

MS30-P17 Two-step spin transition and superstructure in an iron(II) coordination network based on flexible bitopic ligand 1-(tetrazol-1-yl)-3-(1,2,3-triazol-1-yl)propane

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The spin crossover (SCO) in iron(II) systems bring a lot of attention due to the possibility of switching between high (HS, S=2) and low (LS, S=0) spin state using different stimuli like temperature, pressure, AC magnetic field or light. The SCO is usually accompanied by change of other properties like: magnetic, optical, structural, dielectric, etc. In particular, it is connected with the step change of the Fe-ligand bond lengths. The structural distortion caused by the modification of structural parameters of chromophore FeN₆ propagates further, changing also the second coordination sphere. The spread of the deformation on the whole crystal leads to the appearance of the cooperative effects, including structural bistability, which is a basis for the potential applications in molecular electronics [1].

A majority of the structural studies concentrate only on the investigations of the two stable states LS and HS. The knowledge only of the crystal structures of the initial and final phases is not sufficient to establish correlations between the structural and magnetic properties of the SCO system.

[Fe(ptrtz)₃](ClO₄)₂·CH₃CN (where ptrtz=1-(1,2,3-triazol-1-yl)-3-(tetrazol-1-yl)propane) is a interesting SCO compound with 2D coordinated network, because exhibits two step complete SCO and only 25% of iron(II) ions undergo HSgLS transition during the first step [2].

A detailed inspection of the diffraction data provides very weak satellite reflections ($h + 1/2$, $k + 1/2$, $l + 1/2$) what is evidence for long-range ordering of the HS and LS Fe(II) iron ions within chains. Research of the superstructure of [Fe(ptrtz)₃](ClO₄)₂·CH₃CN will increase the understanding of propagation processes of the structural distortions and as a result allow to rationally design new materials. In particular, it will aid in increasing of the cooperative character of SCO in the polymeric systems by the choice of proper ligands bridging the SCO centres.

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Keywords: iron(II) compounds, two-step spin transition, superstructure

MS30-P18 Synthesis and structure characterization of biologically active triphenyltin complexes with thioamides

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It has been proved that organotin compounds have anticancer properties but the exact mechanism of antitumor action is still unknown^[1,2]. Analysis of relationships between drug structure and the biological response can be a key to understanding cytotoxic activity. New organotin (IV) complexes with heterocyclic thioamides 2-mercaptoimidazoline (thimt) and 4,6-diamino-2-mercaptopyrimidine (4,6-dapmt) of formulae [Ph₃SnCl(thimt)] (**1**) and [Ph₃Sn(4,6-dapmt)] (**2**) have been synthesized and characterized by FT-IR, NMR, and X-ray diffraction. Deprotonated ligands bond to a metal through the sulfur atom. In both complexes of tin centers are 5-coordinated in less (**1**) or more (**2**) distorted (fig. 1). In **1** the coordination is by three carbon (equatorial plane), one chlorine and one sulphur atoms. In **2** weak Sn-N interactions complete the coordination sphere around the tin. It's the unique example of the structure of Ph₃SnXY system with axial-equatorial arrangement of the phenyl groups. Alternatively structure might be viewed as very distorted tetrahedron.^[3]

The complexes **1** and **2** were tested for in vitro cytotoxic activity against LMS (leiomyosarcoma cells), MCF7 (breast), HeLA (cervical) and CCD39LU (normal human lung fibroblast). Both complexes showed a better cytotoxic activity than clinically established chemotherapeutic cisplatin for all three cancer cell lines. Triphenyltin derivatives exhibit different chemosensitivity of all cell lines, but the best cytotoxic activity was established for LMS cell lines. Moreover, compounds **1** and **2** have less effect on the proliferation of normal cell types. These results showed that these complexes can be novel antitumor drug candidates.

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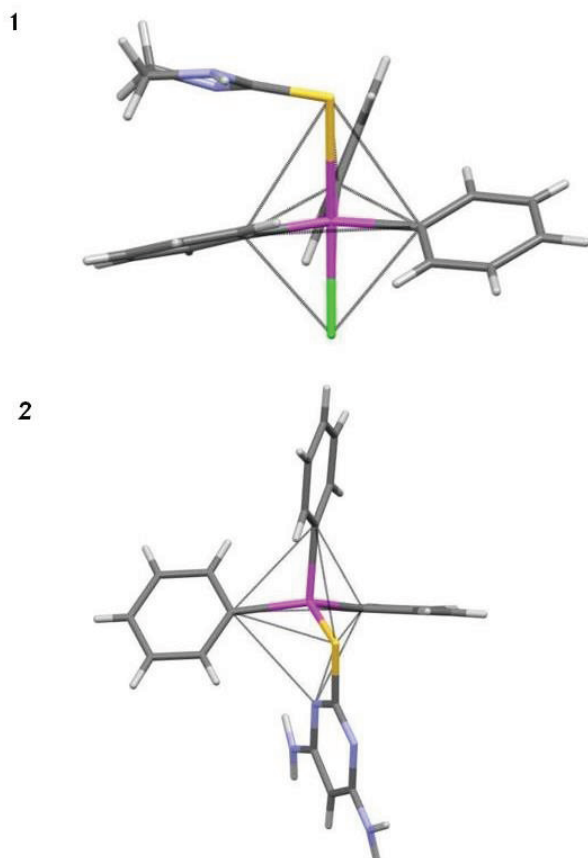


Figure 1. Coordination models of tin cations in (1) and in (2)

Keywords: X-ray crystallography, organotin(IV) complexes, heterocyclic thioamides, antitumor activity,

MS30-P19 X-ray structural analysis and catalytic properties of new thiazoline - carboxylate ruthenium complexes

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X-ray Structural Analysis and Catalytic Properties of New Thiazoline - Carboxylate Ruthenium Complexes

Heterocyclic compounds such as thiazol(in)es, thiazolidines, oxazol(in)es have received large attention. These heterocycles are of importance as pharmaceuticals and ligands for catalysis. The thiazol(in)e ring is present in many biological active natural and synthetic products. There is a great number of publications related to biological activities of thiazoline scaffold. Metal complexes of carboxylate ligands such as picolinic acid, proline, quinoline or isoquinoline carboxylic acid, thiazole or thiazolidine carboxylic acid, bipyridine carboxylic acid are known and investigated their luminescence, structural properties, biological activities [1].

In the proposed study, X-ray diffraction analysis of Ruthenium complexes were performed using an Agilent Diffraction Xcalibur diffractometer equipped with an Eos-CCD detector. Data were absorption-corrected within the CrysAlis program [2]. Structures were solved by SHELXS-97 and refined by means of SHELXL-97 programs [3] incorporated in the OLEX2 program package [4]. Their catalytic activities were evaluated for ATH. These catalyst systems showed excellent activity for a range of ketone and aldehyde substrates tested. Attempts to obtain enantioselective products by lowering the temperature or increasing the catalyst loading, failed the *ee* values. In this work, high yields were obtained in the transfer hydrogenation reaction.

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Keywords: Thiazoline, Ruthenium complexes, Crystal structure, Catalytic analysis