International Journal of Applied Mathematics
Volume 38 No. 11s, 2025
ISSN:1311-1728 (printed version); ISSN: 1314-8060 (online version)

Analysis of the Kamlet-Taft parameter and solvent effects on the RNA Zn molecule.

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Abstract : The RNA Zn molecule's electronic absorption and fluorescence emission spectra swere obtained at room temperature in various organic solvents with variable polarity. The solvent-solute interactions were described using Kamlet Taft parameters. The acquired results demonstrated that a compound's solvatochromic behavior depends on both the polarity of the solvent and the impact of the solvents' hydrogen-bonding characteristics. Based on the data collected, it can be concluded that this RNA Zn molecule has numerous uses, including a DNA cleavage and antibacterial and antifungal properties. In order to comprehend the photoluminescent property of RNA Zn, CIE chromaticity analysis was carried out. Additionally, the optoelectronic properties were examined, including CIE, CRI, and color purity (CIE Coordinates x=0.14,y=0.08). This is appropriate for OLEDs, which are best suited for daylight applications.
Keywords: Kamlet Taft parameters, absorption, fluorescence, solute-solvent interactions, Energy band gap, and CIE chromaticity.

1.Introduction : A derivative of benzothiozole is riluzole Benzothiozole derivatives and their metal complexes have demonstrated significant invitrobiological activity against a variety of bacteria, fungi, and yeast. RNA Zn is a riluzole medication that is combined with matching aldehyde to create riluzole Schiff base Zn metal complex [1-5]. The potential of benzothiozole and similar chemicals as anticancer medicines was demonstrated by a UK cancer research group. The main chemical from this work is phortress. Regardless of estrogen receptor status, this drug has shown efficacy against ovarian, kidney, lung, and colon cancer cells as well as breast cancers.

Compounds used in studies to assess novel products with intriguing biological activities, such as antitumor, antimicrobial, antitubercular, antimalaria, anticonvulsant, anthelmintic, analgesic, and anti-inflammatory activity[6], contain the small and straightforward benzothiozole nucleus. Numerous natural compounds, including bleomycin, epothilone A, lyngbyabellin A, and dolastatin, contain the benzothiozole ring. One special bicyclic ring system is benzothiozole. The synthesis of these molecules is of great interest because of their significant medicinal applications.Benzothizole, a heterocyclic molecule, is used in research as a precursor to larger, typically bioactive substances. Despite having reactive sites that enable functionalization as a

Received : Aug 01,2025

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heterocycle, its aromaticity makes it reasonably stable. The biological activities of derivatives of benzothizole have undergone an intriguing development in recent years.

2.Theory

2.1 kamlet Taft Solvatochromic parameters

The solvent's dipolarity/polarizability index (π*), which measures the solvent's capacity to stabilize a change or dipole through non-specific dielectric interactions, and indices of the solvent's hydrogen-bond donor (HBD) strength (α) and hydrogen-bond acceptor (HBA) strength (β) have also been correlated with absorption transition energy(υ_a), fluorescence transition energy (υ_f), and Stokes shift using the multiple linear regression method proposed by Kamlet and colleagues [7-12].

$$y = y_o + a\alpha + b\beta + c\pi^* \quad (1)$$

where a, b, and c are measurements of the solvents HBD, HBA, and dipolarity/polarizability, respectively, and y is the spectroscopic property under concern and yo is the corresponding spectroscopic property in the gas phase.
In addition to providing information about the solvent's hydrogen bond donor (HBD), α and/or acceptor (HBA), and β ability, which can be assessed using multilinear regression analysis, the solvatochromic effect has been used to determine the magnitude of the solute-solvent interactions, such as the polarizability/dipolarity parameter, π*. To distinguish the impact of non-specific interactions from that of specific interactions, the Kamlet Taft methods have been used [13-14].

