Available online at www.scholarsresearchlibrary.com

Scholars Research Library

European Journal of Applied Engineering and Scientific Research, 2012, 1 (2):73-79
(http://scholarsresearchlibrary.com/archive.html)

ISSN: 2278 – 0041

Relative association and free volume to study molecular interaction in dichlofenac sodium in aqueous solution

Sunanda S. Aswale[1], Shashikant R. Aswale[1], Aparna B. Dhote[2]

[1] Lokmanya Tilak Mahavidyalaya, Wani, Dist. Yavatmal, Maharashtra. 445304.
[2]Nilkanthrao Shinde College, Bhadrawati, Dist. Chandrapur, Maharashtra.

ABSTRACT

Ultrasonic velocity and density of aqueous solution of Dichlofenac sodium is reported at different temperatures, concentrations and at different frequencies. Relative association, free volume, Rao's constant and Wada's constant were calculated from these data. The acoustic and thermodynamic properties are used to study molecular interaction existing in the solution.

Key words: ultrasonic velocity, thermodynamic, free volume, molecular interaction

---

INTRODUCTION

Study of molecular interactions between solute and solvent media has got great importance in many field of science including medicinal chemistry, industrial processes, biochemistry etc. The structure making and structure breaking properties of solute can be studied by measuring viscosity and ultrasonic velocity of an electrolyte in the solutions [1]. Literature survey shows that many researchers have studied the molecular interactions by ultrasonic velocity and viscosity measurement [2-8].

In continuation of our work [9-11], in the present paper we report the ultrasonic velocity, density of aqueous solution of Dichlofenac sodium at different temperatures, concentrations and at different frequencies. From these experimental data the number of thermodynamic parameters namely relative association, free volume, Rao's constant and Wada's constant have been calculated. These parameters were utilized to study molecular interactions occurring in the solution at different temperatures, concentrations and at different frequencies.

MATERIALS AND METHODS

Experimental:
The chemicals used were of analytical grade. Double distilled water was used for preparation of solutions. A special thermostatic water bath arrangement was made for density, ultrasonic velocity and viscosity measurements, in which continuous stirring of water was carried out with the help of electric stirrer and temperature variation was maintained within ±0.01^{0}C multi frequency interferometer (Mittal Enterprises, Model F-83) with accuracy of ±0.03% and frequency 2 MHz, 4MHz, 6MHz were used in the present work for measurement of ultrasonic velocities of solutions. Densities of solutions were measured using specific gravity bottle. These values were

accurate up to ± 0.1 kg/m^3. All the weighing was made on CA-124 (CB/CA/CT series, Contech) digital electronic balance having an accuracy of ± 0.0001g. Viscosities of the solution were measured by Ostwald's viscometer.

RESULTS AND DISCUSSION

From the observed values relative association, free volume, Rao's constant, Wada's constant were calculated.

Relative association is a function of ultrasonic velocity and is calculated by the equation,

$$R_A = \frac{d_s}{d_0}\left(\frac{v_0}{v_s}\right)^{1/3} \qquad \text{........ (1)}$$

Where, v_0 and v_s are ultrasonic velocities in solvent and solution respectively
Where, v_0 and v_s are ultrasonic velocities in solvent and solution respectively.

Free volume is calculated by following equation

$$V_f = [M_{eff} v / K \eta]^{3/2} \qquad \text{...... (2)}$$

Where, M_{eff} is effective molecular weight, K is a temperature independent constant which is equal to 4.28 x 10^9 for all liquids.

Rao's constant and Wada's constant is also a measure of interaction existing in the solution.
Rao's constant is calculated by using following equation.

$$R = [M_{eff}/d_s] v^{1/3} \qquad \text{...... (3)}$$

Wada's constant is calculated by following equation.

