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

Joachim Kusz[1], Maria Ksiazek[1], Robert Bronisz[2], Marek Weselski[2]

1. Institute of Physics, University of Silesia, 40007 Katowice, Poland
2. Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50383 Wrocław, Poland

email: joachim.kusz@us.edu.pl

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 FeN_6 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.

$[Fe(ptrtz)_3](ClO_4)_2 \cdot CH_3CN$ (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 $[Fe(ptrtz)_3](ClO_4)_2 \cdot CH_3CN$ 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.

The work was supported by the Polish National Science Centre (grant number DEC 2011/01/B/ST5/06311).

[1] P. Gutlich, H. A. Goodwin, *Top. Curr. Chem*. **2004**

[2] A. Bialonska, R. Bronisz, J. Kusz, M. Zubko, *Eur. J. Inorg. Chem.* **2013**, 884–893

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

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

Agata Owczarzak[1], Anita Owczrzak[1], Maciej Kubicki[1], Marek Murias[2], Małgorzat Kucińska[2]

1. Adam Mickiewicz University
2. Poznan University of Medical Sciences

email: agataowczarzak@gmail.com

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-mercaptopyrymidyne (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 (leiomyosacroma cells), MCF7 (breast), HeLA (cervical) and CCD39LU (normal human lung fibroblast). Both complexes showed a better cytotoxic activity then 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.

References

[1] S.Tabassum C. Pettinari, J*ournal of Organometallic Chemistry* Volume 691, 2006, 1761–1766

[2] P. J. Smith, *Chemistry of Tin,* Black Academic& Professional: London, 1998

[3] M. N. Xanthopoulou, S.K. Hadjikakou, N. Hadjiliadis , M.Kubicki, *Inorg. Chem*., 2007, 46 (4), 1187–1195