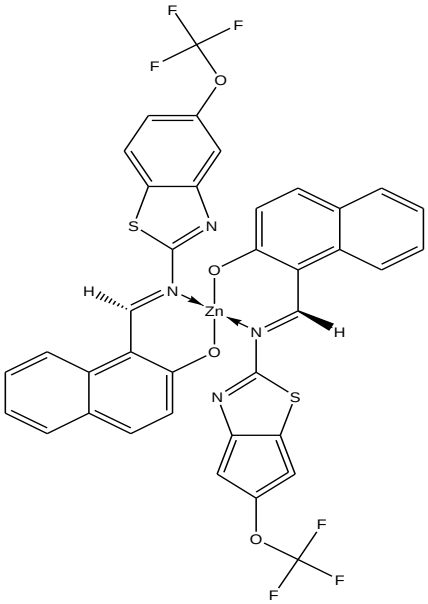

Fig 1: Molecular structure of RNA Zn molecule.

Received : Aug 01,2025

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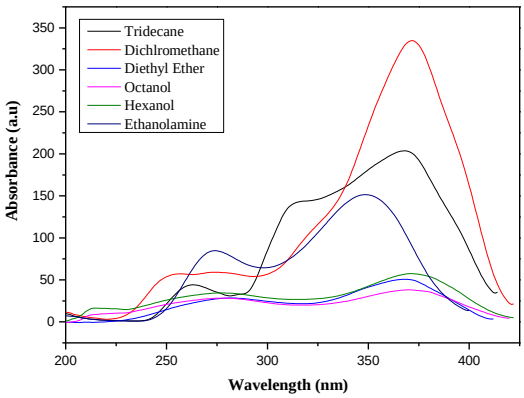

Fig 2: Absorption Spectra of RNA Zn in different solvents.

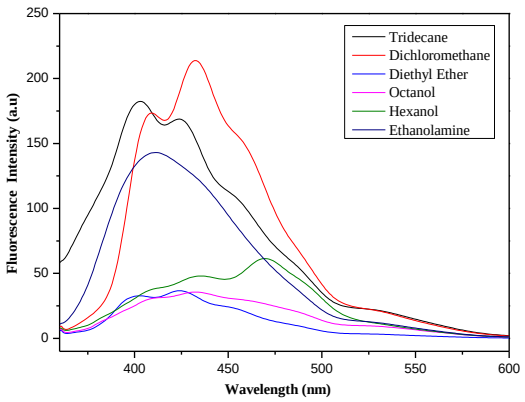

Fig 3: Emission Spectra of RNA Zn in different solvents

3.Materials and Methods

3.1 Materials

The RNA Zn molecule was synthesized [15] using standard methods, and the molecular structure of the molecule is shown in Fig 1. The solvents used in the current study, namely Tridecane, Dichloromethane, Diethyl Ether, Octanol, Hexanol, and Ethanolamine, were obtained from S.D-Fine Chemicals Ltd, India, and were spectroscopic grade.

3.2 Measurement of Absorption and Fluorescence spectra

The RNA Zn absorption spectra were recorded using a Shimadzu UV-1800 UV Vis spectrophotometer over a wavelength range of 200-700 nm, while the fluorescence spectra were obtained using a JASCO FP-8250 Spectrofluorometer with a standard Quartz cuvette. The uncertainty in the measured wavelengths of absorption and fluorescence maxima is + 1 nm. All organic solvents were concentrated at 0.1 mM. The absorption and fluorescence both the spectra were recorded separately for prepared homogeneous solutions of a particular solvent in which RNA Dye molecule dissolved.The experimentally measured values of Absorption, fluorescence spectra and Stokes shift are given in Table 1.

The correlation of Stokes shift ($\overline{\upsilon}_a$-$\overline{\upsilon}_f$) cm^{-1} with various solvent polarity parameters such as orientation polarizability (Δf), hydrogen-bond donor acidity (α), hydrogen bond acceptor basicity (β), and dipolarity/polarizability (π*) showed positive slopes in all cases, indicating that the spectral shift increases with increasing solvent polarity and hydrogen bond strength. The plot of Δυ vs Δf revealed a positive slop of 1673 cm^{-1} , indicating that the excited state is more polar than the ground state and preferentially maintained in solvents with higher dielectric constants, consistent with the Lippert-Mataga model.

