



ACOUSTICAL STUDIES OF SOME PYRAZOLE DERIVATIVES IN DMF AND DMSO SOLUTIONS AT 298.15 K

Shipra Baluja* and Falguni Karia

Physical Chemistry Laboratory, Department of Chemistry, Saurashtra University, Rajkot-360005, India, *E-mail: shipra_baluja@rediffmail.com

ABSTRACT

The density and ultrasonic velocity of some pyrazole derivatives have been studied in dimethyl formamide and dimethyl sulphoxide solutions at 298.15 K. From the experimental data, some acoustical parameters have been evaluated to understand the molecular interaction occurring in these solutions.

Keywords: Pyrazole derivatives, DMF, DMSO, acoustical parameters.

INTRODUCTION

Ultrasonic technology is known to have various applications in various fields (Zell et al., 2007; Datt et al., 2016) such as food (Rani et al., 2012), chemical (Levina et al., 2000; Pelegrinis et al., 2016), water treatment (Doosti et al., 2012), medicine (Sifrash and Hirut, 2011) etc. Further, ultrasonic velocity measurements have been used in investigating various pure liquids (Gardas and Coutinho, 2008; Surayanarayana and Kuppusami, 1976), their mixtures (Naik and Bawankar 2016; Gutta, 2013; Dubey et al., 2009, Prasad et al., 2006) and solutions (Laux et al., 2009; Bhardwaj et al., 2014, Li et al., 2016) to study molecular interactions. Acoustical parameters obtained by density, viscosity and ultrasonic speed provide information about the nature and strength of these molecular interactions (Pandey et al., 1994; Chauhan et al., 2013). It also gives information about bonding between molecules and formation of complex at different temperatures through various interactions.

In continuation of our previous work (Baluja et al., 2008; Bhesaniya and Baluja, 2014; Baluja and Talaviya, 2015), in the present work, some new pyrazole derivatives have been synthesized and their density and sound velocity were measured in N, N, dimethylformamide and dimethyl sulfoxide solutions at 298.15 K. From these experimental data, some acoustical parameters such as isentropic compressibility (κ_s), intermolecular free length (L_f) and solvation number (S_n) have been evaluated in order to study molecular interactions in solutions.

EXPERIMENTAL

The solvents dimethyl formamide (DMF) and dimethyl sulphoxide (DMSO) used in present study were purified by standard method (Riddick et al., 1986).

The pyrazole derivatives have been synthesized in our laboratory and were purified by crystallization in ethanol. The structures of these compounds were confirmed by IR, NMR and mass spectral data. Figure 1 shows the structure of these compounds. The physical constants of these compounds are given in Table 1.

Apparatus and Procedure

Solutions of different concentrations (0.01 to 0.1M) were prepared in DMF and DMSO for the synthesized compounds and were kept at desired temperatures in air tight bottles. An electrical balance (Mettler Toledo AB204-S) with an accuracy of ± 0.1 mg was used for the preparation of solutions.

Measurements of Density, and Ultrasound velocity

Ultrasonic velocity and density measurements of pure solvents and solutions of compounds have been done by using Anton Paar Density and Sound Velocity meter (DSC 5000M) with accuracy of ± 0.5 m/s and ± 0.000005 g/cm³ respectively. The instrument was fully automated and the temperature was automatically controlled. Calibration was carried out using Milli-Q-water (Millipore Pvt. Ltd. Bangalore, India).

RESULTS AND DISCUSSION

The experimental data of density and ultrasonic velocity of pure solvents and solutions are reported in Table 2. Figure 2 shows the variation of ultrasonic velocity with concentration. It is observed from Table 2 and Figure 2 that velocity increases with concentration in both DMF and DMSO solutions for both the compounds.

From the experimental data of density and velocity, some acoustical parameters such as intermolecular free path length (L_f), isentropic compressibility (κ_s) and solvation number have been evaluated by equations reported earlier (Bhesaniya et al., 2014).

