

Polymorphism of methylsalicylatocopper(II) complexes

Miroslava Puchoňová, Ján Moncol', Ján Pavlik, Vladimír Kuchtanin, and Vladimír Jorík

Department of Inorganic Chemistry, Faculty of Chemical and Food Technology, STU in Bratislava, Radlinského 9, Bratislava, Slovakia

Copper complexes containing N-donor ligands are traditionally studied from different points of view, the phenomenon of polymorphism and isomerism of transition metal complexes being one of them. In recent decades, various polymorphs and isomers of carboxylatocopper(II) complexes have been investigated [1,2]. Building upon previous research, we have focused on Cu(II) complexes with various position isomers of methylsalicylate anions (MeSal) in presence of 2-hydroxymethylbenzimidazole (2HMBzim). The synthesis in the presence of 3-methylsalicylate anion led to formation of two complexes with the same composition [Cu(3-MeSal)₂(2-HMBzim)₂] (**1a** and **1b**). The structures of the newly prepared complexes were determined by single-crystal X-ray analysis. The complexes were characterized by spectroscopic methods (IR, UV-vis and EPR spectroscopy). Based on the crystal structures and in accordance with experimental and computational studies it was concluded, that the systems **1a** and **1b** were conformational isomers/polymorphs. With the help of the state-of-the-art computer simulation, it was predicted, that the presence of methanol or acetonitrile as solvents played a pivotal role in folding the molecular components into a specific polymorphic form.

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[1] S. Matejová et al., Polyhedron, 2019, 170, 86.

[2] Z. Repická et al., Struct. Chem., 2010, 21, 1093.