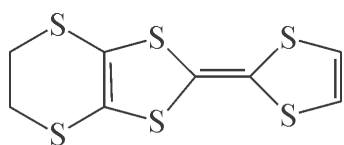


s13.m42.p13 **Peculiarities and Regularities of EDT Based Compounds.** Olga Kazheva^a, Ludmila Kushch^a, Gennadii Shilov^a, Anatolii Chekhlov^a, Grigorii Aleksandrov^b, Oleg Dyachenko^a, ^a*Institute of Problems of Chemical Physics, RAS, Chernogolovka, Moscow Region, 142432, Russia,* ^b*Kurnakov Institute of General and Inorganic Chemistry, RAS, Moscow, 119991, Russia. E-mail: koh@icp.ac.ru*

Keywords: X-ray study; Molecular conductors; Structure-property relationship

The work presents the results of crystal chemical investigation of the first electroconducting radical cation salts based on ethylenedithiotetraphthalvalene (EDT) with anions containing Hg and rare-earth elements: (EDT)₄[Hg_{2.83}I₈], (EDT)₄[Hg_{3.17}I₈], (EDT)₆[Hg₄Br₁₂], (EDT)₃[Hg(SCN)Cl₃]·0.5C₆H₅Cl, (EDT)₁₂{[Hg(SCN)₃(I_{0.2})₂Hg(SCN)₃][Hg(SCN)₃(I_{0.9})₂]}·2C₆H₅Cl, (EDT)₂[Ho(NCS)₄(H₂O)₄], (EDT)₃[Y(NO₃)₅]. The chemical formulas of the salts were determined by X-ray study.



EDT

In the report the following crystal chemical features of the investigated compounds' structures will be discussed:

- all investigated compounds based on EDT with anions containing both Hg and rare-earth elements are characterized by b-packing type of the conducting layers;
- all anionic layers represent polymeric formations or various supramolecular associates (Fig. 1);
- partial population of Hg atom's positions in (EDT)₄[Hg_{2.83}I₈], (EDT)₄[Hg_{3.17}I₈], (EDT)₆[Hg₄Br₁₂] crystals is a typical feature of Hg-containing radical cation salts.

Structure-property relationships will be discussed. This work was supported by the RFBR (grant No. 02-03-32794).

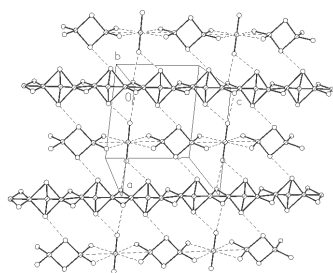


Fig. 1. Anionic layer in (EDT)₄[Hg_{2.83}I₈]

s13.m42.p14 **"Metalloaromaticity" of Metal Chelate Ring. π - π Stacking Interactions in Solid-State Supramolecular Architecture of Copper(II) Complexes with Aromatic Ligands.** Victor Kravtsov, *Institute of Applied Physics, Academy of Sciences of Moldova, Academy str. 5 MD2028, Chisinau, Rep. Moldova. E-mail: kravtsov.xray@phys.asm.md*

Keywords: π - π stacking interaction; Copper complexes; Supramolecular architecture

In recent years, rational design of one- and multidimensional supramolecular architectures assembled from organic molecules and metal ions have been attracting more and more attentions in chemistry and materials science. The aggregation of small supramolecular units into larger arrays using a second supramolecular events represents new approach to complicated metalloorganic assemblies and can lead to new generation of solids with promising properties such as conductivity, magnetism and non-linear optical ones. The possibility of π - π interaction involving metal chelate ring is mostly not well documented in structural discussion. However, understanding and utilization of such non-covalent interaction is of a fundamental importance for the development of supramolecular chemistry and may be ideal example for developing theoretical models of exchange interactions in extended structures.

A number of complexes with heterotopic macrocyclic ligands based on isothiosemicarbazide which incorporate polyether cavity and polyaromatic extended heterocyclic moiety have been studied by x-ray method. The association of these complexes in the crystal demonstrates the diversity of supramolecular architecture, as a function of complexed cations and counter anions. Nevertheless the review of packing patterns in these structures reveals the remarkable repeatability of intermolecular π - π stacking geometry involving bis(salicylidene)isothiosemicarbazide fragments and metal chelate ring. This indicates that stack formation is tolerant towards modification of macrometallocyclic complexes and predominates in the crystal structure formation. New family of mono- and heteronuclear mixed-ligand complexes containing [Cu(AA)(BB)]⁺ building-blocks with aromatic ligands attached to copper(II) and favors the intermolecular stacking interactions involving metal chelate ring has been structurally characterized (AA= acetylacetonate or salicylaldehyde, BB=1,10-phenanthroline or 5,5'-dimethyl-2,2'-bipyridine). Our study reveals that such π - π stacking interactions found in the structures of mononuclear complexes may be transferred to the related polymetallic arrays. The system of π - π stacking interactions is the invariable and determining factor in sustaining extended supramolecular architectures in the crystal of such complexes and can be used as an excellent tool to impart the structural integrity of the discrete pieces and their particular physical properties to the final network assembly. The importance of stacking interaction seems increases for polyaromatic systems.

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