$$W = [M_{eff}/d_s]\, \beta^{-1/7} \qquad \text{...... (4)}$$

Table 1: Thermodynamic parameters of Dichlofenac sodium at 2 MHz

Temp. (K)	Concentration(M)	Ultrasonic velocity (m/S)	Density (kg/ m^3)	Relative association (R_A)	Free volume Vfx10^{-8} (m^3/mole)	Rao's constant (R) (m^3/mole)(m/)$^{1/3}$	Wada's constant (W) (m^3/mole)(N/m^2)$^{1/7}$
303.15	0.001	1524.48	1009.61	1.008	1.20	0.2052	0.3889
	0.01	1563.58	1020.58	1.0108	1.34	0.2052	0.3890
	0.1	1601.30	1038.83	1.020	1.43	0.2087	0.3963
308.15	0.001	1492.57	1003.31	1.0172	0.997	0.2050	0.3886
	0.01	1526.77	1014.72	1.0212	1.05	0.2048	0.3884
	0.1	1564.25	1036.96	1.035	1.25	0.2075	0.3942
313.15	0.001	1454.82	1001.28	1.0265	0.846	0.2037	0.3865
	0.01	1488.29	1008.85	1.0264	0.920	0.2043	0.3875
	0.1	1526.12	1030.52	1.0239	1.12	0.2071	0.3936

Table 2: Thermodynamic parameters of Dichlofenac sodium at 4 MHz

Temp. (K)	Concentration (M)	Ultrasonic velocity (m/S)	Density (kg/ m^3)	Relative association (R_A)	Free volume Vfx10^{-8} (m^3/mole)	Rao's constant (R) (m^3/mole)(m/)$^{1/3}$	Wada's constant (W) (m^3/mole)(N/m^2)$^{1/7}$
303.15	0.001	1669.52	1009.61	1.0015	1.38	0.2115	0.3991
	0.01	1593.80	1020.58	1.0285	1.38	0.2065	0.3912
	0.1	1675.18	1038.83	1.029	1.85	0.2119	0.4014
308.15	0.001	1601.42	1003.31	1.0248	1.11	0.2099	0.3965
	0.01	1598.74	1014.72	1.0371	1.18	0.2080	0.3936
	0.1	1673.37	1036.96	1.035	1.25	0.2075	0.3942
313.15	0.001	1600.17	1001.28	1.0265	0.976	0.2103	0.3971
	0.01	1670.85	1008.85	1.019	1.09	0.2123	0.4005
	0.1	1671.05	1030.52	1.039	1.12	0.2071	0.3936

With increasing concentration and temperature ultrasonic velocity increases suggesting that solute solvent interaction is more. At 2 MHz ultrasonic velocity increases at 303.15 K for 0.01 M while at 4 MHz and 6 MHz for 0.01 M concentration the ultrasonic velocity decreases and at 313.15 K at 4 MHz ultrasonic velocity increases. The solute occupy the interstitial space of water and tend to break the original ordered state of water due to its self association and hence Ultrasonic velocity increases linearly at 2 MHz and 4 MHZ at 313.15 K but at 6 MHz it shows non linearity

Table 3: Thermodynamic parameters of Dichlofenac sodium at 6 MHz

Temp. (K)	Concentration (M)	Ultrasonic velocity (m/S)	Density (kg/ m^3)	Relative association (R_A)	Free volume $Vfx10^{-8}$ (m^3/mole)	Rao's constant (R) (m^3/mole)(m/)$^{1/3}$	Wada's constant (W) (m^3/mole)(N/m^2)$^{1/7}$
303.15	0.001	2298.32	1009.61	0.9068	2.23	0.2353	0.4373
	0.01	2074.14	1020.58	0.9489	2.05	0.2255	0.4217
	0.1	2181.2	1038.83	0.9495	2.75	0.2314	0.4329
308.15	0.001	2295.33	1003.31	0.9216	1.9	0.2367	0.4395
	0.01	2068.8	1014.72	0.9643	1.74	0.2267	0.4236
	0.1	2182.49	1036.96	0.9686	2.06	0.2316	0.4336
313.15	0.001	2290.08	1001.28	0.9226	1.67	0.2370	0.4400
	0.01	2066.84	1008.85	0.9620	1.50	0.2279	0.4256
	0.1	2179.7	1030.52	0.9653	1.90	0.2332	0.4358

