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Applied Chemistry

Elixir Appl. Chem. 62 (2013) 17944-17948

ISSN: 2229-712X

Acoustical studies on molecular interaction of drug Gabapentin in water of various concentrations at different temperatures

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ARTICLE INFO

Article history:

Received: 7 August 2013;

Received in revised form:

28 August 2013;

Accepted: 25 September 2013;

Keywords

Hydrogen bond,
Free volume,
Free length,
Ultrasonic velocity,
Molecular interaction.

ABSTRACT

The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physico-chemical properties and also explain the nature of molecular interactions. The study of thermodynamic parameters to explain molecular interaction of drugs in aqueous or non-aqueous medium provides useful information in medicinal and pharmaceutical chemistry. In present work molecular interaction of aqueous solution of Gabpentin (2-[1-(amino methyl) cyclohexyl] acetic acid) at various concentrations and different temperatures such as 303, 308, 313, 318, 323K was studied by measuring ultrasonic velocity, density and viscosity of the solution. The ultrasonic parameters such as adiabatic compressibility, free volume, free length, acoustic impedance, absorption coefficient, viscous relaxation time, available volume, and Lenard Jones Potential were calculated. These parameters explained formation of hydrogen bond and molecular interaction existing in the solution.

Introduction

The rapid development of ultrasonic techniques for producing powerful ultrasonic vibrations have opened up wide fields of research and technical applications in physics, chemistry, biology, medicine and industry. Ultrasonic is an area of intense scientific and technological research. Science and technology of ultrasonic is widely sought in the recent years for industrial and medicinal application. The literature survey on acoustical studies of solutions reveals that ultrasonic measurements are used to estimate the different elastic properties of the molecule from which the type of molecular interactions can be very well understood.[1-4] The measurement of ultrasonic velocity in pure liquids and mixtures is an important tool to study the physico- chemical properties and also explains the nature of molecular interactions.[5-7]

In the present investigation we tried to study molecular interaction of aqueous Gabpentin (2-[1-(amino methyl) cyclohexyl] acetic acid) solution by measuring ultrasonic velocity, density and viscosity at different concentrations and different temperatures. From the data acoustic parameters such as adiabatic compressibility, free volume, free length, acoustic impedance, absorption coefficient, viscous relaxation time, available volume and Lenard Jones Potential were calculated. Effect of concentration on molecular interaction is studied from acoustic and thermodynamic parameters.

Materials and methods

The chemicals used were of analytical grade. Double distilled water was used for preparation of solutions. 2-[1-(amino methyl) cyclohexyl] acetic acid (Gabapentin) was dissolved in water of various ratio's to prepare different concentration 0.2%, 0.4%, 0.6%, 0.8% and 1.0%. The binary mixture are prepared by using volume percentage(%) by using jobs variation method[8-10].The ultrasonic velocities of aqueous solutions were measured using ultrasonic interferometer (model F05) supplied by Mittal Enterprises, New Delhi operating at the frequency of 2MHZ with the accuracy of ±0.01 ms-1. The densities (ρ) of solutions were determined using specific gravity bottles of capacity 10ml. The viscosities (η) of the solutions are measured using Oswald's viscometer. The different temperatures such as 303, 308, 313, 318 and 323± 0.1K was maintained during the measurement of ultrasonic velocity, density, and viscosity values. The acoustical parameters are calculated from U, ρ, and η using following relation[11-14].

1. Ultrasonic Velocity (U)

The relation used to determine the ultrasonic velocity is given by,

$U = f\lambda$ ms^{-1}

Where, f - Frequency of ultrasonic waves λ - Wave length

2. Adiabatic compressibility (κ)

Adiabatic compressibility which is defined as

$\kappa = (1/U^2 \rho)$ kg^{-1} ms^2 Where, U – Ultrasonic velocity ρ – Density of the solution.

3. Free Volume (V_f)

Free volume in terms of the ultrasonic velocity (U) and the viscosity of the liquid (η) as $V_f = (M_{eff}U/k\eta)^{3/2}$ m^3

Where, M_{eff} is the effective molecular weight ($M_{eff} = \Sigma$ mi xi, in which mi and xi are the molecular weight and the mole fraction of the individual constituents respectively and 'k' is a temperature independent constant equal to $4.28x10^9$ for all liquids.