A positive slope of 533 cm-1 in the Δυ versus α figure suggests that solvents with higher hydrogen-bond donating ability sustain the excited state via specialized H-bond interactions. The Δυ versus β correlation showed a slope of 449 cm^{-1} , indicating that hydrogen bond accepting solvents contribute to excited state stabilization.
The Δυ vs π* figure shows a positive slope of 681 cm^{-1} , indicating that dipolar and polarizable solvents improve solute-solvent dipolar interactions, resulting in a bathochromic (red shift) in

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emission. These findings show that both particular (H-bonding) and non-specific (solvent) factors influence the solvatochromic behavior of the RNA Zn molecule.

Table 1: Experimental absorption, fluorescence characteristics, and Stokes shift of RNA Zn molecules in various solvents.

Solvents	λ_{abs} (nm)	λ_{emi} (nm)	$\overline{\nu}_a$ (cm^{-1})	$\overline{\nu}_f$ (cm^{-1})	($\overline{\nu}_a$-$\overline{\nu}_f$) (cm^{-1})
Tridecane	368	424	27173	23584	3589
Dichloromethane	372	432	26881	23148	3733
Diethyl Ether	368	424	27173	23584	3589
Octanol	367	411	27247	24330	3932
Hexanol	372	435	26881	22988	3893
Ethanolamine	347	411	28818	24330	4322

Table 2: Solvent parameters and solvent polarity functions

Solvents	Polarity Type	ε	n	$E_T(30)$	E_N^T	α	β	π *	Δ*f*
Tridecane	Non Polar Aprotic	2.0213	1.425	31	0.4414	0.00	0.00	0.03	-0.001096119
Dichloromethane	Moderately Polar Aprotic	8.930	1.424	40.7	0.32	0.13	0.1	0.73	0.217170101
Diethyl Ether	Weakly Polar Aprotic	4.2666	1.3530	34.5	0.117	0.00	0.47	0.27	0.164459443
Octanol	Polar Protic	10.3	1.429	48.1	0.537	0.77	0.81	0.40	0.22559407
Hexanol	Polar Protic	13.03	1.418	48.8	0.557	0.77	0.83	0.39	0.243286244
Ethanolamine	Strongly Polar Protic	31.94	1.454	53	0.796	0.86	0.90	0.72	0.263784266

