

Poster Presentation

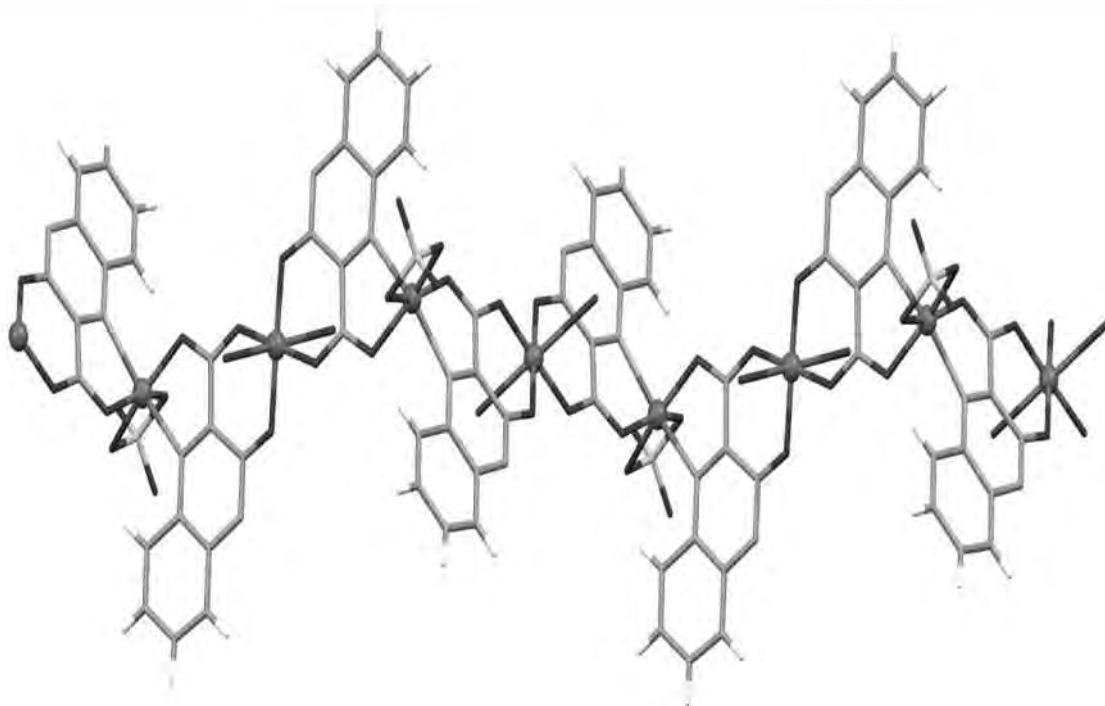
MS83.P27

Copper(II) complexes with 3-hydroxyquinoxaline-2-carboxylic acid

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Hydrothermal and mechanochemical syntheses are extensively used to obtain metal coordination polymers of different dimensionalities. Transition metal complexes with carboxylate based ligands e. g. 3-hydroxyquinoxaline-2-carboxylic acid (3-OHquinoxH) are interesting due to the possible formation of porous structures suitable for gas storage and separation. 1D coordination polymer $\{[\text{Cu}_2(3\text{-OHquinox})_2(\text{SO}_4)(\text{H}_2\text{O})_2]\cdot 4\text{DMSO}\}_n$ (1) was obtained by reaction of CuSO_4 and 3-OHquinoxH in dimethyl sulfoxide (DMSO) solution at room temperature, while mononuclear complex $[\text{Cu}(3\text{-OHquinox})_2(\text{H}_2\text{O})_2]\cdot 2\text{DMSO}$ (2) was formed under hydrothermal conditions. The X-ray crystal structure analysis revealed two differently coordinated Cu(II) ions in 1 (see figure). The first Cu(II) ion in 1 is octahedrally coordinated by two bridging O,O'-bidentate 3-OHquinox ligands and two water molecules in trans position, and the second Cu(II) ion by two bridging N,O'-bidentate 3-OHquinox ligands and one O,O'-bidentate sulfate ion. The Cu(II) ion in 2 is octahedrally coordinated by two N,O'-bidentate 3-OHquinox ligands and two water molecules in trans position. The reaction mixture was also grinded in a ball mill in the presence of H_2O , DMSO or their mixture and the products were identified by powder X-ray diffraction (PXRD). The grinding under these conditions could not be used to prepare pure 1 nor 2, but rather a mixture of both 1, 2, reactants and new, still unidentified, phase. The complex 2 was also studied by DFT methods. The hypothetical complex with two O-bound DMSO molecules is more stable than 2 by 2.9 kcal/mol. The preference for the formation of 2, with two coordinated water molecules, must be assigned to the hydrogen bonds between coordinated water and crystallization DMSO molecules in the crystal structure of 2.



Keywords: copper(II) coordination compounds