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Research Article

STUDY OF MOLECULAR INTERACTION OF DISPERSES RED 54 IN WATER

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Abstract

The densities, viscosities and ultrasonic velocities measurement of disperse red 54 solutions in water were carried out at different temperature and at different concentrations. The acoustic parameters like adiabatic compressibility, intermolecular free length etc were calculated. The variation of these parameters with concentration has been discussed in this work.

Keywords: Disperse red 54, adiabatic compressibility, intermolecular free length.

Introduction

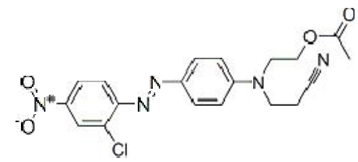
So far, our earth is the only planet in the whole universe, accredited to have life. One of the prime reasons, which support life in our mother-planet, is water. But, anthropogenic activities have caused a great harm to the quality of our lifeline, i.e. water. Anywhere and anytime, water plays an important role for human beings, natural environment, and social development, but the subsequences of used water are represented by polluted municipal and industrial wastewaters (e.g. resulted from mining, metallurgy, metal plating, smelting flux electrolysis, battery manufactories, petroleum refineries, paint and pigments manufacture, printing, photographic industries and the glass production. (Argun, et al,. **2007**). Because of fast depletion of the freshwater resources, there seems to be a crisis of the same. Water pollution is a global concern and, it is the high time that we realize the gravity of the situation. Removing pollutants from water is the crying need of the hour and developing a cost effective and environmentally safe method to achieve the same is a challenging task for researchers. After all, it is the future of mankind, which is at stake.

In recent years, ultrasonic technique has become a powerful tool for studying the molecular behaviour of aqueous solution (Nithiyanantham et al., 2012). Ultrasonic velocity (U) together with density (ρ) and viscosity (η) data furnishes a wealth of information about bulk properties and intermolecular forces (Pierce, 1981). The measurement of ultrasonic velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids and liquid mixtures. 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 (Domanska et al., **2009**). Literature survey shows that very little work has been carried out to understand nature of interaction of dyes and water. Thus, in the present paper, ultrasonic investigation technique has been used of the detection of possibility of specific molecular interactions between dye molecules in water.

Materials and Methods

Chemicals

The Disperse red 54 used as solute was collected from Vap Chem, Surat (Gujarat), and double distilled water used as solvent in this investigation. The dye was dried in a vacuum oven and then stored in desiccators over fused calcium chloride and used without further purification.

CAS No.	Molecular Formula	Formula Weight	Structure
6021-61-0	$C_{19}H_{18}ClN_5O_4$	415.83032	

Solutions

Initial stock solution of 100 ppm was obtained by weighing. Other solutions of various concentrations were prepared by the gradual dilution of the stock solutions by volume. Solutions of disperse red 54 were prepared in double distilled water.

Ultrasonic velocities, densities and viscosities were measured at 293.15 K, 298.15 K, 303.15 K, 308.15 K and 313.15 K. The experimental water bath temperature was maintained constant with temperature stability ± 0.1^{o}C by circulating the coolant liquid from the electronically digitally operated (Plasto Craft Industries) low temperature bath model LTB-10. The densities of the solutions were measured at different temperature by the hydrostatic plunger method. A monopan balance of least count 0.0001g was used to record change in plunger weight dipped in solutions. Ostwald Viscometer was used to determine viscosities of the solutions and solvent at different temperature by suspending viscometer in experimental bath. The ultrasonic velocity was measured in aqueous solutions of disperse red 54 by using an ultrasonic interferometer (model F-81 was supplied by M/s Mittal Enterprises, New Delhi.) at a fixed frequency of 2 MHz having facility to measure ultrasonic velocity at different. The temperature of experimental liquid in measuring cell can be maintained by circulating water through the measuring cell which is specially designed with a double walled cylinder provided with an inlet and outlet. By using thermostat (accuracy ±0.1 K), water is circulated at any desired constant temperature through the outer wall of the cell.

Theoretical equations

From the experimental data of density, viscosity and ultrasonic velocity, various acoustical parameters are evaluated using standard equations:

Adiabatic compressibility

From the ultrasonic velocity (U) and density (d) the adiabatic compressibility can be calculated from the following equation.

$$\beta = 1/ U^2\rho \ kg^{-1} \ ms^{-2}$$

Intermolecular Free Length

Intermolecular Free is used to determine the interaction between the ion and the solvent molecule. The free path length was calculated using the equation

$$L_f = K\sqrt{\beta}$$

Where, *K* is Jacobson's constant which is a temperature dependent coefficient. Jacobson determined the value of K empirically between 0 and 50^{o}C. (Pandey et al 1975, 1979) carried out a critical discussion of temperature and pressure dependence of Jacobson constant and Lf

Acoustic impedance (Z)

The acoustic impedance is given by the product of ultrasonic velocity and density as shown below:

$$Z = U \times \rho \ kg \ m^{-2}s^{-1}$$

Where ρ is the density and U is the ultrasonic velocity in the liquid system.