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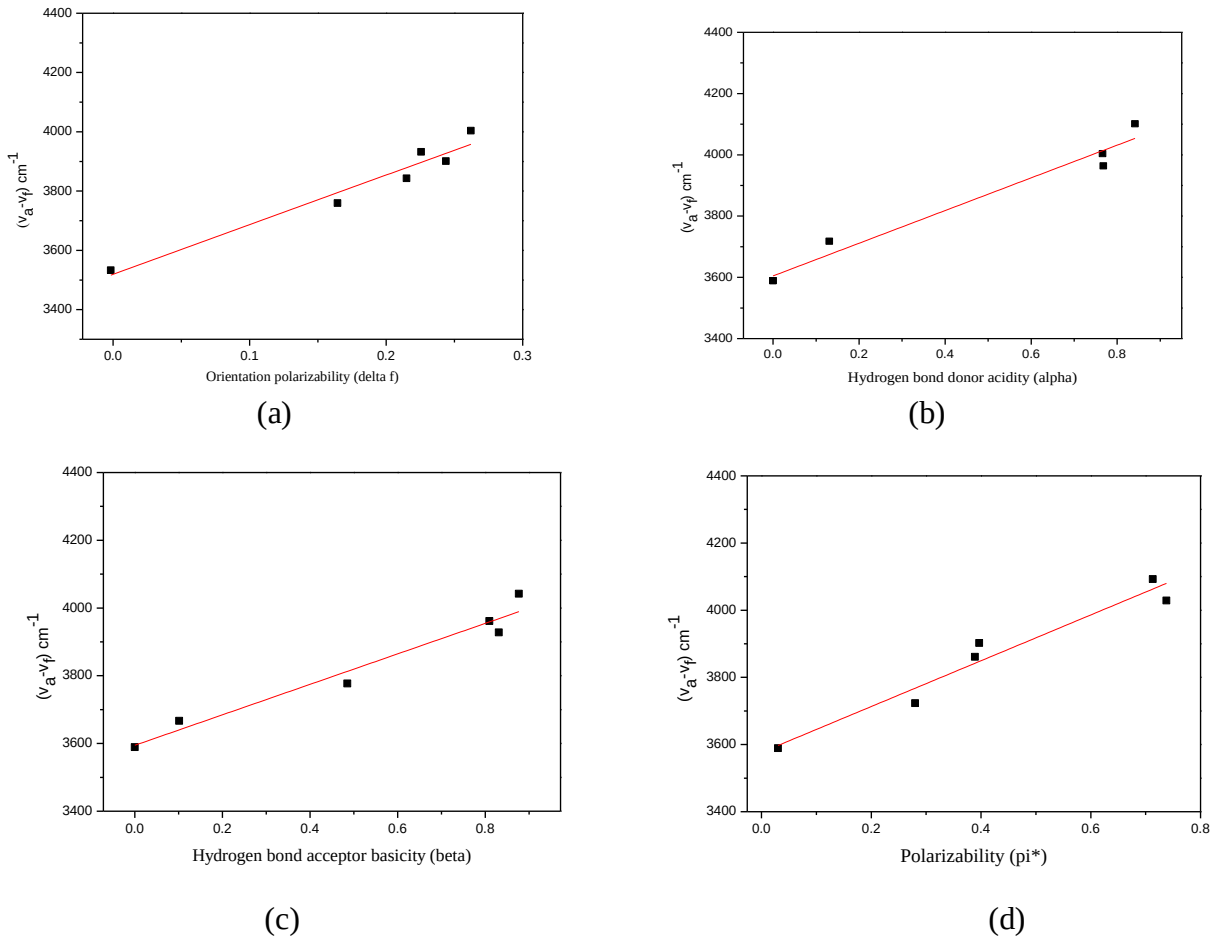

Fig 3: Stoke's shifts vary based on solvent polarity factors, including orientation polarizability (Δf), hydrogen bond donor acidity (α), hydrogen bond acceptor basicity (β), and dipolarity/polarizability (π*).

4.Results and Discussion

4.1 Solvent's Impact on Absorption and Fluorescence Emission Spectra

Figures 2 and 3 present the normalized absorption and emission spectra of RNA Zn in various solvents. The absorption spectra reveal a peak at 350-375 nm, which shifts depending on the dielectric constants of the solvents utilized. Only the longer wavelength is susceptible to solvent polarity, hence absorption variations with solvents have been documented. The emission spectra are obtained by stimulating the material at its longest absorption maxima. The excitation maxima correlate with the longest wavelength absorption band, which has been identified as the intermolecular charge transfer transition.

Table 1 shows the molecule's absorption and emission maxima, as well as the Stokes shift of the absorption and emission peak values in various solvents. The emission spectra reveal a maximum around 400-475 nm. The emission spectra reveal a bigger shift than the absorption

Received : Aug 01,2025

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spectra. Stokes shift magnitudes range from 23148-24330 cm-1. Table 1 shows that when the polarity of the solvent increases, the Stokes shift changes to a bathochromic shift, confirming the π→π* transition.

4.2 Kamlet Taft Solvatochromic Parameters.

Multiple regression is used to determine the individual contributions of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) capacities of solvents to spectroscopic characteristics $\overline{\upsilon}_a$, $\overline{\upsilon}_f$ and ($\boldsymbol{\Delta}\overline{\upsilon} = \overline{\upsilon}_a$-$\overline{\upsilon}_f$). The data for multiple regression analysis using Eq (1), as well as the correlation coefficients in equations 2, 3, and 4.

$$\overline{\upsilon}_a(\text{cm}^{-1}) = 26688 + 121\alpha + 590\beta + 746\pi^* \quad (2)$$

$$\overline{\upsilon}_f\ (\text{cm}^{-1}) = 23386 + 243\ \alpha + 444\ \beta - 140\pi^* \quad (3)$$

$$(\overline{\upsilon}_a\text{-}\overline{\upsilon}_f)(\text{cm}^{-1}) = 3497 + 479\ \alpha - 0.87164\beta - 340\pi^* \quad (4)$$

