MS18-P5 **Physicochemical properties of hybrid organic-inorganic complexes via the charge density studies.** Radosław Kamiński, Roman Gajda, Katarzyna N. Jarzembska, Krzysztof Woźniak, *Department of Chemistry, University of Warsaw*, *Poland*,
E-mail: rkaminski.rk@gmail.com

Hybrid organic-inorganic complexes are very attractive due to their numerous possible applications in modern materials chemistry. They exhibit interesting physicochemical behaviour while being in the solid state. This includes, for example, thermoelectric properties, magnetic high-temperature phase transitions or mechanical properties. Additionally, developments of such new classes of materials can extend our knowledge in the field of so-called crystal engineering.

Recently we have utilized the synthesis and crystallization of different hybrid compounds of transition metal halides with benzene derivatives. A mixing of respective metal halides (*e.g.* $ZnCl_4$, $CoCl_4$, $CdBr_4$) with acetylaniline in acidic conditions resulted in a whole set of new isostructural layered complexes. They all crystallize in the orthorhombic *Cmca* space group. Recently, we have collected high-resolution X-ray diffraction data sets for the cobalt (see figure below) and zinc complexes. In this contribution we present our preliminary charge density studies of the described systems, in terms of the Hansen-Coppens multipole model followed by QTAIM analysis and theoretical periodic computations. Our findings are extended with the recently measured (at 90 K and 120 K) indium complex which shows a structural and magnetic phase transition at 108 K.

Keywords: hybrid organic-inorganic complexes, charge density, structural analysis, layered structures

MS18-P6 **Charge Density Distribution of Diborides.** B.Kodess [ab], V.Khvostov [a]. P.Kodess [b]. [a] VNIIMS, Moscow, Russian Federation, [b] ICS&E, Aurora, CO, USA;
E-mail: kodess@mail.ru

X-ray methods have been developing for determining the parameters of the charge density distribution (CDD) taking into account the features of high accuracy experiments. This procedure a minimize contributions to the uncertainties of measurement results at different stages of the investigation CDD**:** prepare of samples, data collection, initial processing and rejection of the data and refinement model of structure on variety of scale. Improving the accuracy and reproducibility of the results (R=0.7-1%) provides opportunity to use the results both for analysis of the existing theoretical approximations and for analysis a optimal mechanical and electrical properties of different composition. Examples are given for set of diborides of metals. The spheres ((0.25-0.3mm) have been prepared for diborides of A1B2 family (Ń32) also, for which ordinary and high-temperature superconductivity (HTSC) has been found. For the measurements to has been carried out in full Ewald sphere, ŕtomic coordinates and their anisotropic vibration amplitude has been refined and the CDD construct in different sections. Highly-accurate data allow the refinement of a structural type for Mo2B5 which possess of for low-temperature superconductive property. We found vacant lattice site on the position same Boron (B) atoms in Mo2B5 [3]. Its single-crystal data is differ from neutron powder data [3]. This technique (without use multipole expansion even) put into practice for construct the deformation and valence electron distribution maps another diborides, space group P6\mmm, and denotes their layer-wise character with practically two-dimensional honeycomb B planes. The B atoms located in centre of trigonal prism of metal atoms, which adjoin with all facet; and form tri-dimensional structure. The metals and the B lays packed along c-axis in turn. The electron distribution of transition mĺtall is only part-spherical as opposed to Mg in MgB2, however no covalent bonds between metals and B atoms. The calculation [4] show also that for MgB2 graphite-similar B-B interactions is basilar contribution in total energy (for example B-B (68%), B-Mg (23%) and Mg-Mg (9%)) and B2pz – similar state is responsible for weak inter-layer bonding. Such pronounced layer-wise character of structure suggests exciton contribution in HTSC mechanism. The comparison of the characteristics of charge distribution with the results of calculation of the electronic structure of these diborides allows to clarify the direction of further theoretical studies of nature of unique electric properties of diborides.

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