molecular sieves, as shape-selective catalysts, as dessicants, as ion-exchangers, and as hosts in advanced materials. A zeolite's suitability for a specific application is highly dependent upon its structure, so structure analysis is an intrinsic part of zeolite science. However, because most zeolites can only be prepared in polycrystalline form, standard methods of structure analysis cannot be applied.

Over the years, zeolite crystallographers have devised a number of different methods to overcome or circumvent this problem. Initially, physical model building based on information from various sources was the only option available. Interestingly enough, this is probably still the most powerful tool in the zeolite crystallographers toolbox, but it requires experience, talent and intuition. As computing capacity has increased, however, algorithms for automating the model building process have been created. At the same time, methods for improving the quality of reflection intensities extracted from powder diffraction patterns have been devised, and this in turn has allowed single-crystal methodology to be applied with greater success. An overview of some of the more recent developments in this field will be presented.

Keywords: zeolites, powder diffraction, structural analysis software

KN07.25

Acta Cryst. (2005). A**61**, C2

Structure Analysis of Modulated Crystals: Trends and Tendencies

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The superspace theory as developed by DeWolff, Jansen & Janner [1] gave to crystallographers a unique tool for generalization of structural analytical methods to be especially applicable to modulated structures. In many cases the structure analysis can now be performed almost routinely [2]. The superspace approach can also be used to find a systematic way of describing whole families of related structures [3]. The use of CCD and imaging plate systems changed considerably sensitivity of data collection for modulated structures and therefore a need for further improvement of the methods is obvious. The modulation of more complicated systems cannot be efficiently described as series of harmonic functions. Special discontinuous functions already introduced for 3+1 dimensions [4] are to be generalized to 3+2 and 3+3 superspace.

Recently modulations have been found in complicated organic structures including proteins. This opens a various new problems concerning efficiency of methods used for solution and refinement of modulated structures. New techniques such as maximum entropy [5] and charge flipping methods [6] give us a good chance to make such a generalization.

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Keywords: modulated crystal structures, structure analysis, superspace theory

KN08.25

Acta Cryst. (2005). A**61**, C2

High Throughput Technologies in Structural Biology

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During the past few years, progress has been made in developing high throughput technologies for protein cloning, expression, purification, crystallization, crystal imaging, and synchrotron beamline data collection. Recently, we have been able to miniaturize, automate and parrallelize the structural biology processes significantly using nanoliter volume technologies (see http://stevens.scripps.edu/webpage/htsb for examples). Accordingly, significantly smaller amounts of materials can be used at all steps, and more parallel experiments can be engineered (genetic and mechanical) within the same space and time constraints. The next phase of this effort includes integration and improved system processing. A description of these technology developments, current status, and examples will be described.

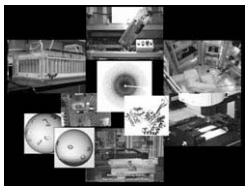

Figure 1. Sample of technologies that have been created in the past few years that include robotics systems for expression, protein purification, imaging, and analysis.

Acknowledgements: I am grateful for the cooperativity of the combined effort of researchers from the Joint Center for Structural Genomics (NIH PSI GM062411), JCIMPT (NIH Roadmap Initiative P50GM073197), Genomics Institute of the Novartis Research Foundation, The Scripps Research Institute, and Syrrx.

Keywords: structural genomics, structure based drug discovery, high throughput structural biology

KN09.25

Acta Cryst. (2005). A**61**, C2

Structure Solution of Pharmaceutical Compounds from Powder Diffraction Data

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A significant part of contemporary medicine is based on the discovery and development of drugs, which are often molecules of ten to thirty non-hydrogen atoms. It is important to know the crystal structures of drug compounds and candidates for various reasons: fundamental understanding of structure and bonding vis-à-vis physiological action, the physical and chemical properties of polymorphs which are frequently encountered in drugs, and the relevance of polymorphism to patent protection and limits thereon. As it happens, many of these materials are available only as powders, and therefore any structural information must be obtained from powder diffraction.

Advances in instrumentation and data analysis techniques, both commercial and in the public domain, are proving equal to the task. However, judging from the literature, structure determination from powder data SDPD is still an obscure art, practiced by relatively few crystallographers. This is despite the outreach activities of a significant number of the innovators of SDPD, who have been working to develop and promulgate powder techniques.

I will review the state of the art and present some new results, such as the structures of chloramphenicol palmitate polymorphs.

Keywords: ab-initio powder structure determination, pharmaceutical structure determination, polymorphism

KN10.25

Acta Cryst. (2005). A**61**, C2-C3

Quasicrystal Structure Analysis. The State of the Art

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The quasicrystal is an aperiodic solid showing Bragg peaks with noncrystallographic symmetry. It is recently clarified that the structure of quasicrystals can be analyzed by using a newly developed direct method and a structure refinement which is based on a higher-dimensional cluster model. They are equally applicable to decagonal and icosahedral quasicrystals since all quasicrystals seem to consist of some atom clusters (or building units)[1].

For the initial model building, the low-density elimination method (LDEM) is efficient [2]. This gives rough shape and size of occupation domains (OD) of a quasicrystal, which specify the location of atoms in a higher-dimensional space.

An initial model for the structure refinement is obtained from the rough ODs determined by LDEM by considering atom clusters, which are included in its crystal approximants. The distribution of atom clusters can not, however, be determined uniquely because of the existence of random phason strain, which is seen in all quasicrystals. This is usually inferred from high-resolution electron microscopy images or simply assumed based on a quasiperiodic tiling. The