The variation of intermolecular free path length (L_f) and isentropic compressibility (κ_s) with concentration is shown in Figures 3 and 4 respectively. It is observed that both intermolecular free path length (L_f) and isentropic compressibility (κ_s) decrease with concentration. This might be due to the aggregation of solvent molecules around solute molecules, indicating there by the presence of solute-solvent interaction for both compounds in both the solvents DMF and DMSO. Thus, there exists strong interaction between solvent and compound molecules in both the solvents DMF and DMSO.

This is further confirmed by solvation number. The solvation number (S_n) is a measure of structure forming or structure breaking tendency of a solute in solutions. Figure 5 shows the variation of solvation number with concentration. For both the compounds, S_n values increases with concentration in both the solvents and the values are positive. The positive value of solvation number suggests structure forming tendency of these compounds in both the solvents. Further, as concentration increases, structure forming tendency is found to increase.

Thus, it is concluded that solute solvent interactions exist for both the studied compounds in both the solvents.

REFERENCES

- Baluja, S., Bhalodiya, R., 2013. Study of molecular interactions in solutions of azomethines of sulfamethoxazole in N, N-dimethylformamide and tetrahydrofuran. *Russ. J. Phys. Chem. A*, 87, 2176-2180.
- Baluja S., Talaviya R., 2015. Molecular interactions in solutions of dihydropyridine derivatives in dimethyl sulfoxide at different temperatures. *J. Chem. Biol. Phys. Sci.*, 5(4), 3916-3939.
- Bhardwaj, T., Bhardwaj, V., Sharma, K., Gupta, A., Cameotra, S. S., Sharma, P., 2014. Thermo-acoustical analysis of sodium dodecyl sulfate: Fluconazole (antifungal drug) based micellar system in hydro-ethanol solutions for potential drug topical application. *J. Chem. Thermodyn.* 78, 1-6.
- Bhesaniya, K., Baluja, S., 2014. Molecular interactions in some synthesized pyrimidine derivatives in methanol and DMF solutions at 308.15 K. *J. Mol. Liqds*, 191, 116-123.
- Chauhan, S., Kumar, K., Patil, B. S., 2013. Study of acoustic parameters of proline in lecithin-ethanol mixture at varying temperature. *Ind. J. Pure Appl. Phys.*, 51, 531-541.
- Datt, P., Kapil, J.C., Kumar, A., Srivastava P.K., 2016. Experimental measurements of acoustical properties of snow and inverse characterization of its geometrical parameters. *Appl. Acoust.* 101, 15-23.
- Doosti, M. R., Kargar, R., Sayadi, M. H., 2012, Water treatment using ultrasonic assistance: A review. *Proc. Int. Acad. Ecol. Environ. Sci.*, 2, 96-110.
- Dubey, G. P., Sharma, M., Oswal, S., 2009. Volumetric, transport and acoustic properties of binary mixtures of 2-methyl-1-propanol with hexadecane and squalane at $T=(298.15, 303.15$ and $308.15)$ K: experimental results, correlation and prediction by the ERAS model. *J. Chem. Thermodyn.*, 41, 849-858.
- Gardas, R. L., Coutinho, J. A. P., 2008. Estimation of speed of sound of ionic liquids using surface tensions and densities: A volume based approach. *Fluid Phase Equil.*, 267, 188-192.
- Gutta, S., 2013. Ultrasonic study of acoustical parameters of binary liquid mixtures of methyl benzoate with 1-octanol at 303.15 K, 308.15 K and 318.15 K. *Res. J. Chem. Sci.*, 3, 14-19.
- Laux, D.; Leveque, G.; Cereser Camara, V., 2009. Ultrasonic properties of water/sorbitol solutions. *Ultrasonics*, 49(2), 159-161.
- Levina, M., Rubinstein, M. H., Rajabi-Siahboomi, A. R., 2000. Principles and application of ultrasound in pharmaceutical powder compression. *Pharm. Res.*, 17, 257-265.
- Li Yang, Figueiredo, E. J.P., Santos, M. J., Santos, J. B., Talavera-Prieto, N. M.C., Carvalho, P. J., Ferreira, A. G.M., Mattedi, S., 2016. Volumetric and acoustical properties of aqueous mixtures of N-methyl-2-hydroxyethyl ammonium butyrate and N-methyl-2-hydroxyethyl ammonium pentanoate at $T = (298.15$ to $333.15)$ K. *J. Chem. Thermodyn.*, 97, 191-205.
- Naik, R. R., Bawankar S. V., 2016. Molecular interactions in atenolol—ethanol mixtures: An ultrasonic study. *Chem. Thermodyn. Thermochem. Russ. J. Phys. Chem.*, A 90, 18-21.
- Pandey, J. D., Jain, P., Vyas, V., 1994. Speed of sound, viscosity and refractive index of multi component systems: analysis of experimental data from the bertrand-acree-burchfield equation. *Can. J. Chem.*, 72, 2486-2492.

