



POST GRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY
BHARATA MATA COLLEGE

(Affiliated to Mahatma Gandhi University Kottayam)
(Re-accredited by NAAC with 'A+' Grade, ISO 9001-2015 Certified)
Thrikkakara P. O, Kochi – 682021, Kerala, India

07-08-2023

Certificate for Collaboration

This is to certify that Dr. Jinsa Mary Jacob, Assistant Professor, Department of Chemistry, Bharata Mata College, Thrikkakara has collaborated with the Department of Basic Science and Humanities, SCMS School of Engineering and Technology, Karukutty, 683 576, for the project entitled "Multi-faceted investigation of copper (II) chelates based on an ONS donor thiosemicarbazone: Crystal structures, spectral aspects, DNA binding and computational studies" from 01/03/2023.

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Work Report of the collaborative work with Bharata Mata College, Thrikkakara

This study unveils the synthesis and characterization of a new binuclear copper(II) chelate $[(\text{Cu}(\text{bmpt})_2)]$ (1) and four mixed ligand copper(II) chelates $[\text{Cu}(\text{bmpt})(\text{phen})]$ (2), $[\text{Cu}(\text{bmpt})(\text{bipy})]$ (3), $[\text{Cu}(\text{bmpt})(4,4'\text{-dmbipy})]$ (4) and $[\text{Cu}(\text{bmpt})(5,5'\text{-dmbipy})]$ (5) based on an ONS donor thiosemicarbazone ligand, 5-bromo-3-methoxysalicylaldehyde- N^4 -phenylthiosemicarbazone (H_2bmpt) and 1,10-phenanthroline, 2,2'-bipyridine, 4,4'-dimethylbipyridine, 5,5'-dimethylbipyridine as coligands. The complexes were characterized by various physicochemical methods like CHNS analysis, molar conductivity measurements, magnetic investigations, and an array of spectroscopic techniques including FT-IR, UV-Vis, and EPR. The crystal structures of complexes 3 and 5 were ascertained by single crystal X-ray diffraction method and it was observed that they crystallize as solvates in triclinic P and monoclinic $P2_1/c$ space groups respectively. In both the complexes, copper(II) ion exhibits a distorted square pyramidal arrangement with oxygen, nitrogen, and sulfur atoms of the thiosemicarbazone ligand, along with one of the nitrogen atoms from the heterocyclic base, occupying the square plane while the other nitrogen atom of base occupies the axial position. DNA interactions of the prepared complexes were checked with CT-DNA in Tris-HCl buffer. The absorption titration was performed by the incremental addition of DNA and the complexes exhibit hyperchromism which suggests a groove binding mechanism. Among the complexes, complex 4 exhibits the highest binding value. The FMO analysis of the complexes revealed that the lowest HOMO-LUMO energy gap is exhibited by complex 1 (1.97 eV) indicating that the dimeric complex is the softest and has high chemical reactivity, low stability and high polarizability. Additionally, 3D mapping of the electron density of all the complexes as MEP surfaces were plotted, shedding light on the reactivity of the complexes. The different functions were mapped on the Hirshfeld surface to decipher the underlying reasons for the difference in noncovalent interactions among complexes (3a and 5a) and the results corroborate the crystal structure studies. It also explains the difference in the degree of $\pi \cdots \pi$ interactions among the complexes especially those having involvement of Cu containing metallocycle.

~~Dr. Nithya Mohan~~
8/08/23

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