Refractometric Evaluation of Polarizability Constants of Substituted Furan-Based Schiff Bases Derived From 5-Nitrobenzene-1, 2-Diamine In 90% DMSO-Water

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***Abstract*—Refractometric parameter, polarizability constants of five substituted furan-based Schiff bases derived from 5-nitrobenzene-1, 2-diamine, namely Schiff bases 3a – 3e. Polarizability constants were measured at varying concentrations in 90% DMSO-water binary solvent (0.000625–0.01 mol Kg^{-1}) and temperatures ranging from 298.15 to 318.15ºK. The results reveal that polarizability decreases with increasing temperature and dilution, while increasing with the introduction of heavier and more polarizable substituents on the furan ring. Among the investigated compounds, the iodo-substituted Schiff base shows the highest polarizability at all temperatures and concentrations. The observed trends are explained in terms of molecular size, substituent mass, and electronic effects, confirming the sensitivity of refractometric measurements in establishing structure–property relationships in Schiff bases.**

***Index Terms*—Schiff bases; Polarizability constant; Refractometry; Substituent effect; Temperature dependence; Furan derivatives; 90% DMSO-Water.**

I. INTRODUCTION

Schiff bases are synthetically important compounds because of the presence of the azomethine (>C=N) group which Hugo Schiff [1] discovered in 1864. Different products are obtained from the reaction of primary, secondary, and tertiary amines with aldehydes, and ketones.[2] Imines are obtained from primary amines[3]while secondary amines give enamines. When aryl group substituent is a structural part, such compound is stable, and called Schiff base.[4] Schiff-bases are an important type of ligand with diverse donor atoms having remarkable coordination sites towards transition metals[5-7]due to an azomethine linkage enhancing biological activities.[8-9]Major Schiff bases have been prepared starting from various amines by different methods,[10-11] showing important applications in catalytic reactions, materials chemistry, and industry.[12-13]

Molecular polarizability is a fundamental property related to the ease with which the electron cloud of a molecule can be distorted by an external electric field.[14] It plays a crucial role in determining optical behaviour, intermolecular interactions, and reactivity. Refractometric methods offer a reliable and simple experimental approach to determine polarizability constants and to study the influence of temperature, concentration, and molecular structure.[15]

In the present work, five Schiff bases N^1-((5-methylfuran–2-yl) methylene)-5- nitrobenzene -1,2–diamine (3a), 5–nitro-N^1-((5–nitrofuran–2-yl) methylene) benzene–1,2–diamine(3b), N^1-((4–bromofuran–2-yl)methylene)–5–nitrobenzene-1,2–diamine(3c),N^1-((5–bromofuran–2-yl) methylene)–5-nitrobenzene1,2-diamine(3d) and N^1-((5–iodofuran–2-yl) methylene)–5-nitrobenzene-1,2–diamine (3e) were synthesized from 5-nitrobenzene-1,2-diamine and differently substituted furan-2-carbaldehydes.[16] Molar refractivity and poarizability constant were evaluated.

II. MATERIALS AND METHODS

2.1 Materials

All five Schiff bases (3a to 3e) were synthesized by the condensation of substituted furan-2-carboxaldehydes with 5-nitrobenzene-1, 2-diamine using standard literature procedures. The compounds were purified by recrystallization and characterized by conventional spectroscopic methods (IR, UV–Vis, ^{1}H NMR, ^{13}C NMR and Mass). Dimethyl Sulphoxide (Qualigens) and double distill water.

2.2 Preparation of Solutions
Solutions of each Schiff bases (3a to 3e) were prepared in a 90% dimethyl sulphoxide-water binary solvent at Molal concentrations of 0.01, 0.005, 0.0025, 0.00125, and 0.000625M. Fresh solutions were used for each measurement to ensure accuracy.

2.3 Refractometric Measurement
Density of solution was measured by using density bottle using Digital electronic weighing balance (Model CA-44 Accuracy 0.1mg). Density bottle was kept in transparent walled constant temperature water bath to attain thermal equilibrium for 15 min. Refractive index was measured on thermostatically controlled Abbe's Refractometer (Model LMAR 1317 T Make Labman). Accuracy of refractive index measurement was up to ±0.00001. Temperature of solution was maintained constant by water circulation system surrounding the prism box available with refractometer using specially designed water bath. Refractive index measurements were carried out using a calibrated Abbe's refractometer at temperatures of 298.15, 303.15, 308.15, 313.15, and 318.15 K. Temperature control was maintained using a circulating water bath.

