaramary D,Neeraja P. IOSR J App Chem 2012;5:59-71.
[27] Sarat K Swain, Pragnya P, Priyadarshini. Indian J Pure Appl Phys 2010;48:539-542.
[28] Malasane PR, Aswar AS. Indian J Chem Technol 2005;12:689-694.
[29] Gajendra Bedare, Vivek Bhandakkar, Bhagwat Suryavanshi. Intl J Appl Phys Mathemat 2012;2(3).
[30] Jayakumar S , Kannappan V. JASI Vol XXV 1997.
[31] Bahadur Alisha S , Rao KC. J Pure Appl Ultrason 2001;23:26.
[32] Pradhan SK, Dash SK, Moharan L, Swain BB. Indian J Pure Appl Phys 2012;50:161-166.