The vector analysis of complexes type Cu$_4$OX$_6$L$_4$

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The vector model of chemical structure is based on vector analyses of valence bonds, nonvalence 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$_4$OX$_6$L$_4$, X = Cl, Br; L = ligands with Cl, N, O donor atoms.

Vector analysis is applied to structures of Cu$_4$OCl$_6$(3-pyme)$_4$ (3-pyme = 3-pyridylmethanol) [1] and Cu$_4$OCl$_6$(3-pyet)$_4$ (3-pyet = 3-pyridylethanol) 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$_4$OCl$_6$(OPPh$_3$)$_4$ molecule (highest symmetry, lowest possible vector values) [3] and Cu$_4$OCl$_6$(2-Mepy)$_4$ molecule (steric effects in low symmetry, very high vector values) [4].

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