Pelegrinis, M. T., Horoshenkov, K. V., Burnett, A., 2016. An application of Kozeny–Carman flow resistivity model to predict the acoustical properties of polyester fibre. Appl. Acoust., 101, 1-4.

Prasad, V. S., Rajagopal, E., Murthy, N. M., 2006. Ultrasonic behavior of ternary mixtures containing water, dimethylformamide and t-butanol at 298.15 K. J. Mol. Liq., 124,1-6.

Rani, B., Singh, U., Prasad, M., Chauhan, A. K., Maheshwari, R., 2012. Utilization of ultrasound technological advances in food industry. Int. Res. J. Pharma., 3, 125-127.

Riddick, J.A., Bunger, W.B., Sakano, T., 1986. Organic solvents-physical properties and methods of purification, techniques of chemistry, New York.

Sifrash, M. G., Hirut, B., 2011. The role of ultrasound in determining fetal sex. Ethiop. J. Health Dev., 25, 216-221.

Surayanarayana, C.V., Kuppusami, J., 1976. Free volume and internal pressure of liquids from ultrasonic velocity. J. Acoust. Soc. Ind., 4, 75-82.

Zell, K., Sperl, J. I., Vogel, M. W., Niessner, R., Haisch, C., Acoustical properties of selected tissue phantom materials for ultrasound imaging. Phys. Med. Biol., 52, N475–N484.

Figure 1: Structure of pyrazole derivatives

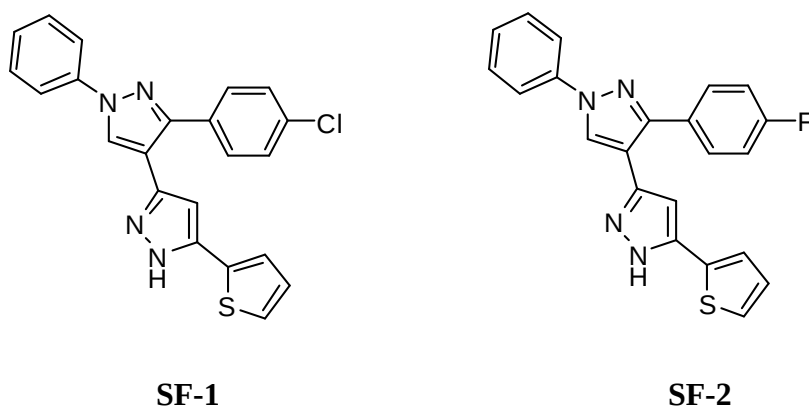
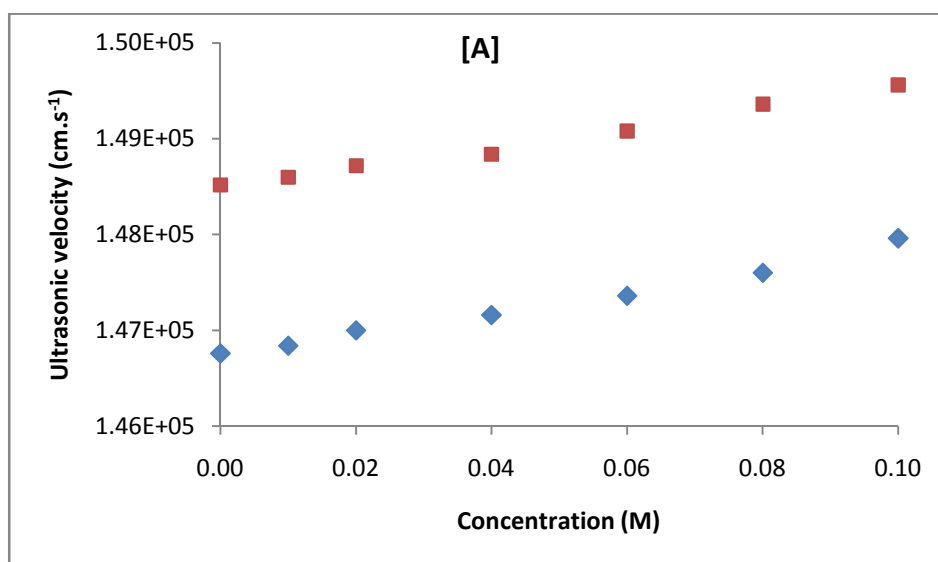


