22nd Iranian Chemistry Conference, 23-25 August, 2023
University of Kurdistan

Comparison of structure, nature of bond, fluorescence response and biological activity of Cu(I) and Ag(I) complexes of a known tetradentate Schiff base ligand derived from tren and its reduced form

Ghazal Zahedi[a], Farshid Hajibabaei[a], Samaneh Sanei Movafagh[a] and Sadegh Salehzadeh[a]*

Department of Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran
Email: saleh@basu.ac.ir

The interaction of metal complexes with deoxyribonucleic acid (DNA) has been a subject of interest in bioinorganic chemistry, especially since the discovery of cisplatin and their analogues [1-3]. In this project, the Ag(I) and Cu(I) complexes of a known tetradentate Schiff base ligand derived from tris(2-aminoethyl)amine (L^1_{sb}) and its reduced form (L^1_r) were synthesized and characterized by CHN elemental analysis, UV-Vis, IR, ^{1}H NMR and ^{13}C NMR spectroscopies. In addition, the structure, nature of the bond, fluorescence intensity and biological activity of them were investigated and compared. DNA interaction studies through the UV-Vis method confirmed that L^1_r and $[AgL^1_r]NO_3$ both have effective interaction with DNA, and the calculated binding constant (K_b) indicated that L^1_r has higher affinity compared to $[AgL^1_r]NO_3$. Density functional theory studies on the above Cu(I) and Ag(I) complexes and several similar complexes showed that the metal−ligand bond dissociation energies (BDEs) in copper complexes are larger than those in Ag(I) complexes.

Keywords: Schiff base, Tris(2-aminoethyl)amine, DNA interaction, Bond dissociation energy.

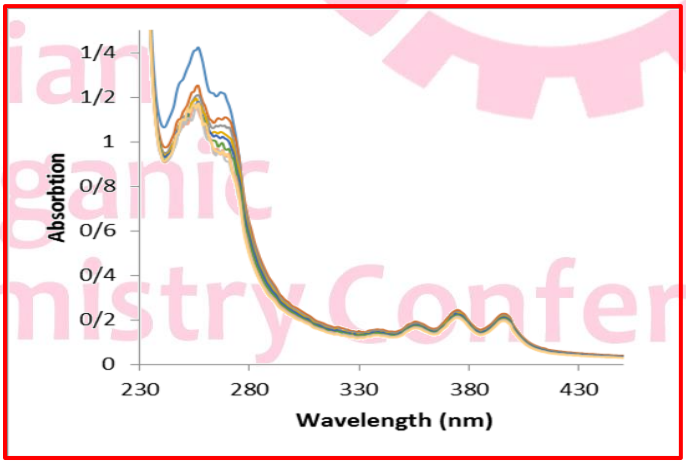


Figure 1. The changes of UV-Vis spectra of L^1_r in the DNA→L^1_r system at room temperature and pH 7.4 ($[L^1_r]$= 5.0×10^{-5} M and [DNA]= 0.0 to 9.7×10^{-5} M).

References

[1] Farrell, N. *Compr. Coord. Chem. II*. **2003,** 9, 809-840.
[2] Gua, T., Hasebe, Y. *Biosens. Bioelectron.* **2012,** 33, 222–227.

[3] Hajibabaei, F., Movafagh, S.S., Salehzadeh, S., Derakhshandeh, K., Gable, R.W. *J. Mol. Struct.* **2023,** 135857.

22nd Iranian Inorganic Chemistry Conference