NONLINEAR ACOUSTICAL PROPERTIES IN AQUEOUS BIOMATERIALS

O.P.CHIMANKAR*, and V.A.TABHANE[@] and G.K.BAGHEL*
*P.G.Department of Physics, RTMNagpur University, Campus, Nagpur-440033 INDIA
Department of Physics, Institute of Science, Nagpur, INDIA

Abstract: *The ultrasonic velocity and adiabatic compressibility are the fundamental parameters used to determine the number of thermo-acoustical parameters. The volume expansivity is used to evaluate reduce volume, fractional free volume, repulsive exponent of intermolecular potential, Moelwyn-Hughes parameter, lattice Gruneisen parameter, Bayer's nonlinearity parameter and averageGruneisen parameter have been evaluated in aqueous glycine,L-arginine and L-methionine with various concentrations at temperature range 293K to 313K. The nonlinear variations of these parameters have been used to explain the molecular interactions, anharmonicity and structural information in aqueous biomaterials.*

Key-words:: Thermo-acoustics, Volume expansivity,Lattice Gruneisen parameter, Bayer's nonlinearity parameter,Moelwyn-Hughes parameter, Anharmonicity,

1. Introduction:

Acoustic and thermodynamic parameters have been extensively used to investigate the properties of liquids and liquid mixtures [1,2]. Such studies have been found to provide information about the intermolecular processes and the structure of liquid state. Thermo acoustic properties throw more light on the internal configurational energy of liquids [3].Many workers have studied the thermo acoustic properties in case of liquids, liquefied gases, molten metals and polymers[4-6]. But the review of literature reveals only few attempt to determined the thermo acoustic parameters in aqueous biomaterials [7,8].

Recently there has been an increased interest in the state of water in the living cell. For the knowledge of water- protein interaction, it is necessary to understand the role and interaction of biological macromolecules in living organisms.[9,10].The biological system contain 70% water. In the view of importance of biomaterials in human biological system, the present work, an attempt have been made to examine and analyze the relationship between different thermo acoustical parameters like reduced volume, fractional free volume, lattice Gruneisen parameter, Moelwyn Hughes parameter, Bayer's nonlinearity parameter average Gruneisen parameter for aqueous glycine,L-arginine and L- methionine at various concentration in the temperature range 293K to313K.

2. Problem Formulation:

The value of volume expansivity (α) is obtained from the graph between densities with temperature. The various thermo acoustical parameters are calculated using following relations:

1 .The molar volume is given by

$$V= M/\rho$$

Where M is the molecular weight and ρ is the density of mixture.

2. Reduced volume is evaluated using

$$Vr= \{1+ \alpha t/3(1+\alpha t)\}^{3}$$

3. Characteristic volume is given by

$$V^*= V/Vr$$

4. Available volume is calculated by

$$Va =V-V^*$$

5 .Fractional free volume is given by

$f = Va/V$

6. Repulsive exponent of intermolecular potential is evaluated by

$n=3\{2/f-5\}$

7. The Moelwyn-Hughes parameterC_1 is defined as

$C_1= \{13/3+ (\alpha T)^{-1}+4/3\ \alpha T\}$

8. Lattice Gruneisen parameter Γ in terms of C_1 is

$\Gamma =C_1-1/2$

9. Bayer's nonlinearity parameter is given by

$B/A = C_1-1$

10. The average Gruneisen parameter is defined as

$\Gamma_a = \gamma-1/\alpha T$

Where $\gamma = Cp/Cv$ is the ratio of the heat capacities.

Experimental details:

The biomaterials glycine,L-arginine and L-methionine used were of E-Merck grade. Triple distilled water was used as a solvent. According to the molecular weights of biomaterials, the solution of glycine, L-arginine and L-methionine are prepared by dissolving into water with molarity of 0.01 M.The concentration of biomaterial is increased in water. The ultrasonic velocity is measured at fixed frequency 2MHz. by employing automatic ultrasonic attenuation recorder (AUAR-102) supplied by Innovative Instrument ,Hyderabad and a frequency counter APLAB-1116.The density in mixture is measured by hydrostatic sinker method .A specially design and fabricated double walled stainless steel cell was used for measurement of ultrasonic velocity. The temperature of fluid mixture was kept constant by the use of thermostatU10 with±0.1^0C.accuracy.The accuracy in density measurement is of 1 in 10^4grams.

3. Problem Solution:

Result and Discussions: The different thermo acoustical parameters V,α,Vr,V*,Va,f,n,C_1, Γ,B/A and Γ_a are evaluated using equation (1-10) are represented in table 1,2 &3 for aqueous solution of glycine,L-arginine and L-methionine at 298K.It is observed that, the volume expansivity(α),fractional free volume(f),repulsive exponent(n),Moelwyn-Hughes parameter(C_1),Bayer's nonlinearity parameter(B/A),Lattice Gruneisen parameter(Γ),and average Gruneisen parameter(Γ_a) are found to show nonlinear behaviors with increase in molar concentration of biomaterial.

The increasing value of the fractional free volume with increase in concentration of biomaterial shows an enhancement of disorder in the liquid due to increased mobility of the molecules in a liquid [11].The value of the f for aqueous biomaterials is about 0.13 as compared to about 0.20 for saturated hydrocarbon liquid ,about 0.15 for fluorocarbon fluids[12] and 0.17 for ternary mixture reported earlier[3].This suggest that free(available) volume in aqueous biomaterial is less than other studies. The small value of fractional free volume or available volume shows the larger size of the molecules in aqueous bio-solutions.

