IJCRT.ORG ISSN : 2320-2882

INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

# A theoretical evaluation of Structure and Biological descriptors of Ru(II) polypyridyl complexes of 2-(3,4,5-Trimethoxy-phenyl)-H-imidazole[4,5-f][1,10]phenanthroline

Navaneetha Nambigari[1,2*] and Sravani Gudikandula[1]

1.Department of Chemistry, University College of Science, Saifabad, Osmania University, Hyderabad - 500004, Telangana State, INDIA.

2.Department of Chemistry, University College of Science, Osmania University, Tarnaka, Hyderabad – 500007, Telangana State, INDIA.

**Abstract:**

The mononuclear Ru(II) polypyridyl complexes of the type $[Ru(NN)_2L](ClO_4)_2.2H_2O$,where NN are 1,10 phenanthroline (1), bipyridyl (2), 4,4'-dimethyl-1,10 - ortho Phenanthroline (3) and 4, 4' dimethyl 2, 2'-bipyridine (4), and 'L' is an Intercalator ligand, TMIP=2-(3,4,5-Trimethoxy-phenyl)-H-imidazole[4,5-f][1,10]phenanthroline were studied by various computational methods.

The stability of the Ru (II) complexes helps in determining the binding ability with CT-DNA which was investigated by molecular modeling - a computational study. The energy of these complexes are 445.65 (1) 430.66 (2), 399.59 (3) and 380.64Kcal/mole (4) respectively. These values indicate that TMIP complex $[Ru(phen)_2TMIP]^{+2}$ indicative of the higher stability owing to substitution over the ancillary ligand.

The DNA binding affinities order of these complexes: 1 > 2> 3 > 4, indicating that the unsubstituted complex has better affinity to DNA implying the role of the auxiliary ligand. Electronic characteristic and HOMO - LUMO gap of the Ru complex is less than the Intercalator hence kinetically labile.

**Key words:-** Polypyridyl, Biophysical Studies, DNA, Photo cleavage and Intercalation.

## I. INTRODUCTION

Metal coordinated complexes have been used as drugs to treat a variety of illnesses, including those with antimicrobial, anticancer, anti-diabetic, anti-arthritic, antiulcer, and anti-malarial properties. The development of new medications for cancer therapy is a crucial field of research. Because they can cleave DNA under physiological settings, metal complexes have drawn attention in recent decades for the development of metal-based anticancer medications [1-3]. Recent progress in the field of medicinal chemistry has been provided by the discovery of cisplatin and its analogues for the treatment of cancer. These platinum drugs have a wide range of clinical uses, but they have serious limitations because of their high toxicity, range of side effects on normal cells, inactivity against many other cancer cell lines, and tendency to metastasize [4]. This motivated scientists to look for other possible metal-based anticancer drug options, and as a result, complexes of different transition metals were synthesized and tested for their anticancer activities [5]. Due to their rich photochemical reactions and photo physical characteristics, Ruthenium (II) polypyridyl complexes have drawn a lot of interest as substrates for DNA binding among the documented DNA binders [6-8].

Ruthenium complexes containing dipyridophenazine (dppz) ligand have been extensively researched due to their remarkable photophysical characteristics and robust DNA binding [9, 10]. By substituting on the dppz ligand, a number of derivatives of $[Ru(phen)_2(dppz)]^{+2}$ (phen is 1,10-phenanthroline) have been created [11]. It was discovered that altering the intercalating ligand's structure resulted in adjustments to the intercalated complex's orientation. A number of ruthenium complexes have been suggested as possible anticancer substances. Compared to platinum compounds, these complexes have exceptional anticancer efficacy and decreased overall toxicity; in certain situations, their anticancer activity surpasses that of cisplatin. $[Ru(bpy)_2(dppz)]^{+2}$ where bpy = 2,2'-bipyridine shows cytotoxicity at low half-maximum inhibitory doses ($IC_{50}$). Ru (II) complexes have been produced recently, possibly as a result of their structural composition, solubility, lipophilicity, charge, and photophysical properties, which may make them targets for cells [12–14]. According to more recent research, ruthenium (II) polypyridyl complexes can effectively cause apoptosis and exhibit high cytotoxicity in vitro [15 - 19].

The stability of novel Ruthenium(II) polypyridyl complexes derived from TMIP - [2-(3,4,5-Trimethoxy-phenyl)-H-imidazole [4,5-f][1,10]phenanthroline] were determined theoretically by Semi empirical methods using Gaussian software.. The binding association of CT-DNA to these complexes was examined by using UV-Visible absorption titration, Fluorescence emission and viscosity experiments [20, 21].

## II. METHODOLOGY, RESULTS AND DISCUSSION

Ground state geometries and analysis of frontier molecular orbitals (FMOs) of Ruthenium (II) complexes have been theoretically studied by the Semi empirical method using PM6 were performed with the Gaussian09 package [22, 23]. DFT calculation is also applied to understand the change in structural or geometrical parameters through calculations of bond length, bond angle, and torsional angle of metal complexes [24] Besides, the stability and reactivity of ligands and their complexes are investigated through the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) energies of the ligand upon binding to metal. In this study, the geometrical and electronic properties of the ligand and Ruthenium (II) polypyridyl complexes are studied.

