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Molecular Interaction Study of N-(4-bromophenyl) Maleanilic Acid and N-(4-bromophenyl) Maleimide in Aqueous Dimethyl Sulphoxide at 308.15 K

Dnyaneshwar D. Lokhande

Department of Chemistry, K. P.G. Arts, Commerce and Science College, Igatpuri, Dist. Nashik-422 403, Maharashtra,, INDIA

* *Correspondence: E-mail: ddlokhande1175@gmail.com*

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ABSTRACT: Apparent molar volume, limiting apparent molar volume, semi-empirical parameter, Falkenhagen and Jones-Dole viscosity coefficients were evaluated for N-(4-bromophenyl) maleanilic acid and N-(4-bromophenyl) maleimide in 80% aqueous dimethyl sulphoxide at 308.15 K. From theses parameters, molecular interactions and their extent present in the solution were predicted.

Keywords: Dimethyl sulphoxide; N-(4-bromophenyl) maleanilic acid; density; apparent molar volume; Jone Dole viscosity coefficient.

INTRODUCTION: Maleimide is an important heterocyclic moiety in biology[1-3] and pharmacology[4-7] due to its multi-functional nature. Density, viscosity, apparent molar volume, limiting apparent molar volume and Jones-Dole viscosity coefficients 'A' and 'B' are very useful in predicting the type and extent of molecular interactions as well as to understand different biochemical aspects at the body temperature. The results can be interpreted in terms of solute-solute, solute-solvent and solvent-solvent interactions in these systems. Dimethyl sulphoxide is an aprotic solvent and is strongly associated due to highly polar S=O group. The study of dimethyl sulphoxide is important because of its application in medicine[8-9]. Density and viscosity of some 4-substituted N-phenyl maleimides in aqueous dimethyl sulphoxide have been studied at 308.15 K[10]. The study of molecular interactions present in N-(4-bromophenyl) maleanilic acid and N-(4-bromophenyl) maleimide at 298.15 and 303.15 K in aqueous dimethyl sulphoxide has been reported earlier[11]. In the present article the study has been extended at higher temperature and results were interpreted for the same compounds.

MATERIALS AND METHODS: N-(4-bromophenyl) maleanilic acid (a) and N-(4-bromophenyl) maleimide (b) were synthesized[12] and purified by recrystallization.Triple distilled water and analytical reagent grade dimethyl sulphoxide of minimum assay of 99.9% (SD Fine Chemicals) were used for preparation of solution in the range 0.002 M to 0.01 M at room temperature.

The bicapillary pycnometer and Ubbelohde viscometer was calibrated[13] using triple distilled water. The desired temperature was maintained with the helpof thermostatic water bath. The solutions of different concentrations were prepared in80 % aqueous dimethyl sulphoxide.The flow time was recorded by using digital stop watch. The solution densities and viscosities were determined at 308.15K. Apparent molar volumes, ϕ_v were obtained by following equation[14-15].

$$\phi_v = \frac{1000(\rho_0-\rho)}{c\,\rho_0} + \frac{M_2}{\rho_0}$$

Where, M_2, C,ρ_0 and ρ are the molar mass ofsolute, concentration (mol. L^{-1}) and densities of the solvent and the solution respectively.

The apparent molar volumes$\phi_v$were plotted against the concentration as per the Masson's equation[16].

$$\phi_v = \phi o_v + S_v C^{1/2}$$

Where ϕo_v is the limiting apparent molar volume and S_v is semi empirical parameterwhich depends on the nature of solvent, nature of solute and temperature.The viscosity data was analysed using Jones-Dole equation[17].

$$\frac{\eta_r - 1}{C^{1/2}} = A + B\,C^{1/2}$$

Where, $\eta_r = \eta/\eta_o$(relative viscosity),η and η_o are viscosities of the solution and solvent respectively. C is the molar concentration.The intercept (A) of linear plot of $(\eta_r\text{-}1)/C^{1/2}$vs $C^{1/2}$predicts the extent of solute-solute interaction while slope (B) reflect the extent of solute-solvent interaction.

RESULTS AND DISCUSSION: Parameters such as density, viscosity, apparent molar volume and relative viscosity for N-(4-bromophenyl) maleanilic acid and N-(4-bromophenyl) maleimide in 80 % aqueous dimethyl sulphoxide at 308.15K are reported in Table 1. Density and apparent molar volume $\phi_v$for both acid and imide were found to be increased with concentration. The more negative $\phi_v$values in acid (a)are may be due to strong molecular association. Fig.1 shows linear plots of ϕ_v vs $C^{1/2}$ of maleanilic acid and maleimide solution at 308.15K respectively. Limiting apparent molar volume (ϕo_v) and semi empirical parameter (S_v) were obtained from linear plots are listed in Table 2. The high positive value of 'Sv'indicates the presence of strongsolute-solute interactions. Maleanilic acid (a) has more solute-solute interactions than maleimide (b). Viscosities of the solutions were found to be increased with concentration. Fig. 2 shows variation of $(\eta_r\text{-}1)/C^{1/2}$ vs $C^{1/}2$ at 308.15K. The values of viscosity coefficients 'A' and 'B' obtained from the linear plots are reported in Table 2. Falkenhagen coefficient (A) represent the extent of solute-solute interactions and Jones-Dole coefficient (B) measures the order and disorder introduced by solute in solvent (solute-solvent interactions). Positive values of 'A' shows the presence of strong solute-solute interactions while negative values of 'B' shows weak solute-solvent interactions at low temperature. The high value of 'A' for an acid (a) indicates the presence of stronger solute-solute interactions than that for maleimide.