It is evident from the aforementioned equations that the primary solvent impact for the title molecule is the non-specific dielectric interaction (π*). However, the contribution of the HBD and HBA factors cannot be ignored. The above relations show that HBA (β) influence is more than HBD (α) for $\overline{\upsilon}_a$ and $\boldsymbol{\Delta}\overline{\upsilon}$, while HBD (α) influence is greater than HBA (β) for $\overline{\upsilon}_f$.[16-17]

4.3 Optical Property of RNA Zn molecule

4.3.1 CIE Chromaticity of RNA Zn Molecule

The color coordinate values for Tridecane, Dichloromethane, Diethyl Ether, Octanol, Hexanol, and Ethanolamine were determined using Osram Sylvania CIE coordinate software (10) as shown in Fig 4. The corresponding x and y values are tabulated in Table 3. These coordinates are close to the range for ideal blue light as defined by the National Television Due to the electron-drawing properties of RNA Zn, the CIE coordinates of the molecule in various solvents roughly match the range for perfect blue light (0.14, 0.08).

Photometric characteristics, including Correlated Color Temperature (CCT) values for RNA Zn in various solvents, were determined to be between 1820K and 5825K. The Du'v' numbers represent the error between the test lamp's color temperature and the molecule's CCT, as calculated by software (11). The molecule's ability to replicate colors in comparison to natural light or an ideal source is measured by its Color Rendering Index (CRI), which was found to be roughly 25% for RNA Zn. The average color purity in various solvents is 90.37%, which is a crucial characteristic for evaluating the possible uses of organic compounds. Overall, the RNA Zn molecule has comparatively strong chromaticity, which makes it appropriate for OLEDs and a variety of display applications. (12). The following formula is used to determine the color purity of RNA Zn.

$$\text{Color purity} = \frac{\sqrt{(X-X_i)^2+(Y-Y_i)^2}}{\sqrt{(X_d-X_i)^2+(Y_d-Y_i)^2}} \quad (5)$$

Where (Xi, Yi) is the color coordinate of white light, (Xd,Yd) is the CIE coordinate of the major emission wavelength, and (X,Y) are the CIE chromaticity coordinate values of the compound

Received : Aug 01,2025

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under study. Table 1 in this report displays the (Xi, Yi) = (0.310, 0.316), (Xd, Xd) = (0.14,0.08), and (X,Y) values. The color purity is 90.45%, 96.34%, and 96.30%, according to Table 1. 78.33%, 83.69%, and 97.13% for the solvents under study at an excitation wavelength of 350 nm. For WLED (White Light Emitting Diode) applications, the computed chromaticity coordinates for RNA Zn in ethanolamine are close to standard chromaticity for outstanding blue color, making them promising blue generators.

Table 3 : Colorimetric properties of RNA Zn

Solvents	x	y	u^I	v^I	CCT	D u^I v^I	CRI	Color purity
Tridecane	0.1598	0.1013	0.1641	0.2340	2439	-0.1624	17.5	90.45
Diethyl Ether	0.1585	0.0816	0.1731	0.2005	1853	-0.1953	7.375	96.34
DCM	0.1563	0.0832	0.1696	0.2031	1914	-0.1928	4.875	96.30
Octanol	0.1614	0.1445	0.1464	0.2948	5825	-0.1064	28.625	78.33
Hexanol	0.1486	0.1351	0.1374	0.2812	2692	-0.1221	14.25	83.69
Ethanolamine	0.1580	0.0792	0.1739	0.1961	1820	-0.1996	5.5	97.13