**Computational details - Geometric optimizations**

Ground state geometries and frontier molecular orbital (FMOs) of Ruthenium (II) complexes have been theoretically studied by the Gaussian09 package by performing the Semi-empirical PM6 method in the gas phase. The molecular geometry, the highest &lowest occupied molecular orbital (HOMO, LUMO) energies, and Mulliken atomic charges of the molecules are determined from optimized geometry (in Gas). Atomic charges of the ligand and Ru complex are calculated by the Mulliken method [25].

s. The molecular properties, such as the chemical potentials (Pi), HOMO-LUMO gap (Eg), absolute hardness(η), absolute electronegativity (χ), absolute softness (σ), global electrophilicity (ω), global softness (S), and electronic charge, Nmax were calculated according to the equations 1 – 8 [26, 27].

$$Eg = E_{LUMO} - E_{HOMO} \quad (1)$$

$$\chi = (E_{HOMO} + E_{LUMO}) / 2 \quad (2)$$

$$\eta = (E_{LUMO} - E_{HOMO}) / 2 \quad (3)$$

$$\sigma = 1 / \eta \quad (4)$$

$$Pi = -\chi \quad (5)$$

$$S = 1/2\eta \quad (6)$$

$$\omega = Pi^2/2\eta \quad (7)$$

$$\Delta NMax = -Pi\eta \quad (8)$$

From the HOMO - LUMO energy gap (Eg) reactivity of the complex can be accessed; the narrow gap suggests high complex reactivity [26, 28].

The analytical and spectral studies depict an octahedral coordination of Ru(II) complexes which were further verified by their molecular modelling studies. The 3D optimized structures of metal complexes were presented in **Fig. 1.** The energy minimization process was iteratively performed to determine the total energy, which is as follows: 445.65 (phen), 430.66 (bpy), 399.59(dmp) and 380.64 kcal/mol (dmb). The values of the total energy suggest that unsubstituted ancillary ligand complexes are more stable. Further conformational investigation of Ru (II) polypyridyl complexes, including bond length, bond angles, torsion angles, and intercalator lengths data.

**Table 1. Bond lengths of 3D conformers of synthesized Ru (II) Complexes**

| .No | Complex | Metal Intercalator length(Å) Ru - N | Total Energy (KCal/mol ) | M-$N_1^a$ | M-$N_2^a$ | M-$N_3^b$ | M-$N_4^b$ | M-$N_5^b$ | M-$N_6^b$ |
|---|---|---|---|---|---|---|---|---|---|
| . | $[Ru(phen)_2TMIP]^{+2}$ | 14.1257 | 445.65 | 1.9525 | 1.9515 | 1.9528 | 1.9522 | 1.9523 | 1.9530 |
| . | $[Ru(bpy)_2TMIP]^{+2}$ | 14.1289 | 430.66 | 1.9540 | 1.9531 | 1.9506 | 1.9507 | 1.9521 | 1.9504 |
| . | $[Ru(dmp)_2TMIP]^{+2}$ | 14.2234 | 399.59 | 1.9543 | 1.9537 | 1.9512 | 1.9510 | 1.9518 | 1.9513 |
| . | $[Ru(dmb)_2TMIP]^{+2}$ | 14.1280 | 380.64 | 1.9522 | 1.9521 | 1.9514 | 1.9511 | 1.9515 | 1.9515 |

The bond lengths calculated using Gaussian 9.0 programs. (a: nitrogen bonded to metal. a: N1 and N2, N of TMIP ligand bonded to metal) N3, N4, N5 and N6 are polypyridyl(phen/dmp/bpy/dmb).
1=$[Ru(phen)_2TMIP]^{2+}$; 2=$[Ru(bpy)_2\ TMIP]^{+2}$ 3= $[Ru(dmp)_2TMIP]^{2+}$; 4 =$[Ru(dmb)_2\ TMIP]^{+2.}$