4. Acoustic impedance (Z)

The acoustic impedance is computed by the formula

$Z = U\rho$ $kgm^{-2}s^{-1}$

Where U –Ultrasonic velocity ρ –Density of the solution

5. Free Length (L_f)

Jacobson[15] introduced the concept of the free length in liquids. He suggested the following relation to calculate the intermolecular free length.

$L_f = (K/U \rho^{1/2})$ m

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Where U - Ultrasonic velocity of liquid ρ - Density of liquid
K - Jacobson temperature dependent constant defined as
$K = (93.875 + 0.345T) \times 10^{-8}$

6. Absorption Coefficient (α/f^2)

The absorption coefficient (α/f^2), also sometimes called attenuation coefficient. It is defined as

$\alpha/f^2 = 8\pi^2\eta/3\rho U^3$

7. Available Volume (V_a)

The available volume (V_a) is a direct measure of compactness and the strength of bonding between the molecules of a liquid or liquid mixture. It can be calculated from following relation

$V_a = V_m(1- U/U_a)\ m^3$

Where V_m is the molar volume and U_a=1600ms^{-1}

8. Lenard Jones Potential (LJP)

The Lenard Jones potential exponent is given by[16]

$LJP = 6Vm/V_a$

Where V_m - the molar volume V_a - the available volume

9. Viscous Relaxation time (τ)

Relaxation time (τ) and absorption coefficient are directly correlated. The absorption of a sound wave is the result of the time lag between the passing of the ultrasonic wave and the return of the molecules to their equilibrium position. It is calculated using the relation[17]

$\tau=4\eta/3\rho U^2$ Where η - viscosity of the solution ρ - density of solution U - Ultrasonic velocity of the solution.

Result And Discussion

The measured ultrasonic velocities(U), densities (ρ), viscosities (η) and other acoustical parameters such as adiabatic compressibility (κ), free volume (V_f), free length (L_f), acoustic impedance (Z), absorption coefficient(α/f^2), viscous relaxation time (τ),available volume (V_a) and Lenard Jones potential (LJP) values at 303, 308, 313, 318 and 323K is given in the tables 1,2 and 3.

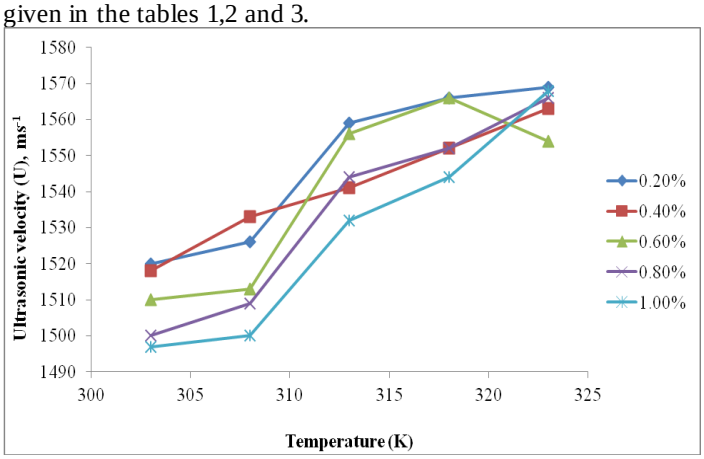

Fig 1. Ultrasonic velocity versus temperature

Figure 1 From the graph it is observed that the velocities are increases with the increasing value of temperature. But it is decrease with increasing solute concentration at particular temperature. Plot has been drawn for various velocities, which are varying with different concentration and temperature. The increase in ultrasonic velocity at higher temperature may be due to solvent-solute interaction and decrease in velocity with increase in concentration may be due to the weakening of intermolecular forces between the molecules.

