

Synthesis and characterization of a cadmium II complex with an oxime ligand.

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Oximes are considered analogous compounds of the imines, which result in the following formula: $RR'C = N-OH$. [1] Oximes are easily obtainable compounds with the ability to form intermolecular hydrogen bonds, giving rise to very stable macrocyclic species. [2] The oximes and the oximate group (obtained by deprotonation of the hydroxyl fraction) contain two possible coordination sites, the imine nitrogen and the hydroxyl oxygen atom. [3] The synthesis of the complex 1 bis- [acetate (O, O') ethanol (di-isatin-3-oxime-N,O)- μ -isatin-3-oxime-O) cadmium(II)]₂·H₂O occurs through the reaction between the isatin-3-oxime ligand and cadmium acetate dihydrate dissolved in ethanol in the ratio 2:1. The synthesis of the complex 2, [(di-isatin-3-oxime-N,O)- μ -isatin-3-oxime-O) cadmium(II)]₂·H₂O·DMSO, occurs through the reaction between the isatin-3-oxime ligand dissolved in dimethylsulfoxide with the cadmium acetate dihydrate in ethanol at a 3:1 ratio. The ligands were previously deprotonated with potassium hydroxide and the solutions of the reactions were kept under reflux for three hours. After a slow evaporation of the solvents, yellow crystals were isolated, which were capable of X-ray diffraction in single crystals. The resolution of the complex structure 1 determined that the coordination sphere of each metal ion is formed by two oxime ligands as bidentates, one of which acts as a bridge between the two cadmium (II) ions through the carbonyl oxygen atom of the protonated ligand. The complex also has two co-ligands, one of monodentate behavior, ethanol and acetate acting as bidentate. However, the complex presented dodecahedral geometry, with the coordination of the acetate in bidentate form and ethanol in the monodentate form occurring in the axial part, and the pentagonal base is formed by donor atoms of the oxime ligand, leading to the coordination number eight. In complex 2, the coordination number is seven, where each metal center is coordinated by two protonated bidentate isatin-3-oxime ligands; and a deprotonated chelator that also acts as a bridge through the nitrogen and oxygen atoms of the oxime fragment. There is also the presence of a water molecule and *N,N*-dimethyl sulfoxide acting as the solvate of crystallization. This complex of *trans* and centrosymmetric configuration presents a distorted pentagonal bipyramidal geometry. The characterization and elucidation of these structures allows the study of the different forms of coordination adopted by the oxime ligand and as well as in the planning of new structures with specific purposes within the bioinorganic area as well as in other areas of application.

[1] ARAÚJO, C.R.M.; GONSALVES, A.A. Revista Virtual Química . Vol.7, Nº4, pág.1469-1495, 2015.[2]TOMA, H.E . Química de coordenação, organometálica e catálise. Volume 4 Coleção de Química Conceitual. Editora Blucher, São Paulo, 2013.[3] ALOMAR,K.; HÉLESBEUX,J-J, ALLAIN, M.; BOUET,G. Journal of Molecular Structure . Vol. 1019, pág.143–150, 2012.