Table 1: Physical constants of pyrazole derivatives.

Compound code	Molecular formula	Molecular weight	M.P. °C	% yield	R _f value
SF-1	C ₂₂ H ₁₇ N ₄ SCl	404.5	142	68	0.84
SF-2	C ₂₂ H ₁₇ N ₄ SF	388	148	65	0.76

Table 2: The density and ultrasonic velocity of SF-1 and SF-2 in both the solvents at 298.15 K.

Conc. M	Density gm/cm ³	Ultrasonic velocity m/sec	Density gm/cm ³	Ultrasonic velocity m/sec
SF-1			SF-2	
DMF				
0.00	0.9485	1.4676	0.9485	1.4676
0.01	0.9518	1.4684	0.9487	1.4684
0.02	0.9520	1.4700	0.9489	1.4688
0.04	0.9528	1.4716	0.9511	1.4700
0.06	0.9529	1.4736	0.9528	1.4708
0.08	0.9586	1.4760	0.9538	1.4616
0.10	0.9599	1.4796	0.9572	1.4636
DMSO				
0.00	1.0953	1.4852	1.0953	1.4852
0.01	1.0957	1.4860	1.0963	1.4860
0.02	1.0961	1.4872	1.0969	1.4880
0.04	1.0972	1.4884	1.0973	1.4904
0.06	1.0979	1.4908	1.0978	1.4924
0.08	1.0985	1.4936	1.0985	1.4948
0.10	1.1006	1.4956	1.0990	1.4968

Figure 2: The variation of ultrasonic velocity with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15 K.