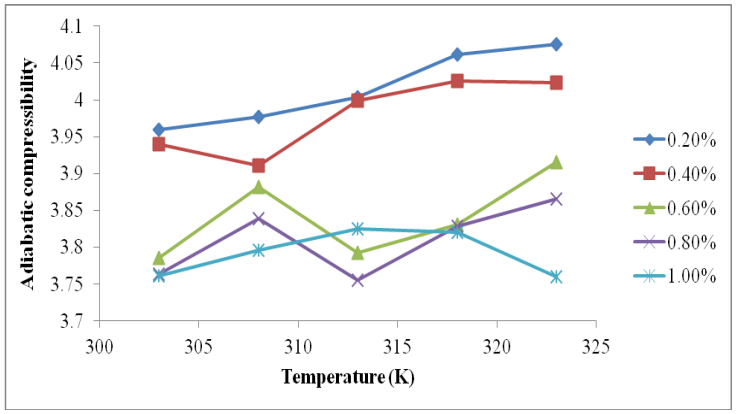

Fig 2. Adiabatic compressibility versus temperature

Figure 2 describes the variation of adiabatic compressibility with different values of temperature as well as concentration. It was found that adiabatic compressibility increases with the increasing value of temperature which clearly indicates that the molecules at higher temperature are forming a more loosely bounded system[18-20]. It was concluded that the velocity in general decreases with increase of temperature irrespective of its molecular weight and concentration.

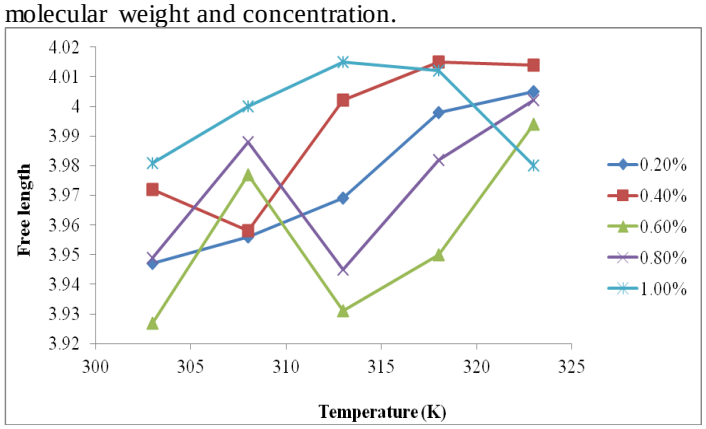

Fig 3. Free length versus temperature

Figure 3 Variation of ultrasonic velocity in solution depends upon the increase or decrease of molecular free length after mixing the component, based on a model for sound propagation proposed by Eyring and Kincaid[21]. It was found that, intermolecular free length increases linearly on increasing the percentage of solute in solution. The intermolecular free length increase due to greater force of interaction between solute and solvent by forming hydrogen bonding. The same trend also observed an increase intermolecular free length with increasing temperature.

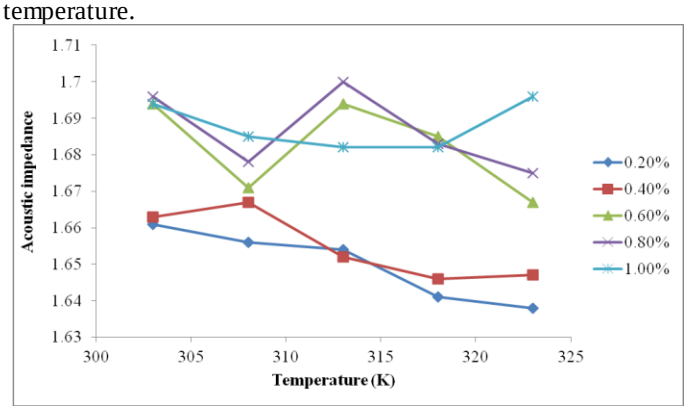

Fig 4. Acoustic impedance versus temperature

Figure 4 represents the plots between acoustical impedance and temperature. The trend in the variation of impedance with temperature is reverse to that of ultrasonic velocity.

