

The dangerous statistics

Marian Koman, Gregor Ondrejovič, and Ján Moncol'

*Fakulta chemickej a potravinárskej technológie STU, Oddelenie anorganickej chémie
ÚAČHTM, Radlinského 9, 812 37 Bratislava, Slovakia*

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 $\text{Cu}_4\text{OCl}_6\text{L}_4$, L = ligands with N and O donor atoms. In Cambridge Structural Database are 69 crystal structures with such a composition. The $\text{Cu}_4\text{OCl}_6\text{L}_4$ molecule is regarded as a supramolecular model of interactions between ligand L and hypothetical "round-shaped" coordination tetra-receptor Cu_4OCl_6 . For vector calculations each $\text{Cu}_4\text{OX}_6\text{L}_4$ structure is placed into the three dimensional Cartesian coordinate system with the central oxygen atom O placed in origin 0. Studied ligands are compared and described by molecular structural dynamics and corresponding shifts of electron densities by means of bond lengths (O1-Cu, Cu-L, Cu-Cl) and structural distances (O1...Cl, O1...L). In this paper, we focused on the study of the deformation of the trigonal-bipyramidal coordination polyhedron of copper atoms. The ligands L were divided into four groups depending on the presumed electron density on the donor atoms. The principles of vector methods and calculations have been described¹⁻³.

Grant Agencies (Slovakia: APVV-18-0016) are acknowledged for the financial support.

- [1] Ondrejovič G., Moncol' J. (2015) Structures of $\text{Cu}_4\text{OCl}_6\text{L}_4$ complexes studied by vectoranalysis. Book of Abstracts – XXV. International Conference on Coordination and Bioinorganic Chemistry, Smolenice: 101. ISBN 978-80-89597-25-3
- [2] Ondrejovič G., Moncol' J. (2017) Advanced structural analysis of coordination $\text{Cu}_4\text{OX}_6\text{L}_4$ molecules. Book of Abstracts – XXVI. International Conference on Coordination and Bioinorganic Chemistry, Smolenice: 82. ISBN 978-80-8208-014-1
- [3] Ondrejovič G., Moncol' J., Koman, M. (2020) The crystal structure of tetrameric copper(II) complexes, Hirshfeld surface analysis, and vector analyses of $\text{Cu}_4\text{OCl}_6\text{L}_4$ complexes with N-donor ligands. Chem. Pap. 74, 3755-3766.