

Diorganotin dihalides, R_2SnHal_2 with Hal = Cl, Br, I, belong to the basic chemicals in organotin(IV) chemistry because they are versatile precursors for the preparation of other diorganotin compounds like complexes, hydrolysis products, hydrides and so on. Since the first structural characterization of Me_2SnCl_2 in 1970 by Davies et al. [1] some dozens structures of dihalides were determined but no general classification scheme was evolved. In solid state, many of these dihalides exists as monomers without any intermolecular tin-halide interactions because of intramolecular Lewis-base Lewis-acid adduct formation or because of steric hindrance but especially the common ones with hydrocarbon rests are dominated by intermolecular tin halide interaction with strong effects on intramolecular bond angles and lengths. For this kind of interaction which is often termed *secondary bonding* [2] or *supramolecular architecture* [3] two main types of arrangements were found: 1) side by side with the dipole moments more or less antiparallel (a) to each other or 2) one after another with two equal or different tin halide interactions and a more or less parallel (p) ordering of the dipole moments.

In the course of a systematical study on the crystal structures of diorganotin dihalides we obtained – in addition to the already known structure types - a lot of new ones which gave us the possibility to develop a general classification scheme for the intermolecular tin-halide interaction. To discriminate the different structure types, our scheme takes into account the dipole-dipole interaction represented by the angle bisector between the halide atoms, the crystallographic symmetry elements between the interacting molecules and a tin-halide respectively tin-tin aggregation plane. The poster will show the limitations and options of our scheme covering oligomeric ($2a$, $4a$) arrangements, the different chainlike ones built up by monomers with parallel ($P_0 - P_2$) or antiparallel ($A_0 - A_2$) orientations of the dipole moments, the chainlike ones built up by dimers [$C2(2a_1)$] as well as the band [$B(pp)$] and sheet [$S(2a_1)$] like structure types.

[1] A.G. Davies, H.J. Milledge, D.C. Puxley, P.J. Smith, *J. Chem. Soc. A* **1970**, 2862-2866. [2] N.W. Alcock, J.F. Sawyer, *J. Chem. Soc. Dalton* **1977**, 1090-1095. [3] M.A. Buntine, F.J. Kosovel, E.R.T. Tiekink, *Cryst. Eng. Commun.* **2003**, 5, 331-336.

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Crystal structures of few new β -octamolybdates

Wiesław Łasocha,^{a,b} Alicja Rafalska-Łasocha,^a Wojciech Nitek,^a
^a*Faculty of Chemistry Jagiellonian University, Ingardena 3, 30-060 Kraków, (Poland).* ^b*Jerzy Haber Institute of Catalysis PAS, Niezapominajek 8, 30-239, Kraków, (Poland).* E-mail: lasocha@chemia.uj.edu.pl

Octamolybdates are important and interesting group of compounds. Among the molybdates, they are the most numerous group of compounds. In addition, there are several types of octamolybdates. Why are they important to study, when their applications are not especially numerous yet?. The reason is a desire to understand the rules governing the formation of certain polymetallate anions. These rules are quite complex, the type of anion depends on the reaction time, concentration and type of reactants. An additional element is the richness of anionic forms and their potential applications in crystal engineering. For a deeper understanding of principia of polymetallate construction, structural studies of a group of newly obtained compounds, have been undertaken. We investigated octamolybdates of aniline derivatives with the general formula $NH_2-Ph-R_{(1 \text{ or } 2)}$ and mm2 symmetry.

Synthesis: aqueous solution of molybdic acid and amine, acidified with HCl or CH_3COOH was boiled under reflux for 1-24hrs.

Among the most surprising findings is the fact that; short-term synthesis using 4-methylaniline results in octamolybdate, while the result of a long (24hr) synthesis is pentamolybdate. Similar results were observed in the case of 4-iodoaniline. Interestingly, using 3,5-dimethylaniline exclusively trimolybdate is produced, regardless of the reaction time. In the case of 4-fluoroaniline and 4-chloroaniline, 24-hour reactions conducted under the same conditions, have resulted in a complex polycrystalline material, which has not been fully explored yet.

