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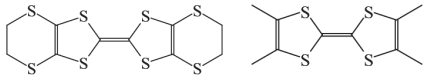
Radical cation salts and charge transfer complexes based on tetrathiafulvalene (TTF) and their derivatives constitute a wide class of organic materials with transport properties ranging from insulating to superconducting. The iron group metal bis(1,2-dicarbollide) complexes $[3,3'\text{-M}(1,2\text{-}C_2B_9H_{11})_2]^-$ (M = Fe, Co, Ni) have been proposed as counterions for synthesis of new radical cation-based molecular materials. Substitution of hydrogen atoms in these complexes for various atoms and groups opens practically unlimited perspectives of their modification.

In this report we describe synthesis, crystal structure and electrical conductivity of tetrathiafulvalenium salts of iron bis(dicarbollide) anion $[3,3'\text{-Fe}(1,2\text{-}C_2B_9H_{10})_2]^-$: $(ET)_2[3,3'\text{-Fe}(1,2\text{-}C_2B_9H_{11})_2]$ (**1**) and $(TMTTF)[3,3'\text{-Fe}(1,2\text{-}C_2B_9H_{11})_2]$ (**2**).



The geometry of the $[3,3'\text{-Fe}(1,2\text{-}C_2B_9H_{10})_2]^-$ anion are similar in the salts. The dicarbollide ligands are mutually rotated by 180° producing *transoid* conformation (Fig. 1).

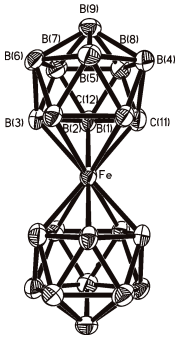


Fig. 1. $[3,3'\text{-Fe}(1,2\text{-}C_2B_9H_{10})_2]^-$ anion in (**1**). Hydrogen atoms omitted for clarity.

Both radical cation salts prepared were found to be semiconductors. The activation energy of (**1**), E_a, was found to be ~0.07 eV, the room temperature conductivity is 1.5×10^{-2} $\Omega^{-1}cm^{-1}$, whereas for (**2**) it is lower than 10^{-10} $\Omega^{-1}cm^{-1}$.

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Keywords: organic conductors, X-ray study, structure-property relationship

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Crystal structure of human tyrosylprotein sulfotransferase

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Post-translational protein modification by tyrosine sulfation plays an important role in extracellular protein-protein interactions, with implications in immune response, inflammation, hemostasis, and viral infection including that of the human immunodeficiency virus (HIV). The sulfation reaction is catalyzed by the Golgi enzyme called the tyrosylprotein sulfotransferase (TPST). Here we present the first crystal structure of the human TPST (hTPST) complexed with a substrate peptide and a degradation product of the sulfate donor, 3'-phosphoadenosine-5'-phosphosulfate (PAPS). At 1.9Å resolution, the structure shows that the bound substrate peptide forms an L-shaped structure and a short parallel β-sheet with a loop following the PAP-binding site. The central region of the substrate peptide that encompasses the acceptor tyrosine residue interacts specifically with several residues of hTPST2. The anchoring of the central region of the substrate peptide at a fixed distance from the 5'-phosphate of PAP underscores the selectivity of hTPST2 for tyrosine-containing peptide as a substrate. The structural information, in conjunction with the mutational analysis data, provides a molecular basis for substrate-binding and catalysis, and explains how TPST can accommodate a variety of substrate proteins.

Keywords: keyword-1 crystal structure, keyword-2 post-translation

MS31.P15

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Additional ligand in the ru coordination sphere of hoveyda-type catalysts. Part II

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We report new structures of sulphon and sulphoxide derivatives of a II generation Hoveyda-type catalyst [1]. This catalyst is a one of the most important and effective from all catalysts of the metathesis reaction [2].

Last year we reported, that water molecule was found in the ruthenium coordination sphere of some compounds [3]. This year we present the first structure of the sulphon derivative (Fig. 1), which was possible to obtain only due to the presence of another additional ligand: 3-bromopyridine [4]. We observe that the ruthenium atom is coordinated by oxygen from the sulphon group and thus a 6-membered ring is formed.

We also compare structures of the catalysts containing no additional molecules i.e. the catalyst with water and with 3-bromopyridine. It appears that the 3-bromopyridine moiety interacts with catalyst in the solution, which changes the colour of the solution. This also has a significant influence on the catalyst activity and determines the reaction rate at room temperature. Finally, it does