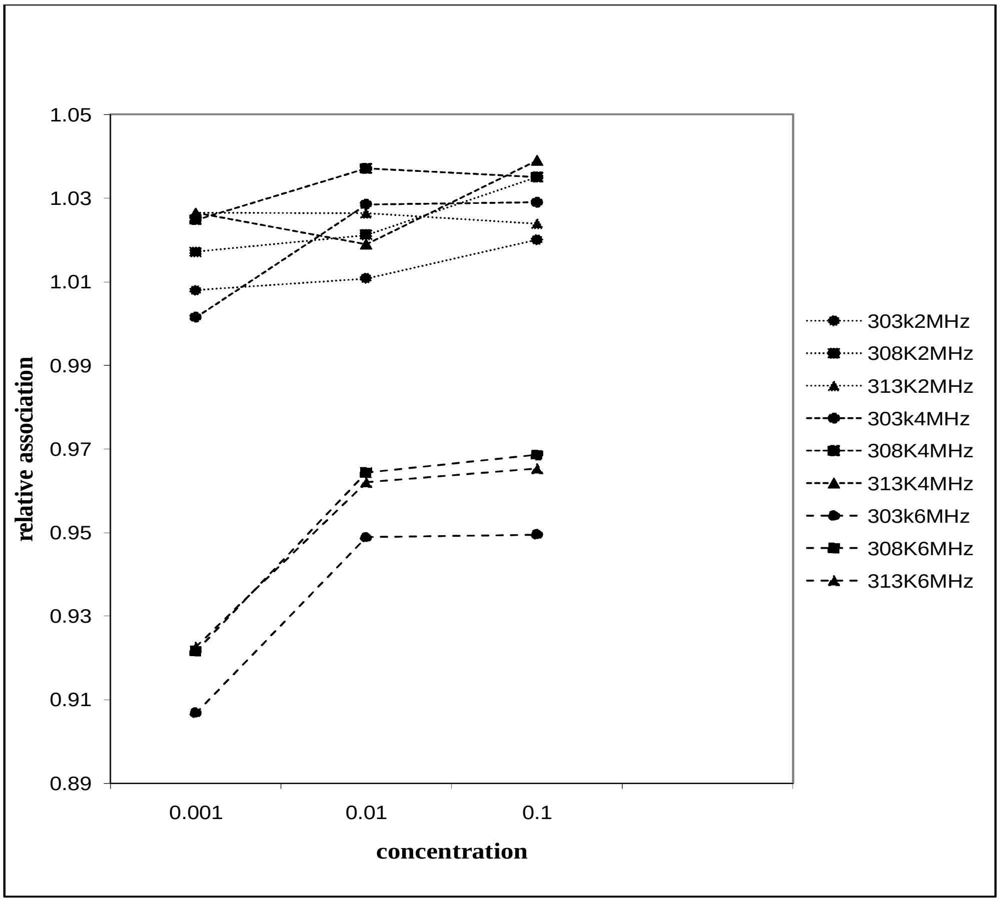

Fig 1: relative association at different concentrations, temperatures and at different frequencies.

