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Comparative Study of Molar Refraction and Polarizability Constants of Novel 1-Furyl-3-(substituted phenyl)-2-propene-1-one in Different Percentages of Solvents

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The refractive indices and densities of 1-furyl-3-(substituted phenyl)-2-propene-1-one **(I–VI)** in different percentages of dioxane-water, ethanol-water and acetone-water mixtures have been measured. The data have been used to calculate the molar refraction and polarizability constants for the compounds which have been used to detect the nature of dipoles and to compare the 1-furyl-3-(substituted phenyl)-2-propene-1-one **(I–VI)** on the basis of presence of different substituents.

Key Words: Molar refraction and polarizability constant, 1-furyl-3-(substituted phenyl)-2-propene-1-one.

INTRODUCTION

The properties of liquids like viscosity, refractive index and ultrasonic velocity of binary mixtures have been the subject of interest for many workers[1–3]. Dielectric constants and refractive indices of binary mixtures have been studied by Oswal[4]. Study of refractive indices in mixed solvents have been done by Agrawal *et al.*[5–7]. In the present communication, the comparative study of molar refraction and polarizability constant of 1-furyl-3-(substituted phenyl)-2-propene-1-one **(I–VI)** in different percentages of dioxane-water, ethanol-water and acetone-water mixtures on the basis of presence of different substituents have been reported.

EXPERIMENTAL

1-furyl-3-(4-dimethylaminophenyl)-2-propene-1-one **(I)**, 1-furyl-3-(phenyl)-2-propene-1-one **(II)**, 1-furyl-3-(2-nitrophenyl)-2-propene-1-one **(III)**, 1-furyl-3-(4-methoxyphenyl)-2-propene-1-one **(IV)**, 1-furyl-3-(3-hydroxyphenyl)-2-propene-1-one **(V)** and 1-furyl-3-(2-furyl)-2-propene-1-one **(VI)** were prepared in the laboratory and confirmed by elemental analysis, IR and PMR spectral data. The densities of ligand solutions and solvents were determined by a bicapillary

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pyknometer (±0.2%). The refractive indices of solvent mixtures and solutions were measured by using Abbe's refractometer at (30 ± 0.1°C). The accuracy of Abbe's refractometer was within ±0.001 unit. The solvents used were of A.R. grade and doubly distilled water was used. Weighing was made on Shimadzu Japan BL-2204 balance (±0.001 g). Solutions were prepared in different percentages (85, 90, 95 and 100%) of dioxane-water, ethanol-water and acetone-water mixtures.

RESULTS AND DISCUSSION

The molar refraction of solvents (dioxane, ethanol and acetone) and solvent-water mixtures are determined from

$$R_{S\text{-}W} = X_1R_1 + X_2R_2 \quad (1)$$

where R_1 and R_2 are molar refraction of solvent and water respectively.

The molar refraction of solutions in solvent-water mixtures are determined from

$$R_{mixture} = [(n^2 - 1)/(n^2 + 2)] \times [(X_1M_1 + X_2M_2 + X_3M_3)/d] \quad (2)$$

where n is the refractive index of solution, d is the density of the solution, X_1, X_2, X_3 are the mole fractions of solvent, water and solute and M_1, M_2, M_3 are the molecular weights of solvent, water and solute respectively.

The molar refraction of solute is calculated as

$$R_{solute} = R_{mixture} - R_{S\text{-}W} \quad (3)$$

The polarizability constant (α) of solute is calculated as

$$R_{solute} = (4/3)\pi N_0\alpha \quad (4)$$

where N_0 is Avogadro's number.

The data of molar refraction and polarizability constant constant of different solutes are presented in Tables 1 to 6. It can be seen that the molar refraction and polarizability constant of the solute decreases with increase in percentage of ethanol and acetone, which may be attributed to the fact that the dipole in the ligand lies perpendicular to the longer axis of the molecules and increase in the percentage of solvent causes decrease in the dielectric constant of medium. Considerable dipole association takes place, resulting in decrease in molar refraction and polarizability constant because of the mutual compensation of the dipoles. Inversely, with increase in percentage of dioxane, the molar refraction and polarizability constant of the solute increases; this may be because of increase in dielectric constant of the medium resulting in dipole dissociation. These values are large in acetone due to its greater polarity as compared to the less polar ethanol and non-polar dioxane solvent.