Table 1: Densities (ρ) (g.cm^{-3}), apparent molar volumes ϕ_v(cm^3.mol^{-1}), viscosities (η) and relative viscosities (η_r) of N-(4-bromophenyl) maleanilic acid (a) and N-(4-bromophenyl) maleimide(b) in 80 % aqueousdimethyl sulphoxide at 308.15K.

Comp.	Conc. (C) mol dm^{-3}	Conc. √C	Density (ρ) (g/cc)	ϕ_v (cm^3. mol^{-1})	Viscosity (η)	Relative viscosity(η_r)
a	0.002	0.0447	1.09299	-1373.1941	2.78374	1.04076
	0.004	0.0632	1.09317	-604.4646	2.79032	1.04322
	0.006	0.0775	1.09341	-357.4003	2.79706	1.04574
	0.008	0.0894	1.09376	-246.4890	2.80408	1.04837
	0.01	0.1	1.09428	-195.5464	2.81155	1.05116
b	0.002	0.0447	1.09238	-1109.7699	2.73934	1.02417
	0.004	0.0632	1.09254	-476.4286	2.74587	1.02660
	0.006	0.0775	1.09274	-271.4341	2.75249	1.02908
	0.008	0.0894	1.09307	-183.8525	2.76557	1.03397
	0.01	0.1	1.09335	-126.7141	2.77240	1.03653

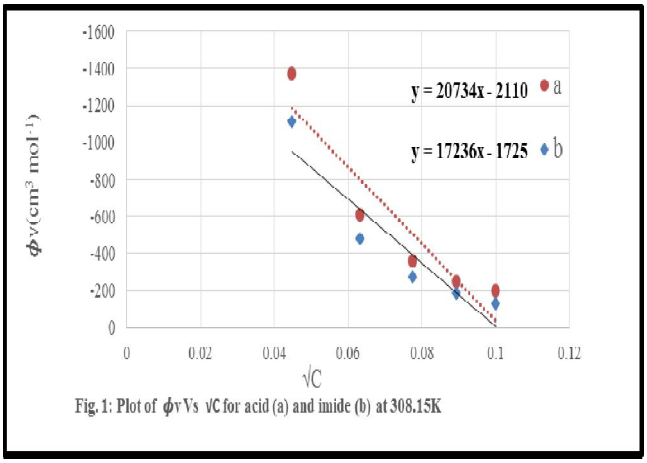

Figure 1: Plot of ϕ_v vs c½ ofN-(4-bromophenyl) maleanilic acid and N-(4-bromophenyl) maleimide in 80% aqueous dimethyl sulphoxide at 308.15K.

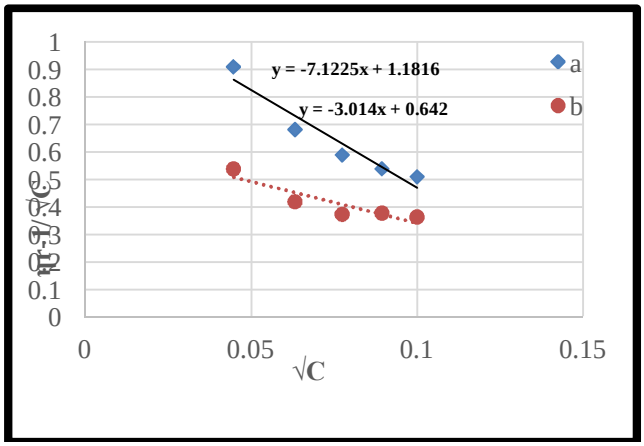

Figure 2: Plot of $(\eta_r\text{-}1)/c^{½}$ vs $c^{½}$of N-(4-bromophenyl) maleanilic acid and N-(4-bromophenyl) maleimide in 80 % aqueous dimethyl sulphoxide at 308.15 K.

Table 2: Masson and Jones-Dole Parameters of N-phenyl maleanilic acid (a) and N-phenyl maleimide (b) in aqueous dimethyl sulphoxide at 308.15 K.

Comp.	ϕo_v	S_v	A ($dm^{3/2}mole^{-1/2}$)	B (dm^3mole^{-1})
a	-2110	20734	1.1816	-7.1225
b	-1725	17236	0.642	-3.014

CONCLUSION: In the present work we have systematically reported apparent molar volume and Jones-Dole viscosity coefficientstudy of N-(4-bromophenyl) maleanilic acid (a) and N-(4-bromophenyl) maleimide(b)in 80 % aqueous dimethyl sulphoxide solution at 308.15K. It was observed that the negative values of apparent molar volume indicate strong molecular association in compound 'a' and 'b'. Positive values of Sv and viscosity constant 'A' indicate the presence of strong solute-solute interaction.The extent of interactions were found to be more in N-(4-bromophenyl) maleanilic acid (a) and N-(4-bromophenyl) maleimide(b). The Jones -Dole and Masson's equations were found to be obeyed for maleanilic acid and maleimide in aqueous dimethyl sulphoxide solution at 308.15K.

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