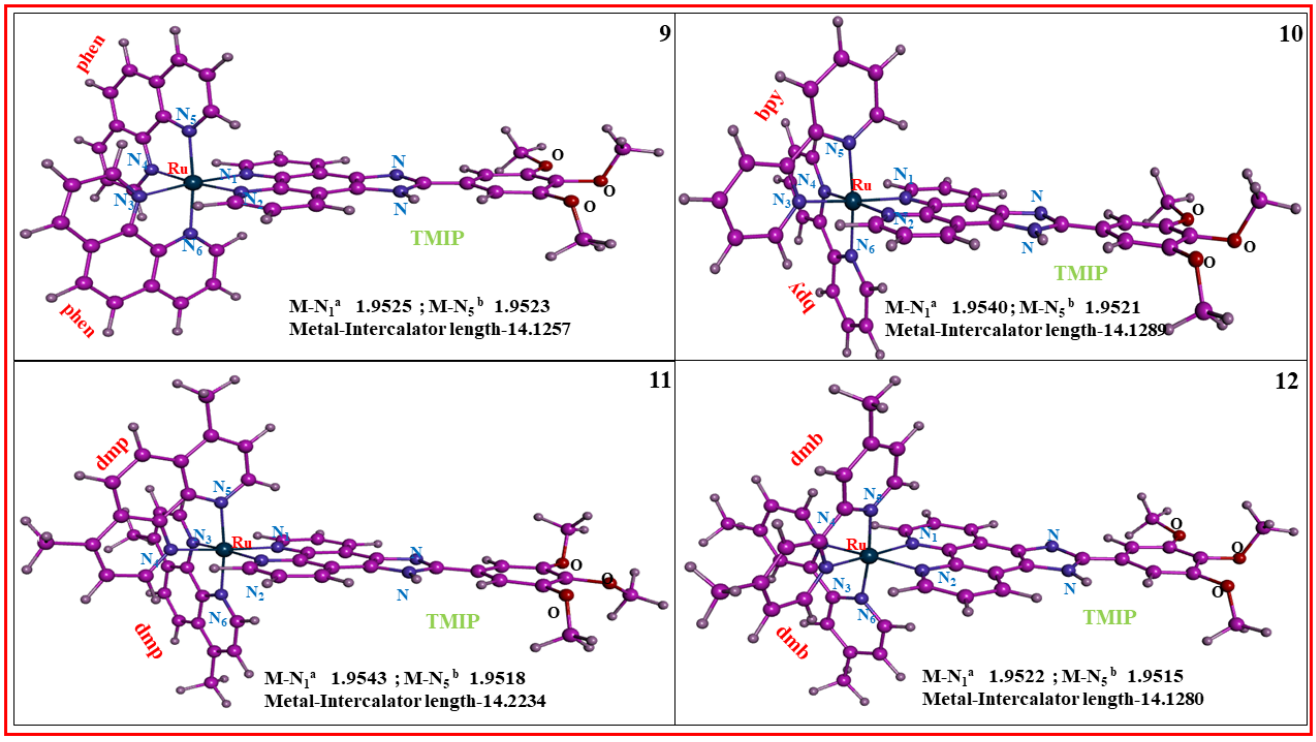


**Figure 1. 3D model of the Ru(II) polypyridyl complexes where; 1.$[Ru(phen)_2TMIP]^{+2}$,2. $[Ru(bpy)_2TMIP]^{+2}$,3.$[Ru(dmp)_2TMIP]^{+2}$,4.$[Ru(dmb)_2TMIP]^{+2}$**

Table 1 displays the structural information (M-N bond length and metal-intercalator length) of the 3D metal complex conformers. Ru - N (N of intercalator-TMIP) bond length is a shorter than N of the auxiliary ligand. The complexes' reported has bond angles ranged from 90.2 to 92.4, close to octahedral geometry. The results demonstrate that the optimised structures of the examined complexes are slighted distorted since these

molecules are stressed and depart from predicted bond angles (90°), as expected in the octahedron. The literature demonstrates that a balance of columbic attractions and Van der Waals repulsions between the metal cation and the donor atoms affects the choice for M-N bond length.

For Metal Polypyridyl Complexes, the frontier molecular energy levels [HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital)] provide insight into the possible electronic transitions. A factor in determining the stability of the structure is the energy gap between the HOMO and LUMO orbitals, crucial parameter for chemical reactivity, which also denotes the molecule's electrophilic and nucleophilic tendencies.

**Table 2** provides information about the electron affinity, ionization potential and LUMO-HOMO gap (Eg) of the ligands TMIP and its complexes. The Koopmans theorem states that the energy difference or Eg gap is used to determine the molecular properties. **Figure 2** shows the 3D Contour surfaces of the frontier molecular orbitals of the Ligand TMIP and Complexes (1-4). The energy gaps in complexes are found to be in the range of 4.9945 TO 5.3479 eV, whereas TMPIP ligand Eg is 7.6116 eV.Metal complexes have a smaller HOMO-LUMO gap.Which indicates the ligand show less chemical reactivity than its Ru (II) complexes. Among the complexes, the phen(complex 1), dmb(complex 4) complexes were more reactive than the bpy(complex-2) and dmp(complex-3) complexes. Soft molecules have a modest HOMO-LUMO gap compared to hard molecules' huge HOMO-LUMO gap, soft molecules will therefore be more polarizable than hard ones. Complexes1 is more vulnerable to nucleophilic attack, according to the HOMO-LUMO calculations. on the imidazole ring of the Intercalator ligand of the complex, The LUMO is localized on the imidazole ring of the Intercalator ligand of the complex, according to the 3D contour diagrams (**Figure 2**). These results indicate that the interaction hub for DNA – metal complex may well comprise the Ru(II) cations, TMPIP, and imidazole rings.