Dioxane-Water < Ethanol-Water < Acetone-Water

TABLE-1
MOLAR REFRACTION FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) DIOXANE-WATER MIXTURES

Percentage of dioxane	Compounds (I–VI)/Molar refraction, [R] cm^3 mol^{-1} at (30 ± 0.1°C)					
	I	II	III	IV	V	VI
100	0.3332	0.5206	0.5408	0.3194	0.3997	0.3030
95	0.2639	0.3910	0.4084	0.2483	0.3210	0.2326
90	0.1601	0.2428	0.2615	0.1465	0.1835	0.1374
85	0.1016	0.1857	0.1979	0.0804	0.1297	0.0751

TABLE-2
MOLAR REFRACTION FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) ETHANOL-WATER MIXTURES

Percentage of ethanol	Compounds (I–VI)/Molar refraction, [R] cm^3 mol^{-1} at (30 ± 0.1°C)					+
	I	II	III	IV	V	VI
100	0.1119	0.1890	0.2163	0.0749	0.1383	0.0763
95	0.1887	0.3677	0.3833	0.1692	0.2277	0.1519
90	0.3250	0.5512	0.5700	0.3122	0.3621	0.2952
85	0.4745	0.6615	0.6925	0.4535	0.5122	0.4205

TABLE-3
MOLAR REFRACTION FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) ACETONE-WATER MIXTURES

Percentage of acetone	Compounds (I–VI)/Molar refraction, [R] cm^3 mol^{-1} at (30 ± 0.1°C)					
	I	II	III	IV	V	VI
100	0.1453	0.2226	0.2488	0.1082	0.1704	0.1082
95	0.2217	0.4010	0.4173	0.2031	0.2613	0.1858
90	0.3585	0.5838	0.6021	0.3448	0.3947	0.3277
85	0.5078	0.6944	0.7264	0.4874	0.5458	0.4526

TABLE-4
POLARIZABILITY CONSTANT FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) DIOXANE-WATER MIXTURES

Percentage of dioxane	Compounds (I–VI)/Polarizability constant, [α] × 10^{-24} cm^3 at (30 ± 0.1°C)					
	I	II	III	IV	V	VI
100	0.1320	0.2062	0.2142	0.1265	0.1583	0.1200
95	0.1045	0.1549	0.1618	0.0983	0.1271	0.0921
90	0.0634	0.0961	0.1036	0.0580	0.0727	0.0544
85	0.0402	0.0735	0.0784	0.0318	0.0513	0.0297

TABLE-5
POLARIZABILITY CONSTANT FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) ETHANOL-WATER MIXTURES

Percentage of ethanol	Compounds (I–VI)/Polarizability constant, $[\alpha] \times 10^{-24}$ cm^3 at (30 ± 0.1°C)					
	I	II	III	IV	V	VI
100	0.0443	0.0748	0.0856	0.0296	0.0547	0.0302
95	0.0747	0.1456	0.1518	0.0670	0.0902	0.0601
90	0.1287	0.2183	0.2258	0.1236	0.1434	0.1169
85	0.1880	0.2620	0.2743	0.1796	0.2029	0.1666

TABLE-6
POLARIZABILITY CONSTANT FOR 1-FURYL-3-(SUBSTITUTED PHENYL)-2-PROPENE-1-ONE (I–VI) ACETONE-WATER MIXTURES

Percentage of acetone	Compounds (I–VI)/Polarizability constant, $[\alpha] \times 10^{-24}$ cm^3 at (30 ± 0.1°C)					
	I	II	III	IV	V	VI
100	0.0575	0.0881	0.0985	0.0428	0.0675	0.0428
95	0.0878	0.1588	0.1653	0.0804	0.1035	0.0736
90	0.1420	0.2313	0.2385	0.1366	0.1563	0.1298
85	0.2011	0.2751	0.2878	0.1931	0.2162	0.1793

From Tables 1 to 6, it can also be seen that the order of molar refraction and polarizability constants in compounds is **III > II > V > I > IV > VI.** The increase in molar refraction and polarizability constants of compound **III** as compared to **II** may be due to the presence of electron withdrawing substituent —NO_2 on phenyl ring, which undergoes interaction with solvent resulting in dipole dissociation, while that of decrease in compunds **I, IV** and **V** as compared to **II** may be due to the presence of electron donating substituents —$N(CH_3)_2$, —OCH_3 and —OH respectively. In compounds **I** and **IV** no such interaction is there between the substituents and solvents due to steric hindrance but to a lesser extent ion-dipole bonding may occur because of electron donating effect of —CH_3 groups, causing dipole association. Compound **VI** has lowest molar refraction and polarizability constant.

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