The high value of repulsive exponent n as compared to earlier reported value of n for other liquid system shows the bulk nature of the molecules. The decrease in n with increase in concentration shows the dissociating nature of molecule, which also indicates the increase in the inter-atomic equilibrium distance. The increase in n thus would show associating nature of molecules The low value of n shows the presence of strong repulsive forces at the slightly larger distances in the liquids than in solids[13].

The Moelwyn-Hughes parameter C_1signifies the nonlinear variation of volume expansivity of the liquid with molar concentration (Cm).The value of C_1 is found to about 10, which is comparable with the value reported earlier for other liquid mixtures The high value of $C_1$is due to larger value of α which indicates the dissociative nature of the liquid mixture. But in present aqueous bio-solution, if

C_1increases then α found to be decreases with concentration and vice-versa. This result shows the associating tendency of aqueous bio-solutions.[14,]

Lattice Gruneisen parameter Γ is governed by the molecular order and structure. Bayer's nonlinearity parameter (B/A) is strongly sensitive [15].The decreasing value of B/A, Γ and Γ_a are attributed to decrease in ultrasonic velocity with concentration of biomaterials. In present aqueous bio-solutions, the increase in B/A, Γ and Γ_a with concentration shows decrease in intramolecular modes of vibration and anharmonicity in liquid mixtures. It also indicates the associating nature and weak intermolecular forces in the bio-solution. The decrease in B/A, Γ and Γ_a shows the increase in intramolecular modes of vibration and harmonicity in the liquid state. This indicates the dissociating nature in aqueous biomaterial solution and is attributed to strong intermolecular forces [11,13].

4. Conclusion:

The present study offers a convenient method for verifying and examining the relation between thermo acoustic, anharmonic and nonlinear properties and correlating with fractional free (available) volume and repulsive exponent of intermolecular potential. From this work it may be concluded that the nonlinear variation of acoustical properties is appropriate for describing molecular order, interactions anharmonicity and structure of molecules in aqueous biomaterials.

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Table 1
Aqueous Glycine

Cm(%)	0.00	0.02	0.03	0.05	0.1	0.2
$\alpha*10^{-3}$	0.5586	0.5583	0.5489	0.5571	0.5745	0.5626
V	18.053	18.028	18.025	18.018	18.044	18.120
Vr	1.1496	1.1495	1.1472	1.1492	1.1534	1.1505
V*	15.703	15.683	15.711	15.678	15.644	15.749
Va	2.3493	2.3450	2.3136	2.3398	2.400	2.3712
f	0.130	0.130	0.1283	0.1298	0.1330	0.1308
n	31.1055	31.1269	31.7453	31.2057	30.1076	30.8523
C_1	10.562	10.566	10.665	10.578	10.402	10.522
Γ	4.7813	4.7830	4.8327	4.7893	4.7012	4.7609
B/A	9.5625	9.566	9.665	9.578	9.402	9.522
Γ_a	3.0036	3.0054	3.057	3.012	2.9204	2.9825

Table 2
Aqueous L-Arginine

Cm(%)	0.00	0.02	0.04	0.05	0.06	0.10	0.14	0.2
$\alpha*10^{-3}$	0.5586.	0.5611	0.5604	0.5583	0.5575	0.5569	0.5590	0.5580
V	18.053	17.986	18.036	18.030	18.017	18.016	18.022	18.048
Vr	1.1496	1.1502	1.150	1.1495	1.1493	1.1491	1.1497	1.1494
V*	15.7036	15.6374	15.6828	15.6844	15.6764	15.6767	15.675	15.701
Va	2.3493	2.3487	2.3528	2.3452	2.3410	2.3388	2.3467	2.3467
f	0.1301	0.1306	0.1305	0.1301	0.1299	0.1298	0.1302	0.130
n	31.1055	30.9479	30.9929	31.1277	31.178	31.216	31.078	31.144
C_1	10.5625	10.5372	10.5445	105661	10.5742	10.580	10.558	10.568
Γ	4.7813	4.7686	4.7722	4.7831	4.7871	4.7902	4.779	4.784
B/A	9.5625	9.5372	9.5445	9.5661	9.5742	9.5804	9.588	9.568
Γ_a	3.0036	2.9905	2.9942	3.0055	3.0097	3.0129	3.0014	3.0069

Table 3
Aqueous L-Methionine

Cm(%)	0.00	0.02	0.03	0.04	0.05	0.06	0.08	1.0
$\alpha*10^{-3}$	0.5586.	0.5571	0.5569	0.5584	0.5586	0.5576	0.5579	0.5540
V	18.053	17.998	17.995	17.993	18.011	17.988	17.995	18.010
Vr	1.1496	1.1492	1.1492	1.1495	1.1496	1.1493	1.1494	1.1485
V*	15.7036	15.6605	15.6591	15.6523	15.667	15.650	15.656	15.680
Va	2.3493	2.3371	2.3363	2.3407	2.3439	2.3376	2.3394	2.3296
f	0.1301	0.1299	0.1298	0.1301	0.1301	0.130	0.130	0.1293
n	31.1055	31.2041	31.2156	31.122	31.105	31.170	31.153	31.387
C_1	10.5625	10.5784	10.5802	10.5652	10.5625	10.573	10.5702	10.6078
Γ	4.7813	4.7892	4.7901	4.7826	4.7812	4.7865	4.7851	4.8039
B/A	9.5625	9.5784	9.5802	9.5652	9.5625	9.5730	9.5702	9.6078
Γ_a	3.0036	3.0119	3.0128	3.0050	3.0036	3.0091	3.0076	3.0271