MS.61.5

Two different types of supramolecular architectures of p-sulphonated thiacalix[4]arene with Zn(dipy)₃: Structure and stability

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Sulfonated calix[n]arenes are of great interest as objects of supramolecular chemistry due to their multi-functional complexation abilities and a variety of the conformational forms.

Previously in [1] we reported the structure of the thiacalix[4]arene tetrasulphonate (TCAS) complex **1** with [Zn(bipy)₃]²⁺ and water. TCAS didn't participate in coordination bonding with metal and possessed a partial cone conformation. At the same time NMR measurements of the solution showed that *1,2-alternate*-TCAS may be bound with the dichelated forms of $[Zn(bipy)_n]^{2+}$ (n = 1, 2) in its bi- or tridentate coordination sites.

Crystals **2** of different colour and habit were found together with crystals **1** in the same flask. But they appeared to be twinned and unstable when exposed to air and so required more gentle treatment.

Recent X-ray diffraction analysis of single crystal **2** has revealed a new type of mixed ligand complex (see picture below). This complex is one of those (n = 1) predicted by NMR studies of the mother solution. It co-crystallizes with two [Zn(bipy)₃]²⁺ per thiacalixarene macrocycle and with disordered solvent. Obviously the evaporation of the solvent from crystal is the cause of its instability.

Time-resolved X-ray powder diffraction experiment of powder **2** was carried out to analyze its decomposition. It has been proved that the decomposition product **3** is crystalline but differs from **1** and **2**. The details of the structural changes during crystal decomposition are presented.

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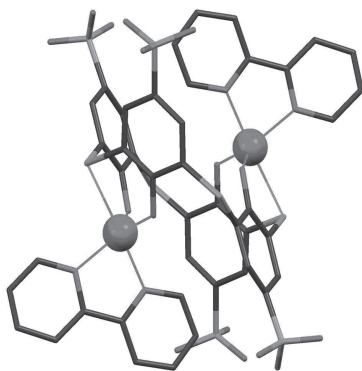
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Crystallography On-A-Chip: using GPU for fast scattering computing

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Efficient computing of scattering of X-ray and neutrons from crystals has been the subject of intense work since computers became available. While the Fast Fourier Transform algorithm is the *de facto* standard for large structures, it can be used strictly only for periodic (crystalline) structures.

However many materials for modern applications cannot be described as triperiodic objects, due to the presence of non-random defects, or inhomogeneous strain fields, such as heterogeneous semiconductor nanostructures. Moreover, it is interesting to compute scattering at positions in reciprocal space which are not dictated by the algorithm (FFT grid) but rather correspond to the actual points measured experimentally (e.g. on the curved surface corresponding to the projection of a 2D detector on Ewald's sphere).

For this reason it is necessary to use efficient algorithms to compute scattering from large numbers (>10⁶) of atoms, for any distribution of points in reciprocal space.

In the last five years new dedicated hardware tools have become available for computing with Graphical Processing Units (GPU) present in modern (consumer) graphics cards. These GPU allow efficient *parallel calculations* with a much higher throughput (up to 1 Tflop/s) compared to microprocessors (typically yielding 1 to 10 Gflop/s per core).

In this presentation, we will explain how GPU can be used for crystallographic computing, and what are the current performance and limits of this "Crystallography-On-A-Chip" approach. Several example of applications have been reported in the last two years [1-3], and we will more specifically focus on results from the PyNX computing library [4-5], which provides a python interface for simple scattering computing, up to 4*10¹⁰ reflections.atoms/s using a GPU, compared to ~10⁸ reflections.atoms/s on a mcroprocessor core.

Applications to the calculation of scattering from nano-structures as well as for Bragg coherent diffraction imaging of strained crystals [6], [7] will be discussed.

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Software libraries in CCP4 Program Suite

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CCP4 is a community based resource in Protein Crystallography with ultimate goal to play a key role in the development of new crystallogtraphic software for academics, not for profit, and for profit research, as well as in eduation and training of scientists, dissemination of new ideas, techniques and practice. The Project was set up 32 years ago, and underwent many changes since that. Currently CCP4 Software Suite contains over 250 programs related to crystallographic computations and structure analysis.

For software collection of this size, appropriate design and organisation of common functionality in libraries is absolutely crucial