more than 10,000Å<sup>3</sup> that shields the proteolytic site. The fact that proteolysis occurs inside a closed chamber is reminiscent of the proteasome structure and for that reason we introduced a new term: the peptidasome. The chamber has no obvious opening for the substrate to enter; yet a bound peptide is found inside and amino acids separated by almost 800 residues in sequence form the active site. The structure suggests a novel mechanism for access to the active site, involving hinge-bending motions that cause the peptidasome to open and close in response to substrate binding.

# Keywords: crystallographic structure, peptide degradation, metalloproteinases

## MS72.29.5

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### **Molecular Machines and Tropical Pathogens**

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The "Type 2 Secretion System" (T2SS) from Vibrio cholerae, enterotoxigenic E. coli (ETEC) and related pathogens is responsible for secreting proteins like cholera toxin (CT) and heat-labile enterotoxin (LT). The T2SS consists of 14-16 different proteins, and spans the inner as well as the outer membrane. We have expressed many components of the T2SS from several bacteria including soluble proteins, integral membrane proteins and multi-protein complexes. Several crystal structures have been elucidated which gives initial insight into the architecture of the inner membrane subcomplex.

The editosome is essential for Trypanosomatids, which are causative agents of sleeping sickness, Chagas' disease and leishmaniasis. For several mitochondrial proteins the pre-mRNA needs to be edited substantially. The editing information is encoded in numerous small "guide RNAs" which are used by the "editosome" to create a mature messenger. The editosome consists of over a dozen different proteins. The structures of editosome ligase and TUTase provide the first views of parts of this complex machinery. **Keywords: type II secretion, RNA editing, tropical disease** 

MS73 MOLECULAR CRYSTALS WITH NOVEL PHYSICAL PROPERTIES *Chairpersons:* Catalina Ruiz-Perez, Annie Powell

#### MS73.29.1

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020464-Bucharest, Romania, E-mail: marius.andruh@dnt.ro The search for new synthetic routes leading to solid-state

architectures with pre-established functions and properties is the heart of crystal engineering. In the last 15 years or so, chemists learned a lot in manipulating the intermolecular forces, in order to design crystalline compounds with useful properties

We are currently developing a synthetic approach aiming at obtaining multimetallic complexes, which is based on the employment of homo- and heterobinuclear complexes as nodes. The following types of cationic species are used: (i) binuclear copper(II) species with end-off compartmental Schiff-base ligands; (ii) alkoxo-bridged copper(II) species; (iii) heterobinuclear 3d-3d' species with macrocyclic compartmental ligands;(iv) heterobinuclear 3d-4f species with side-off compartmental Schiff-base ligands. When the metallic ions are different and paramagnetic, the intra-node exchange interactions, as well as those between the resulting spins may lead to interesting magnetic properties. A particular case is the one concerning the 3d-4f binuclear nodes. The building principle is based on the employment of symmetrical (dicarboxylato anions, bis(4pyridyl) derivatives) or of unsymmetrical spacers (e. g. the isonicotinate anion), which act selectively with the different (3d, 4f) metal ions.

Keywords: coordination chemistry compounds, coordination crystal engineering, magnetic exchange

#### MS73.29.2

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# High Spin and Photomagnetic High Spin Molecules

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As part of our research activities devoted to molecular magnetism, we are interested in synthesising polynuclear compounds showing both large spin ground state and anisotropy. For this purpose, polycyanometalate precursors have been used successfully, with an effective control of the chemistry, which consist to firstly prepare polydentate ligands and their corresponding mononuclear complexes with varied metallic centre such as  $Mn^{II}$ ,  $Ni^{II}$ ,  $Co^{II}$ ,  $Cu^{II}$ , before synthesising polynuclear compounds with tunable geometry. Thus, bi, tri-, tetra-, hexa- and heptanuclear species have been obtained in this way with a spin state value ranging from 3/2 to 27/2.

The step by step rational synthesis allows us to synthesize as well hetero-trimetallic complexes such as CrNi2Mn4 (S=13/2) and several polynuclear species obtained from octacyanometalate precusors, for instance WCu6, WNi6 and WMn6 and the corresponding molybdenium species.

This part of the work devoted to octacyanometalate chemistry paves the way of photomagnetic Single Molecule Magnets. We already succeeded in getting the first photomagnetic high spin molecule !

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Keywords: molecular magnets, photochemistry, cyanide complex

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Crystal Structure-Mobility Correlation in TTF Based Organic Field-Effect Transistors

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Organic Field Effect Transistors (OFETs) have attracted a great deal of interest over the last few years due to their unique processing characteristics and improved electronic mobility. The fundamental material characteristics of organic semiconductors are most clearly measured in single-crystals, but very few have been studied.

Recently, we have reported that crystals of the organic material dithiophene-tetrathiafulvalene (DT-TTF) have a high field-effect charge carrier mobility of  $1.4 \text{ cm}^2/\text{Vs}$ . [1] These crystals were formed by a simple drop casting method, making this material interesting to investigate for possible applications in low cost electronics.

Here, organic single-crystal field-effect transistors (OFETs) based on materials related to DT-TTF are presented and a clear correlation between the crystal structure and the electrical characteristics is observed.[2] The observed relationship between the mobilities in the different crystal structures is strongly corroborated by calculations of both the molecular reorganization energies and the maximum intermolecular transfer integrals.[2,3]

Interestingly, the most suitable materials described here exhibit mobilities among the highest reported for OFETs, and are the highest reported for solution-processed materials. [2,4]

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Keywords: OFETs, TTF derivatives, functional materials