Table 1: Ultrasonic velocity, Density, Viscosity and Adiabatic compressibility values for Gabapentin –Water system of various concentrations at different temperature

Concentration (%)	Temperature (K)	Ultrasonic Velocity U (ms^{-1})	Density ρ (kg/m^3)	Viscosity $\eta/10^{-4}$, (Nsm^{-2})	Adiabatic compressibility $\kappa/10^{-10}$ ($kg^{-1}ms^2$)
0.2	303	1520	1093.20	8.336	3.959
	308	1526	1089.95	7.635	3.977
	313	1559	1086.70	6.884	4.003
	318	1566	1083.45	6.301	4.061
	323	1569	1080.20	5.945	4.075
0.4	303	1518	1091.20	8.341	3.940
	308	1533	1087.95	7.333	3.911
	313	1541	1084.70	6.801	3.999
	318	1552	1081.45	6.087	4.025
	323	1563	1078.20	5.597	4.023
0.6	303	1510	1095.60	8.674	3.786
	308	1513	1092.35	7.678	3.882
	313	1556	1089.10	7.181	3.792
	318	1566	1085.85	6.451	3.831
	323	1554	1082.60	5.958	3.915
0.8	303	1500	1094.4	8.817	3.764
	308	1509	1091.15	7.643	3.839
	313	1549	1087.9	6.962	3.755
	318	1552	1084.65	6.376	3.828
	323	1556	1081.14	6.018	3.866
1.0	303	1497	1094.8	8.892	3.761
	308	1509	1091.55	8.007	3.796
	313	1532	1088.3	7.457	3.825
	318	1544	1085.05	6.65	3.820
	323	1568	1081.8	6.224	3.760

Table 2: Free length, Acoustic impedance, Absorption coefficient and Relaxation time values for Gabapentin –Water system of various concentrations at different temperature

Concentration (%)	Temperature (K)	Free Length $L_f / 10^{-11}$ (m)	Acoustic impedance Z $/10^7$ ($kgm^{-2}s^{-1}$)	Absorption coefficient $\alpha/f^2/10^{-15}$ ($Npm^{-1}s^2$)	Relaxation time $\tau/10^{-13}$ (s)
0.2	303	3.947	1.661	5.708	4.400
	308	3.956	1.656	5.745	4.422
	313	3.969	1.654	6.045	4.629
	318	3.998	1.641	6.276	4.774
	323	4.005	1.638	6.365	4.832
0.4	303	3.972	1.663	5.183	4.011
	308	3.958	1.667	4.919	3.824
	313	4.002	1.652	5.468	4.195
	318	4.015	1.646	5.360	4.101
	323	4.014	1.647	5.613	4.295
0.6	303	3.927	1.694	4.396	3.475
	308	3.977	1.671	4.505	3.520
	313	3.931	1.694	4.602	3.631
	318	3.950	1.685	4.527	3.556
	323	3.994	1.667	5.010	3.893
0.8	303	3.949	1.696	3.982	3.162
	308	3.988	1.678	3.959	3.116
	313	3.945	1.700	4.067	3.230
	318	3.982	1.683	4.134	3.254
	323	4.002	1.675	4.378	3.428
1.0	303	3.981	1.694	3.746	2.981
	308	4.000	1.685	3.574	2.833
	313	4.015	1.682	3.856	3.039
	318	4.012	1.682	3.885	3.065
	323	3.980	1.696	3.924	3.120

Table 3: Available volume, free volume, and Molar volume and Lenard Jones Potential values for Gabapentin –Water system of various concentrations at different temperature

Concentration (%)	Temperature (K)	Available volume $Va/10^{-4}$ (m^3/mol)	Free volume $V_f/10^{-4}$ (m^3/mol)	Lenard Jones Potential (LJP)
0.2	303	8.300	6.805	115
	308	7.677	7.809	129
	313	4.253	9.419	234
	318	3.527	10.820	282
	323	3.216	11.840	309
0.4	303	8.610	6.886	117
	308	7.035	8.478	143
	313	6.195	9.567	162
	318	5.040	11.410	200
	323	3.885	13.080	209
0.6	303	9.500	6.537	106
	308	9.189	7.590	110
	313	4.647	9.078	218
	318	3.591	10.760	282
	323	4.858	11.990	208
0.8	303	10.620	6.408	96
	308	9.668	8.011	105
	313	5.418	9.584	188
	318	5.100	10.960	200
	323	4.675	12.000	218
1.0	303	11.110	6.404	93
	308	9.816	7.858	105
	313	7.335	8.634	141
	318	6.041	10.370	171
	323	3.452	11.720	300