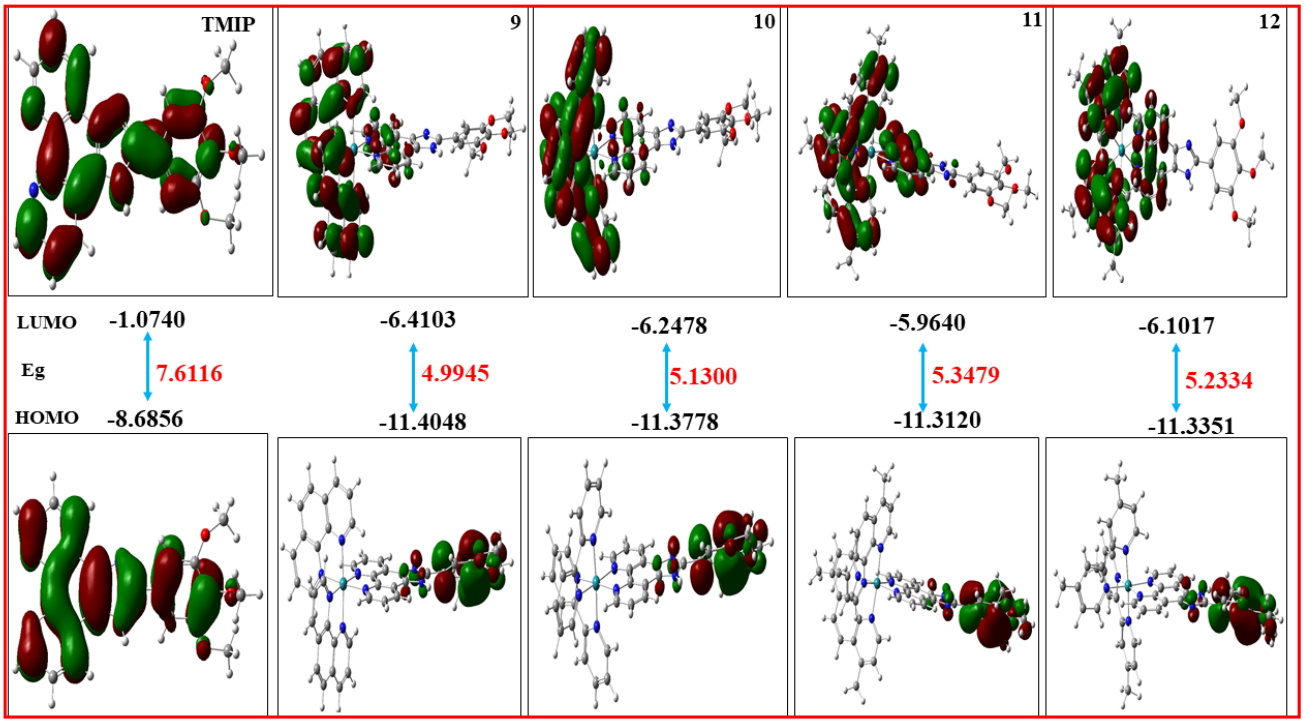


Figure 2.HOMO-LUMO energy gap of the metal complexes (1) $[Ru(phen)_2TMIP]^{+2}$, (2) $[Ru(bpy)_2TMIP]^{+2}$, (3) $[Ru(dmp)_2TMIP]^{+2}$, (4) $[Ru(dmb)_2TMIP]^{+2}$

**Table 2.Data for HOMO, LUMO, IP, EA and LUMO-HOMO gap(ΔE)**

| Ligand and Complex | HOMO(eV) | LUMO(eV) | ΔE, (LUMO-HOMO gap) (eV) | Ionization potential (IP) (eV) | Electron affinity (EA) (eV) |
|---|---|---|---|---|---|
| TMIP | -8.6856 | -1.0740 | 7.6116 | 8.6856 | 1.0740 |
| 1.$[Ru(phen)_2TMIP]^{+2}$ | -11.4048 | -6.4103 | 4.9945 | 11.3778 | 6.2478 |
| 2.$[Ru(bpy)_2TMIP]^{+2}$ | -11.3778 | -6.2478 | 5.1300 | 11.4048 | 6.4103 |
| 3.$[Ru(dmp)_2TMIP]^{+2}$ | -11.3120 | -5.9640 | 5.3479 | 11.3120 | 5.9640 |
| 4.$[Ru(dmb)_2TMIP]^{+2}$ | -11.3351 | -6.1017 | 5.2334 | 11.3351 | 6.1017 |

The HOMO and LUMO energy values can predict the ionization potential (I) and electron affinity (A). The ionisation potential directly correlates with the HOMO energy, while the electron affinity principally links the LUMO energy. Table 2 provides information on the electron affinity, ionisation potential, and LUMO-HOMO gap (Eg) of the ligand, TMIP, and its complexes. The energy gap in complexes are in the range of 4.9945 eV to 5.3479 eV, TMIP Ligand (7.6116 eV), which indicates the ligand show less chemical activity than the comparable Ru (II) complexes, is found to have a larger energy gap.

Soft molecules have a modest HOMO-LUMO gap compared to hard molecules' huge HOMO-LUMO gap, soft molecules will therefore be more polarizable than hard ones. Complexes1 is more vulnerable to

nucleophilic attack, according to the HOMO-LUMO calculations. The TMIP, imidazole ring of the Intercalator ligand and ancillary ligand of the complex, the LUMO is localized, according to the 3D contour diagrams (**Figure 2**). Reactivity increases with HOMO-LUMO gap length. These results indicate that the interaction hub for DNA – metal complex may well comprise the Ru(II) cations, TMIP, and imidazole rings.

The concept of hard and soft acids and bases was established using the molecular metrics electronegativity, a derivative of total energy, and absolute hardness (η), which were calculated for the prediction of biological and chemical reactivity. A greater global electrophilicity (ω) refers a molecule is more electrophilic.

**Biological and chemical reactivity parameters**

The concept of hard and soft acids and bases was constructed using the molecular metrics electronegativity, a derivative of total energy, and absolute hardness (η), which were calculated for the prediction of biological and chemical reactivity.The degree to which a molecule is electrophilic is known as its "global electrophilicity" (ω). The chemical potential (μ), which is equivalent to a change in charge from a system with a higher chemical potential to one with a lower chemical potential, is the symbol for the global reactivity index. Electronegativity (χ) is the capacity to attract electrons equivalent to the negative of the chemical potential.

The attributes of the biological and chemical reactivity parameters calculated as a result of the energies of the border molecular orbitals (LUMO, HOMO) are listed in **Table 3**. According to Parr et al.[28], the electrophilicity index (ω), a positive and definite quantity, calculates a molecule's degree of electrophilicity. The chemical hardness and potential are comparable to this indicator of total reactivity. This reactivity index monitors the energy stabilization process when the system absorbs an additional electronic charge (N) from its surroundings. When an electrophile obtains an electrical charge, its energy must decrease, so its chemical potential must be negative.

The calculated value of the molecular descriptors shows that the Ru(II) complexes possess improved reactivity as compared to the free ligands TMIP. According to **Table 3** data Complex-1 (phen) has minimum hardness values (η), the higher global electrophilicity (ω), lower chemical potential (μ) and maximum softness values (σ) indicating more reactivity than the other complexes. This trend observed in case of other phen containing metal complexes(5&9) also. The results suggests that the ancillary Ligand in the Ru (II) Polypyridyl complexes affect and alter the reactivity, stability, binding abilities for DNA binding and biological activity.

