MS27 P07

Complexes of M(carbaldehyde-oxime)(M=Pd and Hg): Synthesis and Structural Characterization

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Syntheses and X-ray crystal structure analyses of Hg(II) and Pd(II) complexes with pyridine-2-carbaldehyde-oxime ligand are reported. The complexes are obtained from the reaction of simple Hg(II) and Pd(II) salts ($PdCl_2$ and $HgCl_2$) with pyridine-2-aldoxime (HL). The molecular structures of complexes have been determined by single-crystal X-ray analyses. Structural characterization reveals in Hg(II) case the presence of HgL_2 complex but in Pd(II) case the formation of PdL(HL)Cl complex is observed.

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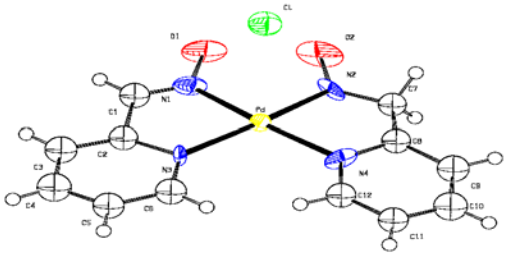

Fig. 1. ORTEP diagram of a symmetric unit of $[PdH(C_6N_2OH_5)_2Cl]$(**1**).

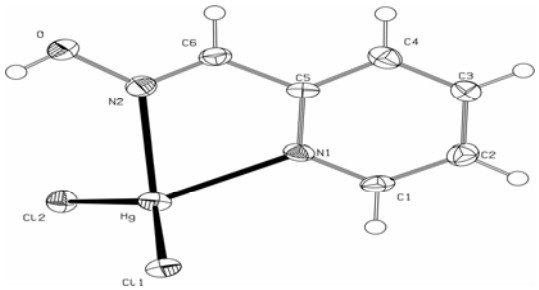

Fig. 2. ORTEP diagram of a unit of $[HgC_6N_2OH_6Cl_2]$(**2**)

MS27 P08

Synthesis and Crystal Structure of 4-Aminoquinolinium Bis(citrato)borate Monohydrate

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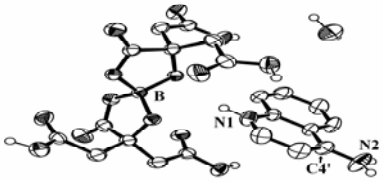
Keywords: single-crystal X-ray, boron compounds, hydrogen bonds

In the course of structural studies of amine salts of boron coordination compounds a new complex – 4-aminoquinolinium bis(citrato)borate monohydrate (I) has been synthesized and its X-ray structural investigation has been carried out. Complex I was prepared by mixing boric and citric acids with 4-aminoquinoline in proportions (molar ratio) 1:2:1 in water solution. Crystals of compound I were obtained by slow evaporation of water from solution.



The structure of the title compound I is formed by univalent cations $[(4\text{-}NH_2)C_9H_6NH]^+$, spiran-type complex anions $[(C_6H_6O_7)_2B]^-$ and crystallization water molecules (fig.). Boron atoms are tetracoordinated as confirms the sp^3 hybridization sphere around them. The bonds B–O(carb.) (average length 1.495(3) Å) are systematically longer than B–O(hydr) (average length 1.448(3) Å). The values of the dihedral angles corresponding to the crossing of two main-square planes of boron-containing heterocycles –C–O–B–O–C– in the two independent complex anions amount to 87.88(6)º and 87.87(6)º. The molecule of 4–aminoquinoline molecule is protonated at the ring N1 atom but not at the amino group nitrogen atom N2 in acidic solutions. The C4'–N2 bond length (1.326(3) Å in average) is approximately equal to the C=N double bond lenght indicating that atom N2 of the amino group must also be sp^2- hybridized. The C–C bonds at C4' atom are somewhat longer (1.424(3) Å in average). The N2 atoms lie almost in the quinoline ring plane (maximum deviation of 0.029(3) Å). Bond angles $C–N^+–C$ are 118.6(5)º. The hydrogen atoms of amino groups, protonated nitrogen atoms, as well as those of hydroxyl groups from two independent complex anions and three of four hydrogen atoms from two independent water molecules are involved in formation of 17 independent O–H...O and N–H...O type hydrogen bonds. Nitrogen