Among anilinium octamolybdates only β -isomers were obtained.

The results indicate that, the creation of a specific polymolybdate type depends on many factors, and structural 'synthons' present in the 'reacting system', may help to describe the resulting structure. However, on their basis, it is much harder to predict resulting anionic species.

All compounds were synthesised for the first time in our laboratory. Structural studies were performed mainly by single crystal methods (Bruker-Nonius), phase composition and structural studies for compound **5** by powder diffraction methods. All compounds were also characterised by IR spectroscopy, SEM, XRD vs. temp and DSC investigations. Some crystallographic data are listed below:

1. $Mo_8O_{26} \cdot 4\{NH_2-C_6H_4-CH_3\}$ – tetrakis(p-toluidinium) β -octamolybdate, Sg. P 2₁/c (14), 8.388(2), 26.669(4), 9.346(3) Å, 103.65(3)°, V=2031.8 Å³, Z=2
2. $Mo_8O_{26} \cdot 4\{NH_2-C_6H_4-F\}$ – tetrakis(p-fluoroanilinium) β -octamolybdate, Sg. P-1(2) 10.567(4), 14.605(3), 15.724(5) Å, 117.16(2), 96.67(4), 97.80(4)°, V=2095.8(8) Å³, Z=2
3. $Mo_8O_{26} \cdot 4\{NH_2-C_6H_4-Cl\}$ – tetrakis(p-chloroanilinium) β -octamolybdate, Sg. P-1(2) 10.586(3), 14.705(5), 16.407(4) Å, 116.26(2), 93.43(2), 98.38(3)°, V=2243 Å³, Z=2
4. $Mo_8O_{26} \cdot 4\{NH_2-C_6H_4-(CH_3)_2\}$ – tetrakis(2,6-dimethylanilinium) β -octamolybdate, Sg. P-1(2), 10.508(5), 11.578(5), 11.686(5) Å, 118.59(5), 93.74(5), 101.146°, V=1204 Å³, Z=1
5. $Mo_3O_{10} \cdot 2\{NH_2-C_6H_4-(CH_3)_2\}$ – bis(3,5-dimethylanilinium) trimolybdate, Sg. P-1(2) 8.936(3), 16.729(4), 7.580(2) Å, 92.20(2), 93.138(3), 98.18(3)°, V=1118.4(4) Å³, Z=2

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Crystal structure of $C_4H_8ONH_2-PbBr_3$ by neutron and X-ray diffraction experiments

akuro Kawasaki,^a Kota Takano,^b Miwako Takahashi,^b Takashi Ohhara,^{a,c} Ken-ichi Ohshima,^b Katsuhiro Kusaka,^d Ichiro Tanaka,^d Taro Yamada,^d Takaaki Hosoya,^d Kazuo Kurihara,^a Nobuo Niimura,^d
^a*J-PARC Center, (Japan). Atomic Energy Agency, Tokai, (Japan).*
^b*Institute of Materials Science, University of Tsukuba, Tsukuba, (Japan).*
^c*Research Center for Neutron Science & Technology, Comprehensive Research Organization for Science and Society, Tokai, (Japan).*
^d*Frontier Research Center for Applied Atomic Sciences, Ibaraki University, Tokai Ibaraki (Japan).* E-mail: takuro.kawasaki@j-parc.jp

$C_4H_8ONH_2-PbBr_3$ has a lead-based inorganic-organic perovskites structure. One-dimensional chains of face shearing $PbBr_6$ octahedra are isolated by $C_4H_8ONH_2^+$ cations to be quantum wire, so this material can be regarded as a naturally self-organized one-dimensional system. The crystal structure of the material is orthorhombic with space group of $P2_12_12_1$. $PbBr_6$ octahedra are strongly distorted because of the existence