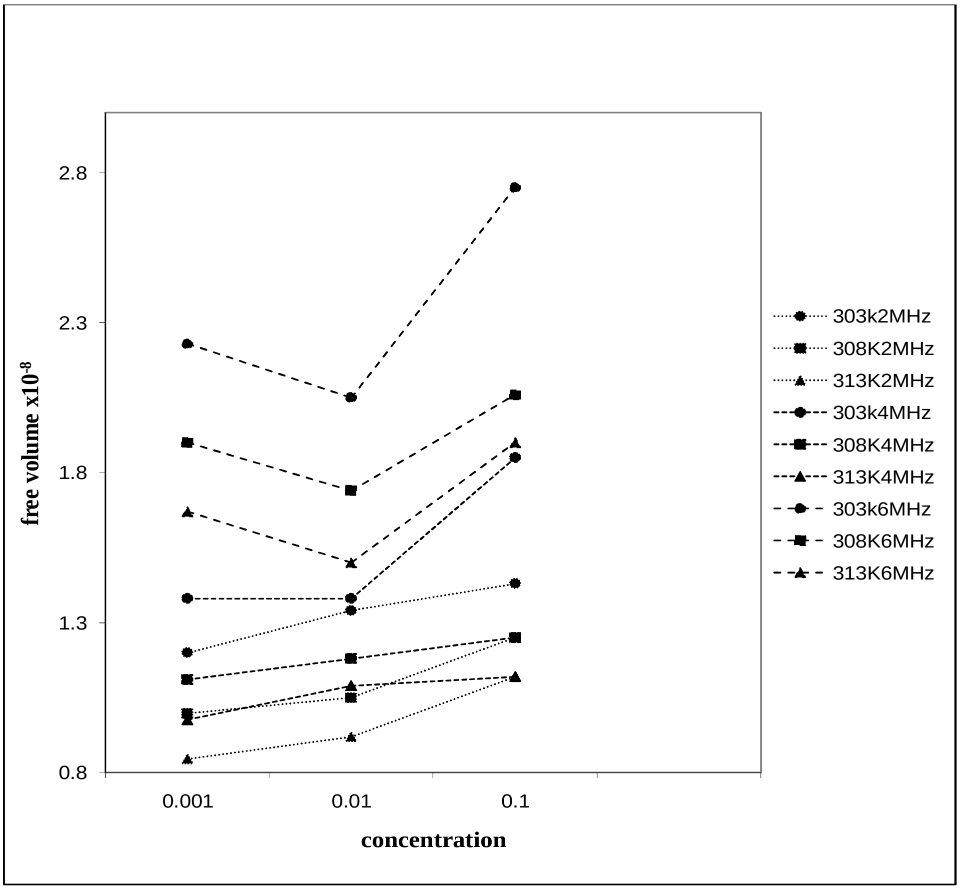

Fig 2: free volume at different concentrations, temperatures and at different frequencies.

Relative association is influenced by two factors [12]
1) Breaking up of associated solvent molecules on addition of solute.
2) The salvation of solute.

From fig-1 it shows that relative association increases with increasing concentration, temperature and also with frequency except at 313.15 K at 2 MHz for 0.1 M solution and at 308.15 K and 313.15 K at 4 MHz it shows non linearity. When solute is added to solvent salvation of solute takes place and hence relative association increases. But at 313.15 K at 2 MHz for 0.1 M solution and at 308.15 K at 4 MHz for 0.1 M and at 313.15 K for 0.01 M solution relative association decreases means that there may be breaking up of water molecules when solute is added to solvent. With increasing concentration and temperature relative association increases but it shows low values of relative association at 6 MHz as compared to 2 MHz and 4 MHz. At high frequency breaking up of solvent molecules takes place and hence relative association has low values. The increase in relative association shows strong solute-solvent interaction.

Free volume is one of the significant factors in explaining the free space and its dependent properties have close connection with molecular structure and it may show interesting features about interactions between liquid mixtures. Fig-2 shows that free volume increases with increasing concentrations and frequencies but decreases with increasing temperatures. When concentration of solute is increased, due to hydrogen bonding in water the molecules of solute may arranged in the solvent in such a way that void space may not be available due to which solute becomes less compressible and hence free volume increases. Increase in free volume shows ion-solvent interaction in solution.

