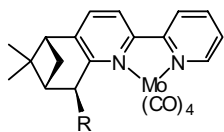


[s9.m3.p31] Few molecules in asymmetric unit; why?

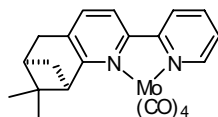
V. Langer, A.V. Malkov, and P. Kocovsky. *Department of Environmental Inorganic Chemistry, Chalmers University of Technology, SE-41296 Göteborg, Sweden and Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, U.K.*

Keywords: 2,2'-bipyridyl-type ligands, packing of molecules, hydrogen bonds.

During synthesis of new chiral 2,2'-bipyridyl-type ligands and studies of their coordination to molybdenum(0), copper(II), and palladium(II)¹, the following compounds has been prepared, crystallized and characterized by single crystal X-ray analysis:



where R = H (**1**) and Me (**2**) and



3

Compound (**1**) exhibits polymorphism: two different kinds of crystals (monoclinic and tetragonal) crystallized from the same batch and could be separated mechanically. In the monoclinic form of (**1**), there are two molecules in the asymmetric unit, while in the tetragonal form of (**1**), just one molecule per asymmetric unit is found. For compounds (**2**) and (**3**) there are again two molecules per asymmetric unit. But in all cases the compounds are enantiomerically pure.

Why this feature occurs? What is governing the simultaneous growth of the polymorphs? Is it specific for this system or is it of more general nature? Are the symmetrically independent molecules in the solid state also chemically different? We believe the hydrogen bonds are the explanation.

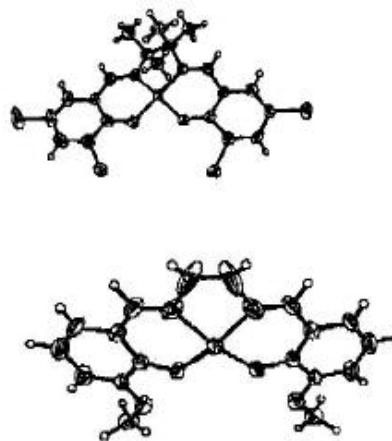
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[s9.m3.p32] Structural behaviour of Ni(II) and Cu(II) complexes with N₂O₂ Schiff base ligands: the effect of molecular conformation on crystal packing.

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Keywords: molecular interactions, supramolecular assemblies.

Cu(II) and Ni(II) complexes with Schiff base ligands derived from salicylaldehyde have long been used in homogeneous catalysis^{1,2} and used recently as heterogeneous electrocatalysts³. Special application has been the stereoselective catalytic ability of the optically active complexes⁴. We present here a systematic study of the structural effects on packing due to the different conformations adopted by the complex molecules. These different conformations are promoted by the introduction of substituents on both the ethane diiminic bridge and on the aldehyde moiety. The steric hindrance imposed in each case implies different constrictions and distortions affecting the overall geometry of the molecule and creating new packing motifs. Molecular and crystal structures of new Ni(II) and Cu(II) complexes will be presented and discussed.



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