Relative Association (RA)

The relative association can be calculated as

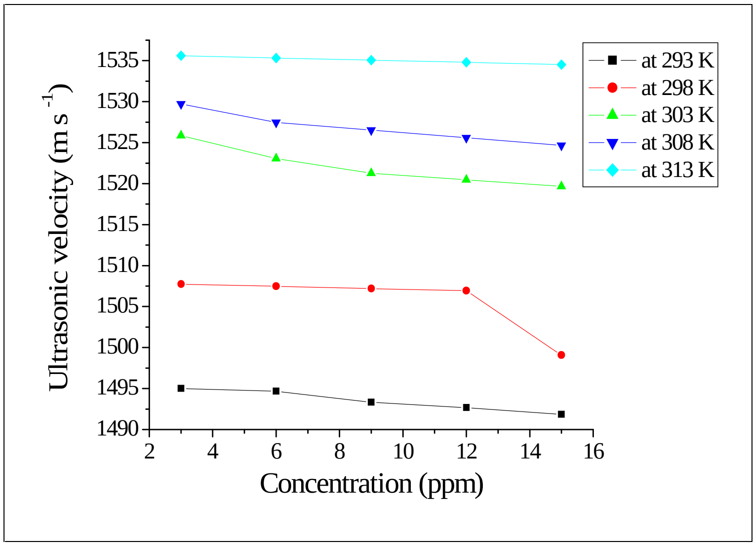
$$RA = (\rho / \rho_0) (\upsilon_0 / \upsilon)^{1/3}$$

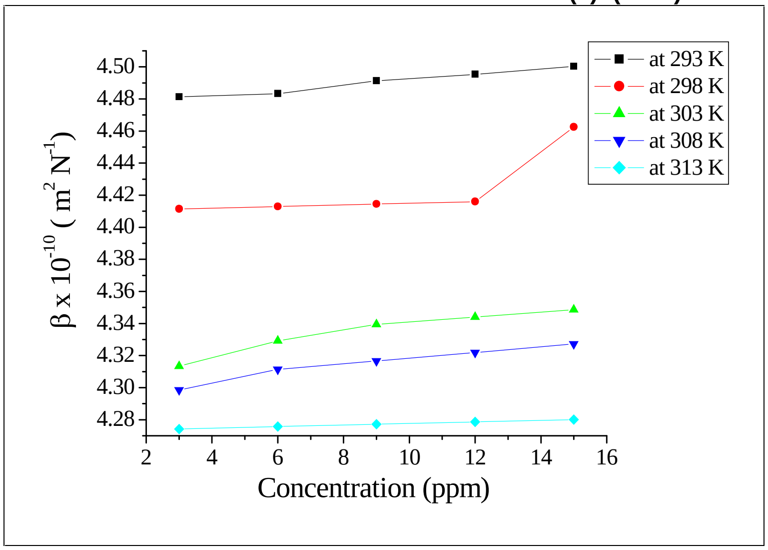
where ρ_0 = density of solvent, υ_0 = ultrasonic velocity of solvent**.**

Results and Discussion

Table 2: Experimental values of densities (ρ), viscosities (η), ultrasonic speeds (U), adiabatic compressibility (β), intermolecular free length (L_f), acoustic impedance (Z) relaxation time (τ) and relative association (RA) of Disperse Red 54 at different temperature.

Temp. (K)	Conc. (ppm)	ρ (Kg m^{-3})	η (10^{-3} Nsm^{-2})	U (ms^{-1})	β (10^{-10} m^2N^{-1})	L_f (10^{-11} m)	RA
293	3	998.414	1.0045	1495.00	4.4813	4.3079	0.9972
	6	998.417	1.0048	1494.67	4.4833	4.3089	0.9973
	9	998.421	1.0058	1493.33	4.4913	4.3127	0.9976
	12	998.424	1.0057	1492.67	4.4953	4.3146	0.9977
	15	998.429	1.0087	1491.83	4.5003	4.3170	0.9979
298	3	997.183	0.8863	1507.73	4.4114	4.3162	0.9977
	6	997.187	0.8922	1507.47	4.4129	4.3169	0.9978
	9	997.189	0.8929	1507.20	4.4145	4.3177	0.9978
	12	997.191	0.8962	1506.93	4.4160	4.3185	0.9979
	15	997.194	0.9007	1499.07	4.4625	4.3411	0.9997
303	3	995.761	0.7960	1525.87	4.3133	4.3095	0.9960
	6	995.763	0.7966	1523.07	4.3292	4.3174	0.9967
	9	995.764	0.7977	1521.27	4.3394	4.3225	0.9970
	12	995.767	0.8005	1520.47	4.3440	4.3248	0.9972
	15	995.768	0.8015	1519.67	4.3486	4.3270	0.9974
308	3	994.119	0.7207	1529.73	4.2986	4.3436	0.9996
	6	994.124	0.7215	1527.47	4.3114	4.3500	1.0001
	9	994.129	0.7222	1526.53	4.3166	4.3527	1.0003
	12	994.131	0.7228	1525.60	4.3219	4.3553	1.0005
	15	994.135	0.7232	1524.67	4.3272	4.3580	1.0007
	3	992.174	0.6543	1535.60	4.2742	4.3726	0.9996
	6	992.175	0.6548	1535.33	4.2757	4.3733	0.9996
313	9	992.178	0.6548	1535.07	4.2772	4.3741	0.9997
	12	992.181	0.6571	1534.80	4.2786	4.3748	0.9997
	15	992.184	0.6593	1534.53	4.2801	4.3756	0.9998