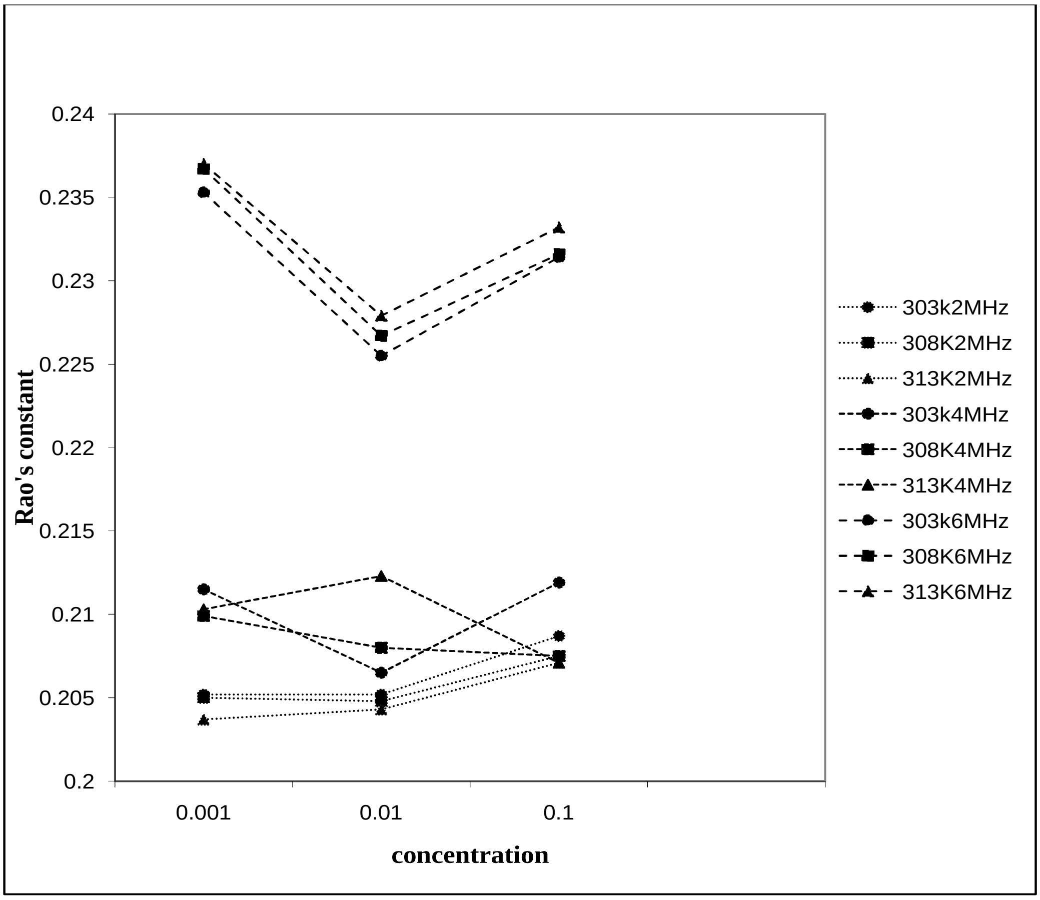

Fig 3 : Rao's constant at different concentrations, temperatures and at different frequencies.

Rao's constant shows non linearity with increasing concentration, temperature. Wada's Constant at 2 MHz increases with increasing concentration and decreases with increasing temperature. But at 4 MHz and 6 MHz it shows non linearity. Many authors [13-14] have interpreted molecular interaction in terms of non linear change of Rao's and Wada's constant.

Fig- 3 and fig- 4 shows that with increasing frequency Rao's constant and Wada's constant increases indicates that availability of more number of solute molecules in a given region thus leads to a tight packing of medium. Increase in Rao's constant and Wada's constant with increasing frequency shows strong solute-solvent interaction existing in the solution.

CONCLUSION

Ultrasonic velocity, density have been measured for aqueous Dichlofenac sodium solution at different concentrations, temperatures and at different frequencies. Relative association, free volume increases shows solute-solvent interaction present in the solution. Also with increasing frequency Rao's and Wada's constant increases shows strong solute-solvent interaction exist in the solution.

