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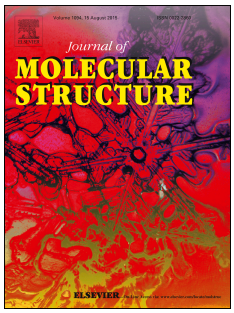

[Dichlorido (2-(2-(1H-benzo[*d*]thiazol-2-yl)hydrazono)propan-1-ol) Cu(II)]: Crystal structure, Hirshfeld surface analysis and correlation of its ESI-MS behavior with [Dichlorido 3-(hydroxyimino)-2-butanone-2-(1H-benzothiazol-2-yl)hydrazone Cu(II)]

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Abstract

In the present work, Cu(II) complexes of 2-(2-benzo[d]thiazol-2-yl)hydrazono)propan-1-ol (L^1) and 3-(hydroxyimino)-2-butanone-2-(1*H*-benzothiazol-2-yl)hydrazone (L^2) are synthesized and characterized by various spectro-analytical techniques. The structure of Cu(II) complex of L^1 i.e., $[CuL^1Cl_2]$, is unambiguously determined by single crystal X-ray diffraction method. While similar efforts were unsuccessful in the case of Cu(II) complex of L^2 i.e., $[CuL^2Cl_2]$. Hence, to avail the structural facts, various cationic/anionic fragments or adducts formed during positive/negative mode electrospray ionization (ESI) of CuL^1Cl_2 and CuL^2Cl_2 have been identified with the help of their charge, monoisotopic masses and isotopic distributions. The similarity in the ESI behavior of two complexes has inferred their structural resemblance, which is further supported by DFT optimized structures, EPR spectral studies and analytical measurements. The EPR spectral behavior ($g_{||} > g_{\perp} > 2.02$) of the complexes are attributed to an axial symmetry with the dx^2-y^2 ground state having square pyramidal Cu(II) ion. CuL^1Cl_2 has crystallized in monoclinic crystal system in $P2_1/c$ space group. The molecular complex has ring-metal (*Cg*-Me) interactions of the type Cg···>Cu, which contributes to the crystal packing. The Cl···H (30.6%) interactions have the major contribution among all intermolecular contacts and have played a vital role in the stabilization of the molecular structure, which is extended to 3D network through C—H···*Cg* and *Cg*-*Cg* interactions.

Keywords

Copper complexes of benzothiazol hydrazone, Crystal structure of the copper complex, Hirshfeld analysis of metal complex, ESI-MS of a coordination complex.