**Table 3. Biological and Chemical reactivity parameters of synthesized ligands and its Ru(II) complexes**

| Complexes | η | σ | ω | μ | χ | S | ΔNmax |
|---|---|---|---|---|---|---|---|
| 1.TMIP | 3.8058 | 0.2627 | 3.1284 | -4.8798 | 4.8798 | 1.9029 | 1.2822 |
| 2.$[Ru(phen)_2TMIP]^{+2}$ | 2.4972 | 0.4004 | 15.8863 | -8.9075 | 8.9075 | 1.2486 | 3.5669 |
| 3. $[Ru(bpy)_2TMIP]^{+2}$ | 2.5650 | 0.3898 | 15.1395 | -8.8128 | 8.8128 | 1.2825 | 3.4357 |
| 4.$[Ru(dmp)_2TMIP]^{+2}$ | 2.6739 | 0.3739 | 13.9520 | -8.6380 | 8.6380 | 1.3369 | 3.2303 |
| 5.$[Ru(dmb)_2TMIP]^{+2}$ | 2.6167 | 0.3821 | 14.5241 | -8.7184 | 8.7184 | 1.3083 | 3.3318 |

**Mulliken charges**

Mulliken charges (produced by the Mulliken population analysis) can be used to calculate partial atomic charges when using computational chemistry techniques, especially those of the linear combination of atomic orbitals molecular orbital approach. The Mulliken atomic charge is one of the essential components that is directly related to the vibrational characteristics of the molecule. This element influences electrical structure, dipole moment, and polarizability, among other chemical characteristics[29]. It helps us comprehend how the electrical structure is impacted by atomic displacement[30].

The Mulliken population analysis-derived net atomic charges of BFIP ligand and its Ru complexes, which were shown in **Table 4**. The extraordinary negative charge on N(1), N(2), N(3), N(4), N(5), and N(6) atoms are due to their electron withdrawing nature. The N1 and N2 electron withdrawing is more as indicated by highly negative charge as shown in **Table 4**.

All of the complexes, carbon atoms have positive charge distributions, with the exception of the carbon atoms that are attached to electronegative atoms, which have exceptionally high positive charges because these electronegative atoms withdraw partial charges, and the carbon atoms that are attached to nitrogen of phen, which have negative charge distributions, which may lead to a more electropositive nature of the Ru (II) atom. The charge distribution of $[Ru(phen)TMIP]^{2+}$ complex represented that the carbons attached with electronegative atoms (Oxygen and nitrogen) are positively charged; meanwhile, these electronegative atoms withdraw partial charges, making it positive, whereas C's bonded to N's are partial negative may be due to the "greater electropositive character of Ru(II) atom".

The charges on the Ru atom in the complexes (1-4), as shown in **Figure 3**, **Table 4** were 0.7299, 0.8036, 0.8042and 0.7398 (e) respectively. These values are much lower than the formal charge of +2. Due to a higher overall charge transfer from the ligand (L) to Ru in complex (1) than in complexes (2,3, and 4) Ru acquires a lower positive charge. Additionally, a reduced negative charge on 'N' in the methyl substituent complexes (dmp and dmb) indicates less charge transfer to it compared to the other complexes, accumulating a low positive charge at the Ru.

The net charge of each hydrogen atom is positive. Due to their electron-withdrawing properties, the nitrogen atoms (polypyridyl- phen, dmp, bpy, and dmb) and the N1 and N2 of the TMIP ligand linked to metal have a significant negative charge. **Table 3** indicates that the N1 and N2 electron withdrawal is more pronounced. The electron density is centred around the nitrogen of the imidazole ring of the intercalator ligand, as shown by the 3D contours of the TMIP ligand and its Ru complexes in **Figure 3**.

The attributes of the biological and chemical reactivity parameters calculated as a result of using the energies of the border molecular orbitals (LUMO, HOMO) are listed in Table 7.The chemical hardness and potential indicate total reactivity, which is found to be higher for phen complex. A molecule with a narrow frontier orbital gap has a higher chemical reactivity and is often more prone to polarization due to its limited kinetic stability [59].

According to the data in Table 3 and **Figure-3** the charges over the central metal atom Ru in 9-12 complexes were as follows, 0.775, 0.800, 0.734, 0.749(e) respectively. The variation in the positive charge from its formal charge is due to the electron charge transfer from the ligand to Ru. This kind of electron shift from ligand to metal is more in case of metal complex-11 hence this complex shows less positive charge. Nitrogen's in the ligand TMIP & metal complexes acquired negative charge's but compared to the metal complex nitrogen's, intercalating ligand imidazole ring nitrogen's have greater negative charge due to high electron density. Carbon atoms in the ligand and complexes acquired positive charge. In the ligand carbon atoms attached to nitrogen atoms gained negative charge after complex formation. All the oxygen atoms have shown negative charges due to its electronegativity character.