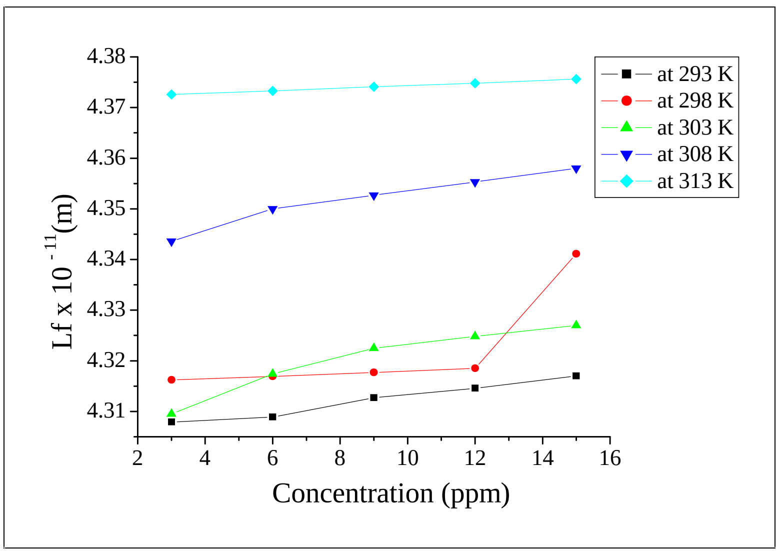


Figure: Plot of variation of ultrasonic velocity (U), intermolecular free length (L_f), adiabatic compressibility (β), with concentration of Disperse Red 54 at different temperature.

It is observed from the table 1 that, density of the solutions increases linearly with the increase in the concentration of the solute for disperse red 54 under investigation at all the temperatures. The density of the solutions decreases with increase in the temperature of the solution which may be due to movement of solute molecules away from each other at elevated temperature. At lower temperatures, the molecules are closer together and they move more slowly. Now, for simple molecules, the line between "can't move" and "moves easily" is pretty distinct. Once the molecules are mobile enough that excluded volume interactions are overcome, and further changes to viscosity are small and mostly due to intermolecular attractive forces.

As a result of this, viscosity of dye solutions decreases with increase in temperature. An examination of Table 1 shows that velocity increases with increase in temperature. As the molecules are moving apart, the intermolecular distance increases which results in increase in L_f. The values of acoustical parameters show that RA increase while β decreases with increase in temperature may be ascribed to the decrease in strength of intermolecular attraction (Larsen et al.,1998 and Hawrylak et al., 2000). The increase of L_f with rise in temperature may be attributed to the fact that the attraction and association in solution decreases with rise in temperature and intermolecular forces weaken.

According to the proposed theory by A. Ali et al., 2005 the decrease in the value of 'L_f' with increase in ultrasonic velocity further strengthens the possibility of dipole-dipole interaction. It can be seen that the acoustic impedance changes similarly with mole fraction and temperature.

The decrease in η indicates weak intermolecular forces between the molecules. The increase in U, L_f and RA can be explained by taking into consideration the loss of weakly polar association and difference in size and shape of component molecules. Such an increase may also be attributed to loose packing of molecules or weak interaction (Rawat and Sangeeta, 2008) which may be brought by weakening of intermolecular forces (Miecznik et al, 2004). The free length increases with increase in temperature as expected due to thermal expansion of the liquids (Rawat et al., 2008). The increase in free length for some cryogenic liquids was observed by earlier workers (Pandey, 1979, 1975).

Conclusion

The increase in U, L_f and RA can be explained by taking into consideration the loss of weakly polar association and difference in size and shape of component molecules. Such an increase may also be attributed to loose packing of molecules or weak interaction Intermolecular forces between the molecules are weakened at elevated temperature. So, the study will be made at room temperature

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