The vector analysis of complexes type $Cu_4OX_6L_4$

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The vector model of chemical structure is based on vector analyses of valence bonds, non-valence interactions and selected interatomic distances in the structure of chemical compounds. The vector structural model is applied to known structures of coordination compounds of the type $Cu_4OX_6L_4$, X = Cl, Br; L = ligands with Cl, N, O donor atoms.

Vector analysis is applied to structures of Cu_4OCl_6(3-pyme)$_4$ (3-pyme = 3-pyridylmetanol) [1] and Cu_4OCl_6(3-pyet)$_4$ (3-pyet = 3-pyridyletanol) molecules [2]. Composition of these molecules differs very slightly in different ligand substituents -CH_2-OH and -CH_2-CH_2-OH. The consequences of the ligand difference for structures of both complexes are presented by means of vector analysis which provides for both structures the sets of quantitative vector parameters. These are compared with structures and corresponding vectors of $Cu_4OCl_6(OPPh_3)_4$ molecule (highest symmetry, lowest possible vector values) [3] and Cu_4OCl_6(2-Mepy)$_4$ molecule (steric effects in low symmetry, very high vector values) [4].

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