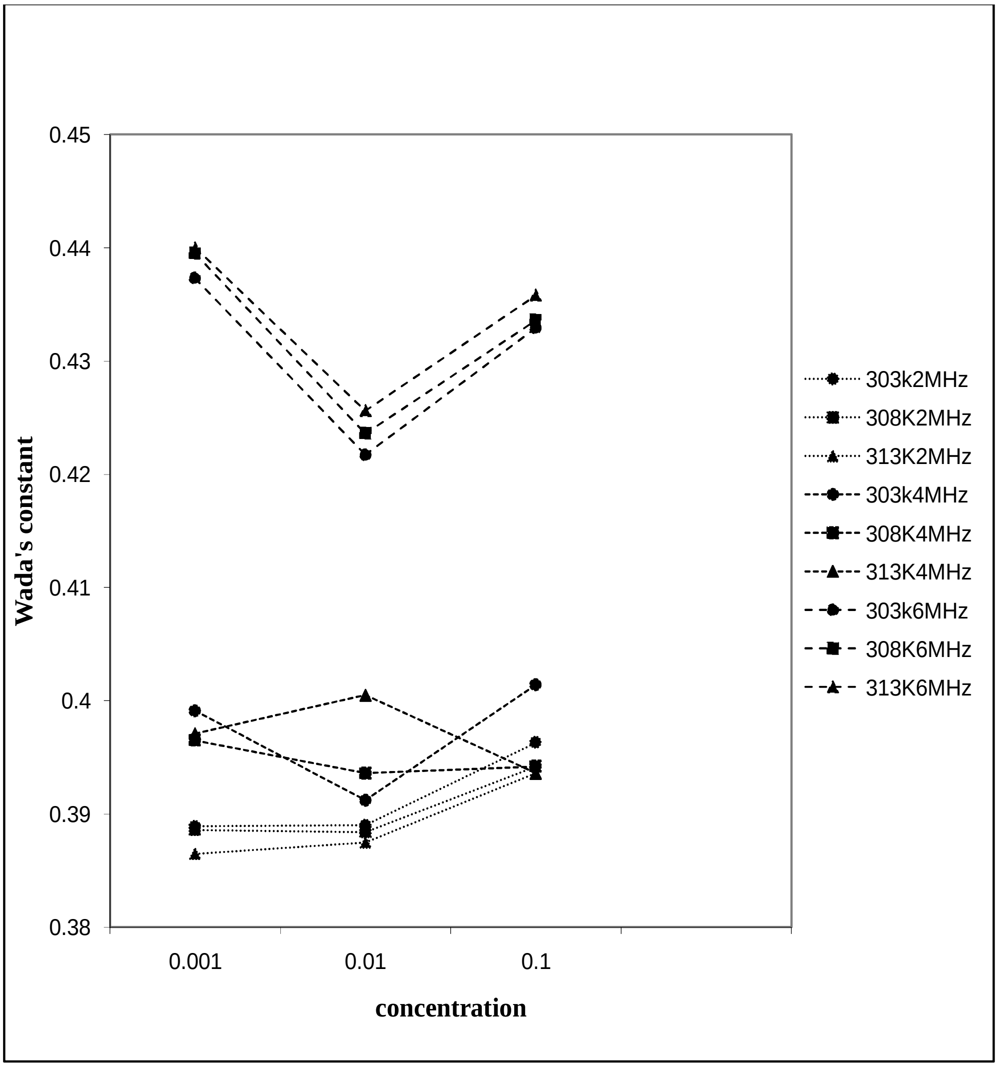

Fig 4: Wada's constant at different concentrations, temperatures and at different frequencies

REFERENCES

[1] S. D. Deoskarkar,M, M. L. Narwade, *Rasayan J. Chem*., **2010**,3(1), 55-59
[2] V. D. Bhandakar, O.P. Chimankar and N. R. Pawar, *J. Chem. Pharm. Res*., **2010**, 2(4), 873-877
[3] P. S. Agrawal , M. S. Wagh, L. J. Paliwal, *Archives of Applied Science Research*, **2011,** 3(2), 29-33
[4] P. Kumar, S. Jayakumar, V. Kannappan, *Indian Journal of Applied Physics,*
[5] A. N. Sonar and N. S. Pawar, *Rasayan J. Chem*., **2010**, 3(1), 38-43
[6] R.Ezhil Pavai and S. Renuka, *International Journal of Research in Pure and applied Physics*, **2011**, 1(2), 6-10
[7] Anjana and Rajinder Bamezai, *Archives of Applied Science Research*, **2011,** 3(1), 370-379
[8] P. Vasantharani, L. Balu, R. Ezhil Pavai and S. Shailajha, *Global Journal of Molecular Sciences*, **2009**, 4(1), 42-48
[9] S.S.Aswale., A. B.Dhote, R. S. Hajare, P. B. Raghuwanshi and S. R. Aswale, Proceeding of Eighteen National Symposium on Ultrasonic NSU-XVIII, Vellore, **2009**, 132-138
[10] S.S. Aswale, S. R.Aswale, D. T. Tayade and P. B. Raghuwanshi, (2008) Proceeding of 1st International Society Bio-Technology Conference-2008, Gangtok**, 2008**, 325-330

[11] S.S.Aswale, P. B. Raghuwanshi, D. T. Tayade. And S. R. Aswale, *J.Indian Chem. Soc*., **2007**, .84, 159-164
[12] Shilpa A. Mirikar, Pravin P. Pawar, and Govind K. Bichile, *Archives of Applied Science Research*, **2011,** 3(5), 233-241
[13] P.N. Gupta, *Acoustica*, **1980,** 237
[14] A. K. Gupta, Krishnakumar, and Birendrakumar Karn, *J. Ind. Council Chem*., **2009**, 26(1), 77-81