XANES and EXAFS based structural investigations of biologically significant cyclicdione copper (II) complexes of arylhydrazone derivatives

PankajAgrawal[1]*,PradeepSharma[2],AshutoshMishra[3]

[1]*Govt.PolytechnicCollege,Sendhwa,MadhyaPradesh,IndiaEmail:pankajphd02@gmail.com
[2]Govt.Holkar(Model,Autonomous)ScienceCollege,Indore,MadhyaPradesh,India
[3]SchoolofPhysics,DeviAhilyaUniversity,KhandwaRoad,Indore,MadhyaPradesh,India

***CorrespondenceAuthor:**PankajAgrawal
*Govt.PolytechnicCollege,Sendhwa,MadhyaPradesh,IndiaEmail:pankajphd02@gmail.com

Abstract:
X-Ray absorption fine structure studies of Schiff base copper(II) complexes were performed. Arylhydrazone derivatives, a primary ligand of copper complexes used in the study, were 5,5-dimethyl-(2-(4-nitrophenyle) hydrazono)cyclohexane-1,3-dione and 5,5-dimethyl-(2-(4-chlorophenyl)hydrazono) cyclohexane-1,3-dione.The crystalline nature and presence of specific functional groups of the copper (II) complexes were confirmed by X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR),respectively.The X-ray absorption near edge structure(XANES) data have been analyzed to calculate the K-edge shift, principal absorption maximum shift, edge width, and chemical shift. The experimental value of chemicalshift is in accordance with the principal absorption maximum shift, indicating that the copper is in an oxidation state +2 in the sample. Effective nuclear charge (ENC) and percentage covalency were calculated from chemical shift and edge width, respectively. The first shell bond length was calculated using extended X-ray absorption fine structure (EXAFS) following different graphical methods. Fourier transforms of the normalized spectra have also been used to obtain bond length.

Keywords:XANES, EXAFS, XRD, FTIR, Chemical Shift, Athena, EdgeWidth