Viera Murašková et al., Chem Sci J 2018, Volume 9
DOI: 10.4172/2150-3494-C2-021

8th European Chemistry Congress

June 21-23, 2018 | Paris, France

Synthesis, crystal structure, spectral and magnetic properties of iron (III) complexes with pyridoxal Schiff base ligands

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Synthesis, crystal structure, spectral and magnetic properties of mononuclear $[Fe\{N(C_9H_{10}N_2O_2)_3\}].7.5H_2O$ and dinuclear $[Fe_2(\mu\text{-}C_{18}H_{18}N_3O_7)_2]\cdot 3(H_2O)\cdot 0.38(O)$ iron(III) complexes based on pyridoxal and glycine are reported. In both cases of complex preparation, an unexpected Schiff base ligand was formed by the catalytic effect of a trivalent iron ion. The presence of water played a role in the formation of a dinuclear complex due to hydrolysis of its mononuclear intermediate. The reaction mechanism of mononuclear and also dinuclear complex formation was proposed. Structural analysis of the dinuclear complex showed that each Fe(III) center has a distorted octahedral $FeNO_5$ core and two Fe(III) atoms are connected with two alkoxo-bridging ligands. The mononuclear complex with the octahedral FeN_3O_3 core of the hexadentate tripodal ligand coordinating to the iron in the facial mode, reveals a trigonal distortion. In the crystal lattice of both complexes, the noncovalent interactions, hydrogen bonds, and π-π stacking interactions expand the mononuclear units to a 3D supramolecular network. In the mononuclear complex, a positional disorder of pyridoxal hydroxymethyl group was identified, which partly undergoes a cyclization forming a five-membered ring with the imine moiety. The two configurations with a different magnetic behavior occur in the ratio 79.5: 20.5. The values of the axial zero-field splitting D parameter of the high-spin state Fe(III) complexes were obtained from the whole temperature range (2-300K) analysis of experimental magnetic susceptibility data. Moreover, in the case of a dinuclear complex, an antiferromagnetic exchange interaction between the two Fe(III) ions was identified and included in the calculation..

Biography

Viera Murašková is a postgraduate student at the faculty of chemical technology at the university of chemistry and technology, Prague (UCT Prague), Czech Republic.

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