Acoustical impedance values also suggest strong molecular interaction between the components at increasing solute concentration. But it is decreases with increasing temperature at all concentrations. It suggests the solute-solvent interaction is less at higher temperatures due to thermal agitation.

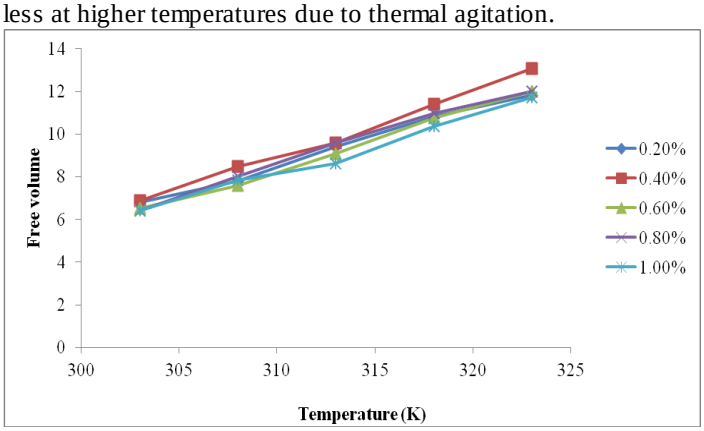

Fig 5. Free volume versus temperature

Figure 5 The increase in free volume shows that the strength of interaction increases gradually with the increase in solute concentration and also increase temperature. It represents that there is strong interaction between the solute and solvent molecules. This molecular interactions between like and unlike molecules are influenced by structural arrangements along with shape and size of the molecules.

Figure 6 shows variation of relaxation time with concentration and temperature. Acoustic relaxation time decreases with increasing concentration. But increases with increasing temperature for all concentrations. The dispersion of ultrasonic waves in system contains information about the characteristic time of relaxation process that causes the dispersion. Increase in relaxation time indicates that degree of cooperation for relaxation of the molecules increases which increases the bulk of cluster when solute is added to solvent.

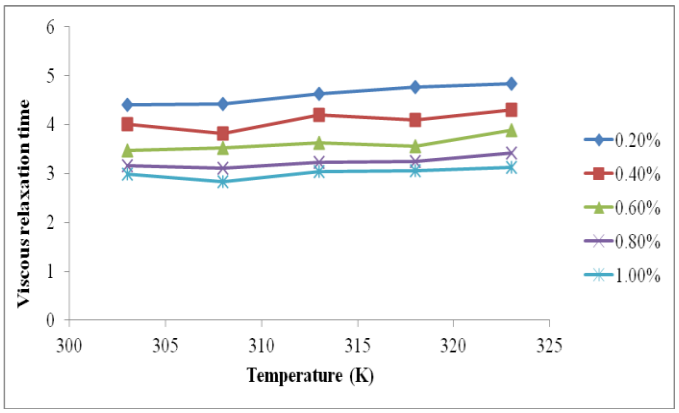

Fig 6. Viscous relaxation time versus temperature

Conclusion

Ultrasonic studies have been carried out in the aqueous solutions of Gabapentin at five different temperatures (namely 303K, 308K, 313K, 318K and 323K) for the percentage concentration ranging from 0.2% to 1.0% with a difference of 0.2%. It is concluded that there exist a significant molecular interactions in the liquid mixtures. The trend of increase in adiabatic compressibility and free length with increase of temperature further concludes the possibility of molecular interaction. This interaction indicates that there is a possibility of some complex formation such as hydrogen bond in the present system.

Acknowledgement

Author is thankful to Department of chemistry, AMET University for encouraging the work.

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