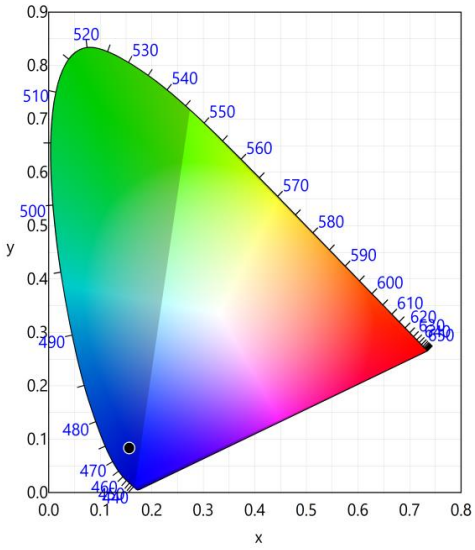

Fig 4 : Plot of color coordinate values for RNA Zn in different solvents with scale of CIE coordinates.

4.3.2 Energy Band gap

The UV-Vis absorption spectra (Fig.2) were recorded, and the optical characteristics of the titled derivative were examined using Tauc's plot. Based on these spectra, we calculated the bandgap

Received : Aug 01,2025

International Journal of Applied Mathematics
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energy of the RNA Zn molecule. As a result, the plots of $(\alpha h\upsilon)^2$ versus Photon energy hυ for the solution phase of the titled compound are shown in (Fig.). The graph's linearity for every solvent under study attests to the direct permissibility of electronic transitions. The arrows therefore illustrate the linearity. The linear region of Fig. 5 (Eg) is extended to find the energy band gap (Eg). Table (4) displays the measured Eg values.

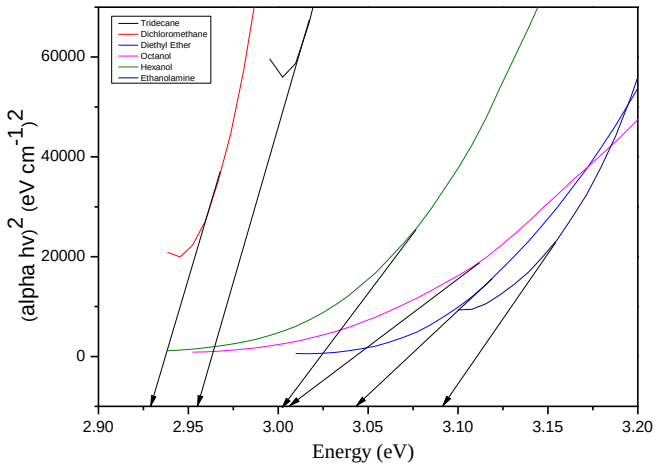

Fig 5: Tauc's plot for optical Energy Band Gap (Eg) in different solvents

Table 4: Energy band gap estimated using Tauc's plot method.

Solvents	Energy bandgap (eV)
DCM	2.9281
Octanol	3.0064
Hexanol	3.0017
Tridecane	2.9540
Ethanolamine	3.0915
Diethyl Ether	3.0432

5. Conclusion

RNA Zn metal complexes have a number of pharmaceutical and medicinal uses, including DNA cleavage, antibacterial, and antifungal properties. The investigated solvents exhibited a small bathochromic shift (red shift) in the photoluminescence emission spectra; this red shift is most likely caused by the solvents' increased polarity. The use of CIE chromaticity analysis helped to comprehend the color tone of the light emitted, providing information on the molecule's

Received : Aug 01,2025

Volume 38 No. 11s, 2025
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photoluminescent properties in various solvents. The molecule's possible appropriateness in particular lighting applications was described by photometric metrics such as CCT, CRI error values, and color purity. The RNA Zn has an average color purity of 97.37% in various solvents, indicating that it may be suitable for display applications. Optoelectronic devices, biological fluorescence indicators, and solvatochromic sensors can all benefit from an RNA Zn molecule with a configurable Eg (2.954-3.194 eV).

Acknowledgement: The authors sincerely acknowledge to USIC- Gulbarga University Kalaburagi and Maharani Cluster University, Bangalore for providing instrumental and Laboratory facilities necessary for this research. The author also expresses gratitude to Department of Physics , Gulbarga University Kalaburagi for providing financial support through the fellowship.

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Received : Aug 01,2025