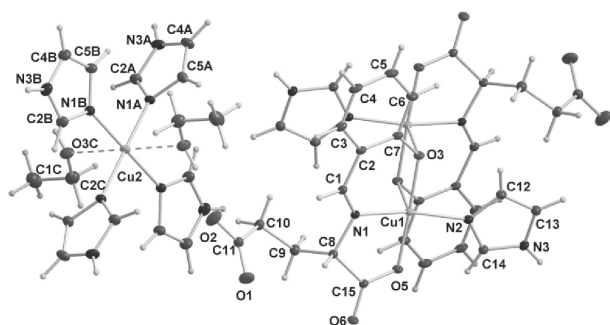


s7.m26.p8 **Novel type of Cu(II) complex containing Schiff base.** Vratislav Langer^a, Pavel Mach^b, Dalma Gyepesová^b, Mária Kohútová^c and Aladár Valent^c, ^aDepartment of Environmental Inorganic Chemistry, Chalmers University of Technology, SE-412 96 Göteborg, Sweden, ^bInstitute of Inorganic Chemistry, Slovak Academy of Sciences, SK-845 36 Bratislava, Slovak Republic and ^cDepartment of Chemical Theory of Drugs, Faculty of Pharmacy, Comenius University, SK-832 32 Bratislava, Slovak Republic. E-mail: langer@chem.chalmers.se

Keywords: Cu(II) complex; Schiff base; B3LYP method

Recently, special interest has been devoted to the group of copper(II) complexes containing Schiff bases, derived from salicylaldehyde and various amino acids, and N-, or O- donor neutral ligands due to their biological activities. From this group of substances the structures of (*N*-salicylidene-*rac*-glutamato) (1-methylimidazole)Cu(II) [1], (*N*-salicylidene-*rac*-glutamato) (2-methylimidazole)Cu(II) [2], (*N*-salicylidene-*L*-glutamato) (2-ethylimidazole)Cu(II) [3] and aqua(*N*-salicylidene-methylester-*L*-glutamato)Cu(II)monohydrate [4] have been determined. Electronic structure of these compounds has been investigated by the B3LYP method. A continuation of these studies is a new complex *trans*-bis(ethanol)tetrakis(imidazole)Cu(II)(2+) bis[μ -(*N*-salicylidene-*L*- glutamato-*N,O*)- $\kappa O:\kappa O'$ -(imidazole)Cu(II)](2-) presented here:



This complex has quite spectacular structural features. Both ions are located on inverse centre. The cation is mononuclear, while the anion is binuclear. The quantum chemical calculation of the electronic structure has also been done by the B3LYP method. The more detailed discussion of the structural features of this complex will be presented.

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s7.m26.p9 **Using symmetrised structure components to improve the refinement of an occupancy modulated structure.** A. David Rae^a and Anthony Linden^b, ^aResearch School of Chemistry, Australian National University, Canberra, Australia, ^bInstitute of Organic Chemistry, University of Zurich, Switzerland. E-mail: rae@rsc.anu.edu.au

Keywords: Pseudo symmetry; Disorder; Refinement

The structure of bis(1-chloro-2,2,4,4-tetramethyl-3-oxocyclo butan-1-yl)pentasulfane can be described as a partial ordering of a 1:1 disordered $P2_1/a$ parent structure combined with a doubling of the *c* axis. The pentasulfane chain completes one turn of a helix and this allows any molecule in the structure to be replaced by an inversion related molecule with all but the S and Cl atoms coinciding with a pseudo inversion equivalent. Refinement in $P2_1/n$ of such a simplified model produces good statistics but has serious problems with distances and angles. Using a stacking fault model that refines an ordered structure but uses separate scales for *l* even and *l* odd reflections improves the geometry but the refinement statistics suffer. The refinement problem was resolved by deciding the structure could be described as 0.732(1) of an ordered $P2_1/n$ structure that contributes to all reflections and 0.268 of a 1:1 disordered $P2_1/a$ structure that contributed only to *l* even reflections. The *l* even reflections see an average molecule that is not in exactly the same position and orientation as the average molecule that the *l* odd reflections see. Successful refinement used the Constrained Least Squares Refinement program RAELS and allowed the $P2_1/n$ and $P2_1/a$ components to be refined separately. Details of appropriate constraints and restraints will be given. The result implies that a simple stacking fault was not an appropriate model. Rather there is a dominant $P2_1/n$ structure with localised mistakes. The inverted molecule is not included as an exact inversion at exactly 1/2, 1/2, 1/4 or its equivalent.