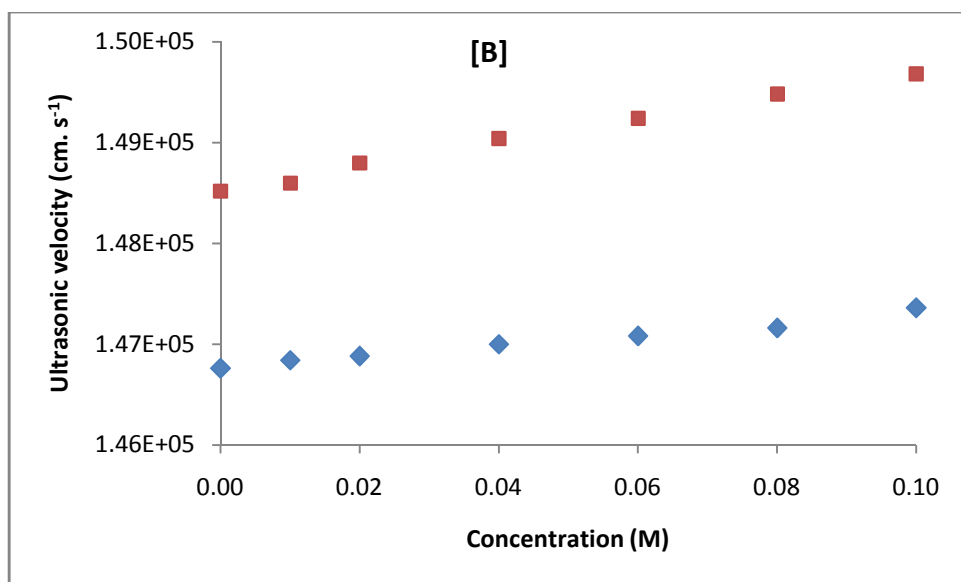
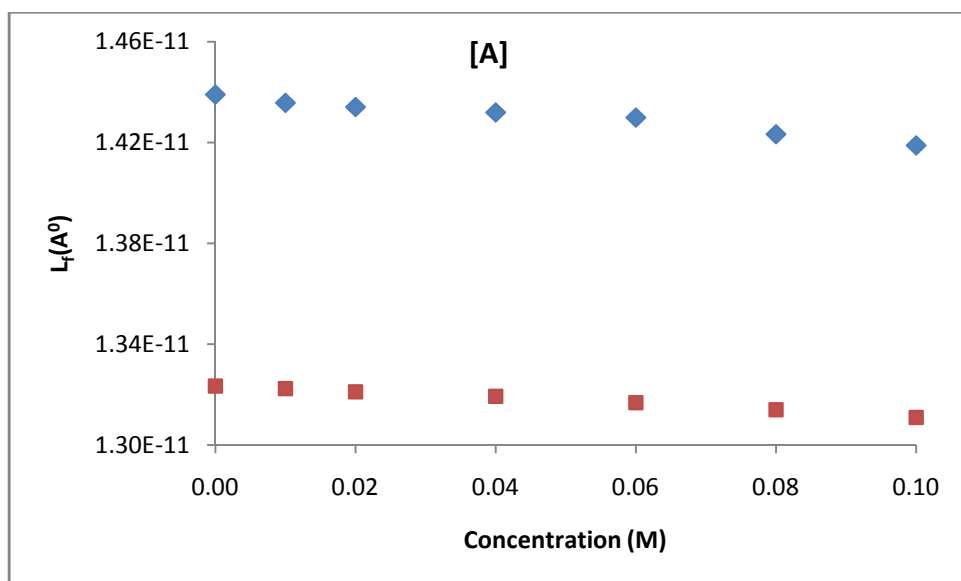


Figure 3: The variation of intermolecular free path length (L_f) with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15K.



