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MS31.26.5
Acta Cryst. (2005). A**61**, C45
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.

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MS32 STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA (INORGANICS)
Chairpersons: Angela Altomare, Holger Putz

MS32.26.1
Acta Cryst. (2005). A**61**, C45
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.

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MS32.26.2
Acta Cryst. (2005). A**61**, C45
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.

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MS32.26.3
Acta Cryst. (2005). A**61**, C45-C46
Are Well Known Phase Diagrams Really Well Known ?

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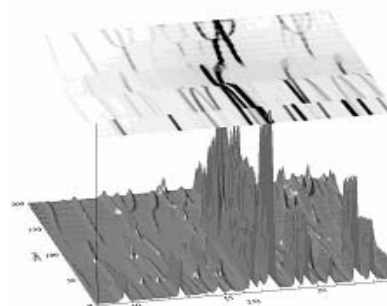
Phase diagrams, which show the preferred physical states of matter at different temperatures and/or pressure, are available for many common substances near ambient conditions. The number of previously unidenti-fied polymorphic phases increases con-siderably even for "well known" com-

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

pounds (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.