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Keywords: anion, hydrogen bond, motif

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Molecular-Level Devices and Machines

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The chemical, bottom up approach, based on the concepts of supramolecular chemistry, can be very useful to design and construct interesting nanostructures.

By using this approach, the macroscopic concepts of a device and a machine can indeed be straightforwardly extended to the molecular level [1]. A *molecular-level* device can be defined as an assembly of a discrete number of molecular components designed to achieve a specific function. Each molecular component performs a single act, while the entire assembly performs a more complex function, which results from the cooperation of the various molecular components. A *molecular-level machine* is a particular type of molecular-level device in which the component parts can display changes in their relative positions as a result of some external stimulus.

Molecular-level devices and machines operate via electronic and/or nuclear rearrangements and, like macroscopic devices and machines, are characterized by (i) the kind of energy input supplied to make them work, (ii) the way in which their operation can be monitored, (iii) the possibility to repeat the operation at will (cyclic process), (iv) the time scale needed to complete a cycle, and (v) the performed function. In this lecture, we will illustrate examples of recent achievements in this field.

[1] Balzani V., Credi A., Venturi M., *Molecular Devices and Machines - A Journey in the Nano World*, Wiley-VCH, 2003.

Keywords: supramolecular chemistry, photochemistry, electrochemistry

MS32 STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA (INORGANICS)

Chairpersons: Angela Altomare, Holger Putz

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Exploiting Preferred Orientation to Resolve the Intensities of Overlapping Reflections

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In 1999, Wessels *et al.* [1] demonstrated the practical viability of the 'texture method' for resolving reflections that overlap in a powder diffraction pattern. By collecting synchrotron data on a textured polycrystalline sample as a function of sample orientation, more information about the relative intensities of overlapping reflections could be obtained. A full texture analysis is used to establish how the crystallites are oriented in the sample, and then a single set of (single-crystal-like) reflection intensities is extracted via a joint refinement procedure using all diffraction patterns (between 5 and 1296) simultaneously. The data collection and analysis strategies for both reflection and transmission geometries have been described [2]. To develop the method further so that even more complex structures can be accessed, several possibilities are being explored. (1) A new method for preparing textured powder samples using a repetitive pressing procedure has been developed. (2) To optimize the resolution of the data, diagonal displacement of the imaging plate at

the maximum sample-to-detector distance has been evaluated. (3) To improve the resolution still further, an experimental setup with a one-dimensional Si-microstrip detector, has been devised. (4) A new background and scaling procedure has been implemented in the data analysis software.

[1] Wessels T., Baerlocher Ch., McCusker L.B., *Science*, 1999, 284, 477. [2] Baerlocher Ch., McCusker L.B., Prokic S., Wessels T., *Z. Kristallogr.*, 2004, 219, 803.

Keywords: powder diffraction, preferred orientation, structure solution

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New Strategies for the *ab-initio* Structure Solution in EXPO2005

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The full pathway in the *ab-initio* crystal structure solution from powder data has been made more straightforward by the package EXPO2004 [1] which is able to: index the diffraction pattern; identify the most plausible space group; estimate the reflection integrated intensities; solve the crystal structure by Direct Methods, in eventual combination with Monte Carlo approach; refine the structure model by Rietveld technique.

New strategies have been recently introduced in EXPO2004 in order to enhance its power, leading to EXPO2005. Among them the most relevant are: a) an improved algorithm for space group determination; b) a new definition of the background contribution; c) efficient methods for estimating the integrated intensities via a systematic procedure based on coding theory and/or Patterson inversion technique; d) an effective figure of merit able to identify the most plausible phases set; e) a powerful global optimization approach to be applied in case of organic structures; f) a more robust structure refinement procedure.

The EXPO2005 features and applications will be described.

[1] Altomare A., Caliendo R., Camalli M., Cuocci C., Giacovazzo C., Moliterni A.G.G., Rizzi R., *J. Appl. Cryst.*, 2004, 37, 1025-1028.

Keywords: *ab-initio* structure determination, powder software, computational crystallography

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Are Well Known Phase Diagrams Really Well Known ?

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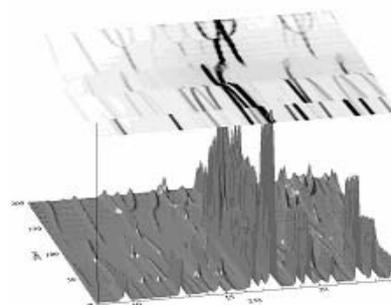


Fig. 1: Temperature dependent powder patterns of RbC_2O_4 [1].

Phase diagrams, which show the preferred physical states of matter at different temperatures and/or pressure, are available for many common substances near ambient conditions. The number of previously unidenti-fied polymorphic phases increases considerably even for "well known" compounds (see Fig. 1) if the technique of high-throughput *in-situ* synchrotron powder diffraction in combination with fast 2D-detectors is applied. The main problem is related to the enormous amount of data which need to be processed efficiently. Techniques to solve part of this problem [2] are presented during the talk.