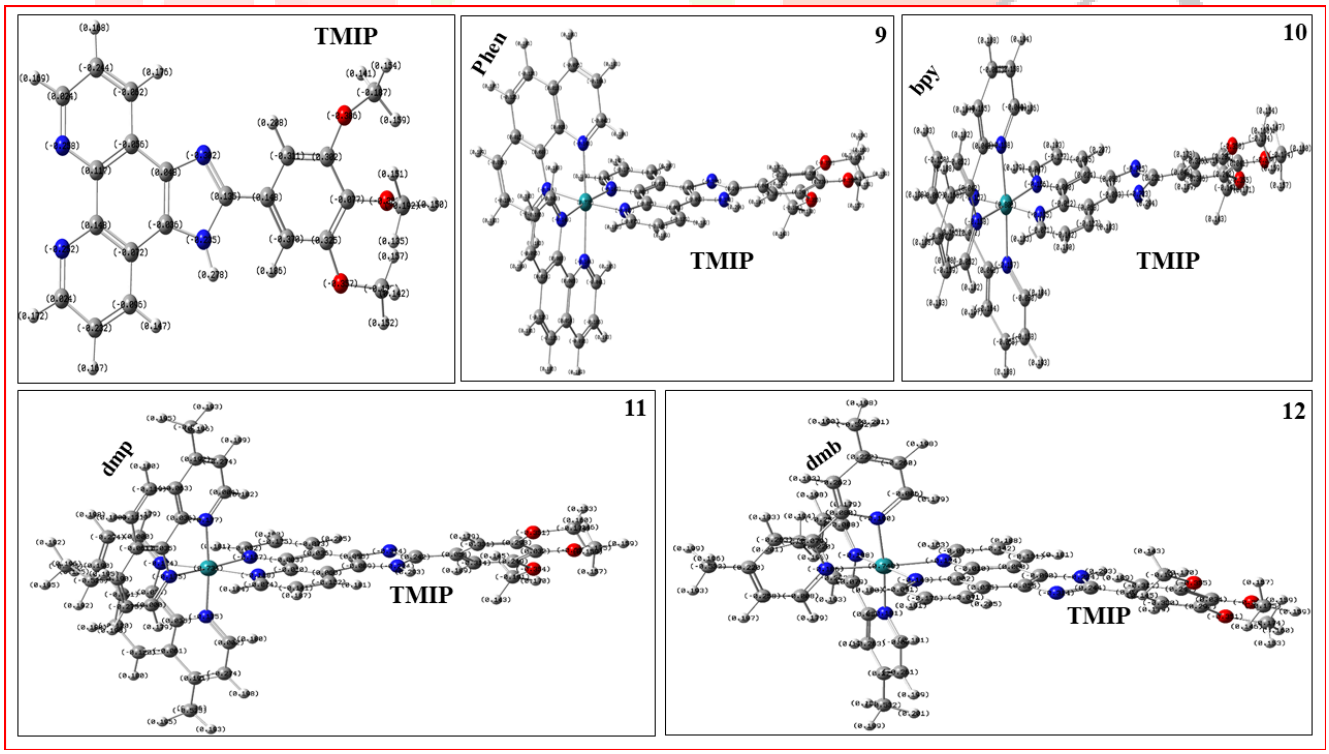


Figure 3. Mulliken charge distribution per atom in TMIP ligand and its Ru Complexes. TMIP.-Ligand,1. $[Ru(phen)_2TMIP]^{+2}$, 2. $[Ru(bpy)_2TMIP]^{+2}$; 3. $[Ru(dmp)_2TMIP]^{+2}$ ;4. $[Ru(dmb)_2TMIP]^{+2}$.

**Table 4. Selective Mulliken atomic charges distribution of TMIP and its metal complexes**

| Atom(No.) | TMIP | A=phen | Bpy | Dmp | Dmb |
|---|---|---|---|---|---|
| Ru | Ru | 0.775 | 0.800 | 0.734 | 0.749 |
| **N6** | - | 0.144 | 0.157 | 0.175 | 0.191 |
| **N5** | - | 0.148 | 0.158 | 0.177 | 0.190 |
| **N4** | - | 0.146 | 0.157 | 0.174 | 0.188 |
| **N3** | - | 0.148 | 0.158 | 0.175 | 0.186 |
| **N1** | 0.258 | 0.147 | 0.156 | 0.137 | 0.124 |
| **N2** | 0.252 | 0.127 | 0.135 | 0.118 | 0.143 |
| **C7** | 0.024 | 0.049 | 0.048 | 0.052 | 0.073 |
| **C8** | 0.023 | 0.073 | 0.071 | 0.074 | 0.051 |
| C9 | - | 0.005 | 0.040 | 0.036 | 0.080 |
| C10 | - | 0.042 | 0.049 | 0.004 | 0.179 |
| **N44** | 0.235 | 0.228 | 0.223 | 0.224 | 0.224 |
| **N45** | 0.302 | 0.314 | 0.315 | 0.314 | 0.314 |
| **O** | 0.387 | 0.350 | 0.350 | 0.351 | 0.355 |

When employing computational chemistry methods, particularly those of the linear combination of atomic orbitals molecular orbital approach, it is possible to compute partial atomic charges using Mulliken charges (generated by the Mulliken population analysis). One of the crucial elements directly connected to the vibrational properties of the molecule is the Mulliken atomic charge. Among other chemical features, this element affects polarizability, dipole moment, and electronic structure [60].

All of the complexes, carbon atoms have positive charge distributions, with the exception of the carbon atoms that are attached to electronegative atoms, which have exceptionally high positive charges because these electronegative atoms withdraw partial charges, and the carbon atoms that are attached to nitrogen of phen, which have negative charge distributions, which may lead to a more electropositive nature of the Ru (II) atom.