III. RESULT AND DISCUSSION

Density and refractive index data were used to calculate molar refractivity (RM) using Lorentz–Lorenz Equation.[17-19] The polarizability constant (α) was calculated from refractive index data using standard refractometric relations based on the Lorentz–Lorenz equation. Average values were taken from repeated measurements to minimize experimental error.

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

Where n – Refractive index of Schiff base solution in 90% DMSO-water.
X_1 - Mole fraction of Dimethyl Sulphoxide
X_2 - Mole fraction of water
X_3 - Mole fraction of Schiff base (3a, 3b, 3c, 3d and 3e)
M_1 - Molecular weight of Dimethyl sulphoxide
M_2 = Molecular weight of water.
M_3 = Molecular weight of solute (Schiff base 3a, 3b, 3c, 3d and 3e).

The molar refraction of ligand is calculated as

$$RM_{ligand} = R_{mixture} - R_{DMSO\text{-}Water} \quad (2)$$

The electronic polarizability, α which is a result of displacement of individual electrons, is proportional to RM. Polarizability of a substance can be determined by measuring the refractive index of the Schiff base solution.

$$RM\ ligand = (4/3)\,\pi N_o \alpha \quad (3)$$

Polarizability constant (α) = 3RM/ 4 π N_o
Where
α – Polarizability constant of Schiff base in 90 % DMSO-water.
No = Avogadro's Constant (6.023 × 10^{23} mol^{-1})

Table-1 Polarizability Constant of Schiff bases 3a, 3b, 3c, 3d and 3e at 298.15- 318.15 K.

Temperature(^{0}K)	Concentration mole fraction	Polarizability Constant (α = × 10^{-23} cm^3)				
		3a	3b	3c	3d	3e
298.15	0.01	0.02408	0.02603	0.02818	0.02819	0.03119
	0.005	0.01645	0.01742	0.01848	0.01849	0.01995
	0.0025	0.01273	0.01322	0.01375	0.01376	0.0145
	0.00125	0.01085	0.0111	0.01138	0.01139	0.01176
	0.000625	0.00988	0.01002	0.01017	0.01018	0.01037
303.15	0.01	0.02407	0.02603	0.02818	0.02819	0.03119
	0.005	0.01644	0.0174	0.01846	0.01847	0.01994
	0.0025	0.01272	0.0132	0.01374	0.01375	0.01448
	0.00125	0.01084	0.0111	0.01137	0.01138	0.01176
	0.000625	0.00986	0.01	0.01015	0.01016	0.01036
308.15	0.01	0.02401	0.02597	0.02812	0.02813	0.03112
	0.005	0.01643	0.01739	0.01845	0.01846	0.01993

	0.0025	0.01266	0.01315	0.01368	0.01369	0.01442
	0.00125	0.01074	0.011	0.01127	0.01128	0.01165
	0.000625	0.00974	0.00988	0.01003	0.01004	0.01023
313.15	0.01	0.02386	0.02582	0.02797	0.02798	0.03097
	0.005	0.01623	0.01719	0.01825	0.01826	0.01972
	0.0025	0.01248	0.01297	0.0135	0.01351	0.01424
	0.00125	0.01059	0.01085	0.01112	0.01113	0.0115
	0.000625	0.00963	0.00977	0.00992	0.00993	0.01012
318.15	0.01	0.02371	0.02567	0.02782	0.02784	0.03083
	0.005	0.01615	0.01712	0.01818	0.01819	0.01965
	0.0025	0.0124	0.01289	0.01343	0.01344	0.01416
	0.00125	0.01051	0.01077	0.01104	0.01105	0.01142
	0.000625	0.00957	0.00971	0.00986	0.00987	0.01006

IV. CONCLUSION

The refractometric investigation of five substituted furan-based Schiff bases revealed that polarizability constants decrease with increasing temperature and dilution, while increasing with the introduction of heavier substituents (Table-1). The iodo-substituted Schiff base exhibited the highest polarizability, followed by brominated, nitro, and methyl derivatives. These results confirm that molecular polarizability is strongly governed by substituent type and molecular structure. The present study highlights refractometry as an effective tool for evaluating optical and electronic properties of Schiff bases and related organic materials.

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