07-Crystallography of Organometallic and Coordination Compounds

A number of antimony(III) aminoxyhexitol acid esters, in which the coordination polyhedron of Sn(IV) is unexceptionally a distorted 5-pentagonal bipyramid, have been found to exhibit certain antitumor activity for a long time (Hu, S. Z. & Lin, W. F., J. Struct. Chem., 1989, 8, 249-256). In order to investigate the mechanism of antitumor activity, the interaction of Sn(IV) complexes with some bases of nucleosides and nucleic acids have been considered in our laboratory. As a preliminary study, SnCl₃ was selected to react with adenosine in the light of complex formation of N-donor ligands such as adenosine, 2',2'-bipyridine and 4-phenylformamidine (Lipka, A., Z. Naturforsch. 1988, 366, 341-346). We report here two crystal structures of the title compounds (CH₃[N(Sn)[Sn(CH₂)₄][O]) and (CH₃[N(Sn)[Sn(CH₂)₄][O]). Complexes of stoichiometry SnCl₃ can feature either six-coordinate polymeric anions as in compound (I), or discrete five-coordinate anions in compound (II). The coumterions are linked through hydroxide bonding with the water molecules, consequently, there are no interactions between Sn(III) and adeninum nitric acid.

Crystal data: \(\lambda(MoK\alpha) = 0.71073 \text{Å}, 296K\)

(I): FW = 454.18, F(000) = 872, monoclinic, P2₁/c, a = 11.94(1), b = 7.649(1), c = 17.544(1) \AA, \(\beta = 103.98(1)\), \(\gamma = 1437.5\) \AA², \(Z = 4\). \(D_m = 2.98, D_0 = 2.08\) Mg/m³, \(\mu = 28.6\) cm⁻¹. \(R = 0.033\) for 2084 observed reflections.

(II): FW = 569.30, F(000) = 576, triclinic, P-1, \(\epsilon = 8.696(1), b = 9.144(3), c = 12.763(2)\) \AA, \(\alpha = 79.50(2), \beta = 74.78(1), \gamma = 83.50(2)\), \(\nu = 960.6\) \AA², \(Z = 2\), \(D_m = 2.03\), \(D_0 = 2.03\) Mg/m³, \(\mu = 21.72\) cm⁻¹. \(R = 0.032\) for 3758 observed reflections.

PS-07.05.15 CRYSTAL STRUCTURE OF (HYDROGEN ETHYLENE-DIAMINETRACETATO) BISMUTH(III) DIHYDRATE. By H. Wang, Z.-H. and X. Z. Huang (Chemistry Department, Xiamen University, Xiamen, China, and R. L. Davidovich, Institute of Chemistry, F. E. Branch, Russian Academy of Sciences, Vladivostok, Russia).

Two modifications of the dihydrate chelate of bismuth(III) with ethylendiamine-N,N',N'-tetraacet_acid (H₂edta), Bi(H₂edta)₂·2H₂O are determined and identified by the method of IR spectroscopy and X-ray powder diffraction analysis (Davidovich, R. L., et al., Koord. Khim. 1988, 14, No. 11, 1511-1516). The α-modification is orthorhombic with cell dimensions \(a = 10.66, b = 18.25, c = 7.35\) Å, which is similar to that of Sn(II)·2H₂O (orthorhombic, \(a = 10.98, b = 18.496, c = 7.341\) Å). The structure is being further investigated.

The crystal structure of the β-modification was determined using single crystal X-ray diffraction methods. The crystals are monoclinic, \(\gamma = 17.85(4), b = 6.84(2), c = 13.21(2)\) Å, \(\beta = 105.78(2)\), \(\nu = 1903.1\) Å³, \(Z = 4\), \(F_w = 534.23, D_m = 2.361\) Mg/m³, \(\lambda(MoK\alpha) = 0.71073\) Å, \(\mu = 117.46\) cm⁻¹, F(000) = 1016, 296K, \(R = 0.034\) for 2003 unique reflections with \(I > 3\sigma(I)\). The structure reveals that the H₂edta⁻ ligand performs a hexadentate chelating function (\(O + 2N\)) and a double bridging function (2O). Features of the exotropic polyhedron of Bi(III) as well as the polymeric structure compared with that of Bi(H₂edta) and \(\text{Sn(II)}\) (Shikhalina, L. M., et al., Koord. Khim., 1991, 17, No. 2, 253-261) will be presented.