The charges on the Ru atom in the complexes as shown in **Figure S14** (Supplementary Information), these values are significantly lower than the formal charge of +2. Due to a higher overall charge transfer from the ligand (L) to Ru in complex (1) than in complex (2), Ru acquires a lower positive charge. Additionally, a reduced negative charge on N in the methyl substituent complexes (dmp) indicates less charge transfer to it compared to the other complexes, accumulating a low positive charge at the Ru. Due to their electron-withdrawing properties, the nitrogen atoms (polypyridyl- phen, dmp, bpy, and dmb) and the N1 and N2 of the TMIPligand linked to metal have a significant negative charge on them.

## CONCLUSION

Ru(II) complexes have been synthesized, characterized, and their interaction with CT-DNA studied. From the biophysical experiments, it is clear that both the compounds can intercalate into DNA base pairs via the TMIP ligand. The complexes 1 binds to DNA more strongly than complex 2 because phenanthroline as an ancillary ligand provide more surface area. Binding affinity follows the order (1)> (2). The experimental results show that Ru(II) complexes exhibited the effect of the DNA light switch.

The HOMO and LUMO gap for a phen complex is 5.7387 eV as compared to the Intercalator (7.5101eV) indicating of kinetic stability and its nucleophilic level of sensitivity. The binding constant information obtained using the absorption and emission techniques is also confirmed by the docking investigations. Therefore this study has widened the scope of developing the Ru(II) –TMIP complexes as a strong DNA probe. All the complexes (**1**, **2**) have good anticancer, antibacterial and anti-fungal activity. The antibacterial activity data for the complexes at various concentrations indicate that the complexes exhibited appreciable activity against gram +ve than gram-ve but were less effective than the standard drug. Therefore, this study has widened the scope of developing these imidazole derivatives as promising biological activity.

## CONCLUSION

Ru(II) complexes have been synthesized, characterized, and their interaction with CT-DNA studied. From the biophysical experiments, it is clear that both the compounds can intercalate into DNA base pairs via the BFIP ligand. The complexes 1 binds to DNA more strongly than complex 2 because phenanthroline as an ancillary ligand provide more surface area. Binding affinity follows the order (1)> (2). The experimental results show that Ru(II) complexes exhibited the effect of the DNA light switch.

The HOMO and LUMO gap for a phen complex is 5.3479 eV as compared to the Intercalator (7.6116eV) indicating of kinetic stability and its nucleophilic level of sensitivity. The binding constant information obtained using the absorption and emission techniques is also confirmed by the docking investigations. Therefore this study has widened the scope of developing the Ru(II) –TMIP complexes as a strong DNA probes. All the complexes (**1**, **2**) have good anticancer, antibacterial and anti fungal activity. The antibacterial activity data for the complexes at various concentrations indicate that the complexes exhibited appreciable activity against gram +ve than gram-ve but were less effective than the standard drug. Therefore, this study has widened the scope of developing these imidazole derivatives as promising biological activity.

## Author Contributions

**Navaneetha Nambigari**:"Conceptualization; Methodology; Resources; Software; Supervision; Roles/Writing – original draft Writing ".

**Sravani Gudikandula**: "Data curation, Formal analysis, Investigation; Validation; Visualization; ".

**Conflict of interest -** On behalf of all authors, the corresponding author states that there is no conflict of interest.

**Acknowledgements**: The authors NN and SG are thankful to The Head, Department of Chemistry and the Principal, University College of Science, Saifabad, Osmania University, and The Head, Department of Chemistry and the Principal, University College of Science, Tarnaka, Osmania University, Hyderabad for the facilities to carry out this work. The authors are thankful to DST FIST, New Delhi, for the Computational Lab facilities to carry out this work.

**Author declarations -** Funding No financial support from any agency.

**Notes**: All data generated or analyzed during this study are included in this published article [and its supplementary information files].

**References:-**

1. Chifotides HT, Dunbar KR. "Interactions of metal − metalbonded antitumor active complexes with DNA fragments and DNA",Acc Chem Res.(2005),38:146–156.
2. Bednarski PJ, Mackay FS, Sadler PJ. "Photoactivatable platinum complexes Anti Cancer Agents," Med Chem.(2007),7:75–93.
3. Dyson PJ et al., "Sensitization of ruthenium nitrosyls to visible light via direct coordination of the dye resorufin: trackable NO donors for lighttriggered NO delivery to cellular targets", J Am Chem Soc.(2008),130:8834–8846.
4. Blanpain C. "Tracing the cellular origin of cancer", Nat Cell Biol. (2013),15:126–134.
5. Galanski M, Jakupec MA, Keppler BK. "Update of the pre-clinical situation of anticancer platinum complexes: novel design strategies and innovative analytical approaches", Curr Med Chem.12 (2005)12:2075–2094.
6. Huang HL et al. "Synthesis, cellular uptake, apopotosis, cytotoxicity, cell cycle arrest, interaction with DNA and antioxidant activity of ruthenium(II) complexes", Eur J Med Chem. 46 (2011)46:3282–3290.
7. Xu L, Xie YY, Zhong NJ, Liang ZH, He J, Huang HL, Liu YJ (2012) Transit Met Chem.(2012),37:197–205.
8. Tan LF et al. "Nucleic acid binding behaviors and cytotoxic properties of a Ru (II) complex," DNA Cell Biol.(2011),30:277–285.
9. Friedman AE et al. "A molecular light switch for DNA: $Ru(bpy)_2(dppz)^{2+}$ J Am Chem Soc. (1990),112:4960–4962.
10. Olson EJC et al. "First Observation of the Key Intermediate in the "Light-Switch" Mechanism of $[Ru(phen)_2 dppz]^{2+}$" J Am Chem Soc.(1997),119:11458–11467.
11. Hartshorn RM, Barton JK. "Novel dipyridophenazine complexes of ruthenium(II): exploring luminescent reporters of DNA", J Am Chem Soc. (1992),114:5919–5925.
12. **Navaneetha Nambigari***, Aruna Kodipaka, Ravi Kumar Vuradi, Praveen Kumar Airva and Satyanarayana Sirasani*. 2022. A biophysical study of Ru(II) Polypyridyl complex, properties and its interaction with DNA. Journal of Fluorescence. 32 (2): 1211 – 1228. Doi: http://doi.org/10.1007/s10895-021-02879-x [IF - 2.226].
13. **Navaneetha Nambigari***, Aruna Kodipaka, Ravi Kumar Vuradi, Praveen Kumar Airva and Satyanarayana Sirasani. 2022. Binding and Photocleavage studies of Ru (II) Polypyridyl Complexes with DNA: An In Silico and Antibacterial activity. Analytical Chemistry Letters. 12 (2), 266 – 282. http://doi.org/10.1080/22297928.20211110

