o.m12.p17 **Structural studies of tributyltin 2-sulfobenzoate.** J. Sykora, J. Brus, A. Smicka, M. Husak. *Department of Solid State Chemistry, Prague Institute of Chemical Technology, Technicka 5, 166 28 Prague 6, Czech Republic; e-mail:sykoraj@vscht.cz*
Keywords: tributylin, crystal sturcture.

Organotin compounds exhibit interesting biological properties[1]. The activity of butyltin compound against certain tumor cell lines of human origin seems very promising[2].

The model compound of tributyltin 2-sulfobenzoate was studied by ^{13}C and ^{119}Sn CP/MAS NMR spectroscopy and the nonequivalence of two tin atoms was determined.

Single crystals were obtained from CH_2Cl_2 and the results of NMR spectroscopy were verified by X-ray structural analysis.

Tributyltin 2-sulfobenzoate crystallizes in space group P 21/c, the independent part is formed by two molecules. The sulfonato group is coordinated to tin atom and both atoms of tin are coordinated by five atoms creating thus trans-C_3SnO_2 trigonal bipyramids (angle O-Sn-O is 174°). The molecules are linked to form helical polymeric chains. These chains are connected by intermolecular hydrogen bonds of carbonyl groups. The distances between tin atom pairs in separate chains are nonequivalent with the Sn(1) – Sn(1) and Sn(2) – Sn(2) distances of 10.00 ? and 7.87 ?, respectively.

These nonequivalent surroundings explain the multiplicity of tin atoms signals in ^{119}Sn CP/MAS NMR spectra.

This work was partially supported within the research project CEZ:MSM 223100002 of Ministry of Education of the Czech Republic and project No. 203/99/0067 of the Grant Agency of the Czech Republic..

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[2] John S. Thayer: Journal of Organometallic Chemistry, 76 (1974) 265-295.

o.m12.p18 **Novel boron coordination compounds with polymeric complex anion. crystal structure of ammonium-cadmium (1:2) bis ((+)-tartrato)borate tetrahydrate.** I. Zviedre[1], V. Belsky[2], J. Ronis[1], J. Schwartz[1]. *[1] Institute of Inorganic Chemistry of the Riga Technical University, Riga, Latvia;*
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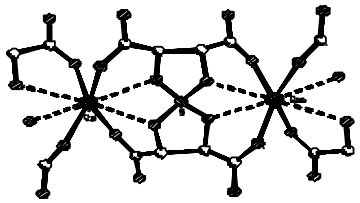
Keywords: boron, crystal structure, polymeric.

Heterospiran complexes with the boron/ligand ratio in the complex anions 1:2 are formed depending on the interaction conditions and the properties of the organic ligands. In the course of systematic investigation of boron coordination compounds ammonium-cadmium (1:2) bis(tartrato)borate tetrahydrate $(NH_4)_3[Cd((+)\text{-}C_4H_2O_6)_2B].4H_2O$ have been synthesized. The well-shaped monocrystals have been obtained. Using the X-ray diffraction analysis method chemical composition and full crystal structure have been determined.

Crystal structure is built from $[NH_4]^+$ cations, polymeric complex anions $[Cd((+)\text{-}C_4H_2O_6)_2B]_n^{3-}$ and four water molecules. The complex anion is formed by bidentatic addition of two *L*(+)-tartaric acid reside to $[B(OH)_4]^-$ and bidentatic addition of four ligands to one cadmium atom.



The boron atom is tetrahedrally coordinated. Bond lenghts are B-O 1.477(3)Å, bond angles on B are from $103.8(2)^0$ to $115.7(3)^0$. The Cd^{2+} ion is coordinated by eight O atoms. Four Cd-O distances are 2.260(3) Å (carboxyl) and four distances - 2.514(2)Å (hydroxyl). The average Cd-O distance is 2.387(3) Å. Coordination polyhedra are distorted square antiprism. Bond distances within the tartrate acid reside: $C(sp^2)$-O are 1.270(6) Å and 1.248(6)Å, aver. 1.259(6)Å; $C(sp^3)$-O are 1.436(5)Å, $C(sp^3)$-$C(sp^2)$ - 1.527(6)Å, $C(sp^3)$-$C(sp^3)$ - 1.526(9) Å. The conformation in the C(1)-C(2)-C(3)-C(4) chain is *trans* with torsion angle -152.7^0. In the course of addition of *L*(+)-tartaric acid molecule due to rotation around the central C-C axis ($\sim 27^0$) the mutual drawing together of the 2,3-hydroxyl groups takes place. he boron containing five-membered heterocycles C-O-B-O-C are approximatelly planar within the range of 0.06 Å.

In the crystal structure the polymeric complex anions $[Cd((+)\text{-}C_4H_2O_6)_2B]_n^{3-}$ forms a infinite chain. The binding of the infinite chains in the three-dimensional crystal structure is realized via hydrogen bonds involving the molecules of crystallization water and ammonium ions. Each complex-anionic chain is associated with four nearest symmetrical anions by complicated system of H-bonds.

Crystal data: a=12.951(2), b=12.951(2), c=6.129(1) Å; V=1028.0(3) $Å^3$, Z=2, tetragonal, $P42_12$, R=0.0303, R_w=0.0783.