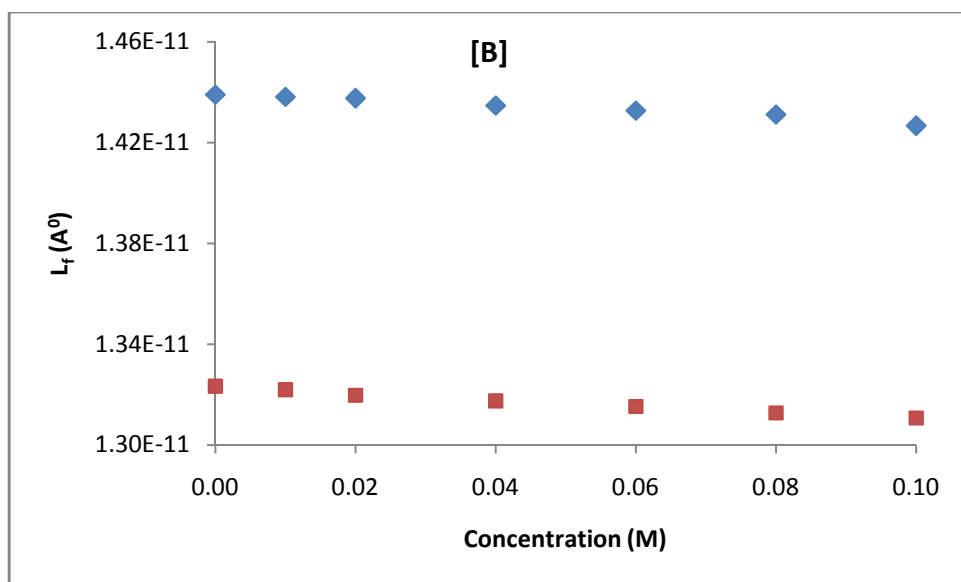
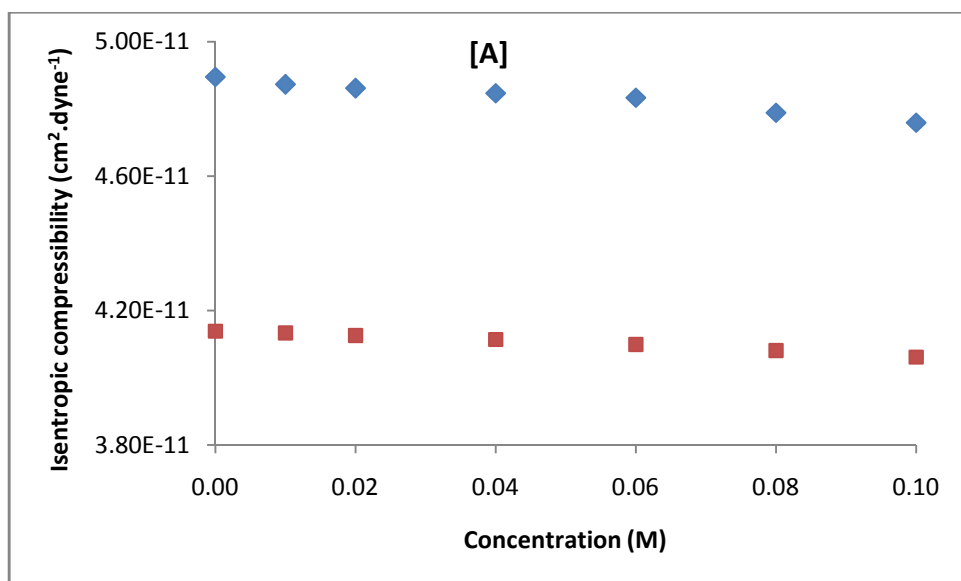


Figure 4: The variation of isentropic compressibility (κ_s) with concentration for [A] SF-I and [B] SF-II in DMF and DMSO at 298.15.



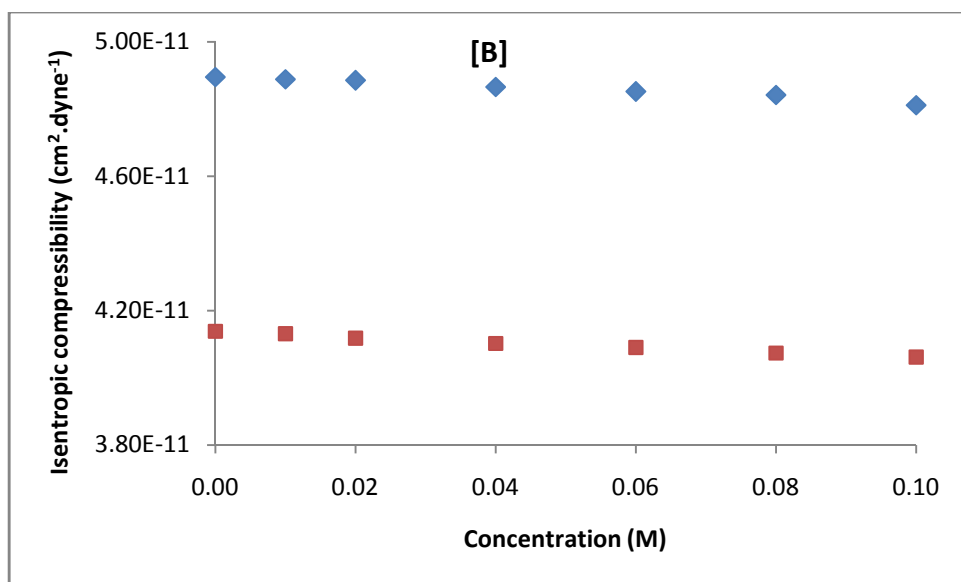


Figure 5: The plot of solvation number (S_n) with concentration for [A] SF-I and [B] SF-2 in DMF and DMSO at 298.15K.