14. ArunaKodipaka, Ravi Kumar Vuradi, Praveen Kumar Airva, **Navaneetha Nambigari***and Satyanarayana Sirasani. 2024. Application of Novel Ruthenium (II) polypyridyl Complexes as robust DNA probes, Optical material and Antimicrobials - An Experimental and DFT approach., Journal of Fluorescence. http://doi.org.10.1007/s10895/-02-03626-8
15. Tan CP et al. "Synthesis, structural characteristics, DNA binding properties and cytotoxicity studies of a series of Ru(III) complexes.," J Inorg Biochem.(2008),102:1644–1653.
16. Puckett CA, Barton JK. "Mechanism of cellular uptake of a ruthenium polypyridyl complex", Biochemistry.(2008),47: 11711–11716.
17. Puckett CA, Barton."Methods to explore cellular uptake of ruthenium complexes", J Am Chem Soc.129 (2007),129: 46–47.
18. Schatzschneider U et al. "Cellular Uptake, Cytotoxicity, and Metabolic Profiling of Human Cancer Cells Treated with Ruthenium(II) Polypyridyl Complexes $[Ru(bpy)_2(N\text{-}N)]Cl_2$ with N-N=bpy, phen, dpq, dppz, and dppn[‡]"Chem Med Chem.(2008),3:1104–1109.
19. Sravani Gudikandula, Aruna Kodipaka,**Navaneetha Nambigari***(2023) Application of Ru (II) Polypyridyl Complexes in Metallopharmaceuticals amd material Science. Mediterranean J. Chem. 13(3): 263-284.
20. Sravani Gudikandula , Navaneetha Nambigari. Correlation of Anti-cancer activity and DNA binding affinity of novel Ru(II) Polypyridyl complex – A Biophysical study", JETIR February (2024), 11 (2) www.jetir.org (ISSN-2349-5162).
21. Sravani Gudikandula, **Navaneetha Nambigari*** (2024) Correlation of Anti-cancer activity and DNA binding affinity of novel Ru(II) Polypyridyl complex – A Biophysical study. J of Emerging Tech. and Inn Res. 11(2): c191 – c201.http://doi.org/10.6084/m9.jetir.JETIR2402225 [IF = 7.95]
22. J. J. P. Stewart, "Optimization of parameters for semiempirical methods. II. Applications," *J. Comp. Chem.*, 10 (1989) 221-64. DOI: 10.1002/jcc.540100209.
23. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, et al., Gaussian 09, Revision D. 01, Gaussian Inc, Wallingford, CT, USA, 2009.
24. Ye Z, Ting L,Qiwen T.Theoretical study on electronic structures and spectroscopy of triarylborane substituted by thiophene. *Bull. Chem. Soc. Ethiop.* 2009, 23, 77.
25. N.A. Ogorodnikova, On invariance of the Mulliken substituent-induced charge changes in quantum-chemical calculations of different levels, J. Mol. Struct., **2009**, 894, 41–49.
26. A.N. El-Ghamaz, M.A. Diab, A.A. El-Bindary, Geometrical structure and optical properties of antipyrine Schiff base derivatives, Mater Sci Semicond Process, **2014**, 27, 521–531.
27. A.Z. El-Sonbati, M.A. Diab, A.A. El-Bindary, S.M. Morgan, Supramolecular spectroscopic and thermal studies of azodye complexes, Spectrochim Acta Part A Mol Biomol Spectrosc, **2014**, 127, 310–328.
28. A.Z. El-Sonbati, M.A. Diab, A.A. El-Bindary, Molecular docking, DNA binding, thermal studies and antimicrobial activities of Schiff base complexes. J. Mol. Liq., **2016**, 218, 434–456.
29. Parr R G, Szentpály L & Liu S **(1999)** Electrophilicity Index. J Am Chem Soc, 121 (1999) 1922 - 1924.
30. Govindarajan M &Karabacak M **(2012)** Spectroscopic properties, NLO, HOMO-LUMO and NBO analysis of 2,5-Lutidine. SpectrochimActa A, 96: 421. doi: 10.1016/j.saa.2012.05.067.

31. Guidara S, Ahmed A B, Abid Y &Feki H, Molecular structure, vibrational spectra and nonlinear optical properties of 2,5-dimethylanilinium chloride monohydrate: a density functional theory approach. SpectrochimActa A, 127 **(2014)** 275 -285. DOI: 10.1016/j.saa.2014.02.028.
32. Ogorodnikova, N. A. On invariance of the Mulliken substituent-induced charge changes in quantum-chemical calculations of different levels.*J. Mol. Struct. THEOCHEM.* 2009, **894**, 41.