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Many crystalline solids can be prepared only as microcrystalline powders and are not suitable for structural characterization by single-crystal X-ray diffraction methods. For such materials, it is necessary instead to tackle structure determination using powder X-ray diffraction data. Although there have been several successful reports of the structure determination of organic molecular solids using traditional strategies for structure solution from powder X-ray diffraction data, the majority of recent work on such materials has exploited the direct-space strategy for structure solution, followed by Rietveld refinement. Indeed, the recent upsurge of activity in this field (in both academic and industrial sectors) has taken place closely in parallel with the development of the direct-space strategy for structure solution, for which a range of different computational implementations are now available. In the direct-space strategy, a hypersurface defined by an appropriate R-factor (in our case the powder profile R-factor) is searched using an appropriate global optimization technique (such as Monte Carlo, simulated annealing or Genetic Algorithm techniques). Our recent research is focused on the development, optimization and implementation of Genetic Algorithm techniques in this field, as well as the application of these techniques to solve the crystal structures of a wide range of different types of molecular materials from different areas of the solid state and materials sciences. The lecture will describe fundamental aspects of the direct-space strategy for structure solution from powder X-ray diffraction data, and will be illustrated by examples selected to highlight the current scope and potential for the application of techniques in this field.

Keywords: structure solution, powder diffraction, molecular solids

KN09

Acta Cryst. (2008). A**64**, C5

Powder diffraction studies of proteins

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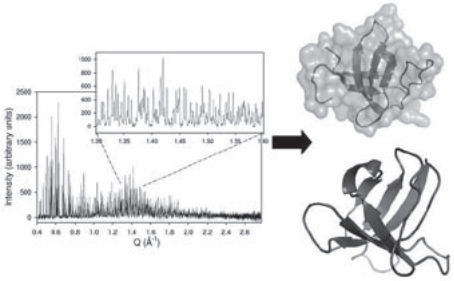
Studying biological macromolecules in the absence of good quality single crystals is a challenging field attracting considerable scientific interest. Modern developments of X-ray powder diffraction have allowed the structural investigation of a range of proteins establishing the method as a useful complementary tool to traditional approaches [1]. Protein powder specimens consist of a large number of randomly oriented diffracting micro-crystals which are usually formed rapidly by batch crystallization under a variety of conditions. An overview of the most recent developments in this field will be presented including: (a) application of the molecular replacement technique and structure refinements of selected proteins (b) methods for successful cryocooling (c) experimental phasing and extraction of molecular envelopes (d) high throughput automated data collection allowing systematic investigations such as screening and phase diagram mapping and (e) application of the method on biologically interesting proteins. Practical applications of the methods will be illustrated by recent examples.



[1] Margiolaki, I. & Wright, J. P. Acta Cryst. (2008). A64, 169-180

Keywords: protein crystallography structures, powder crystallography, synchrotron structural biology research

KN10

Acta Cryst. (2008). A**64**, C5

Structural biology studies of the avian influenza H5N1 virus

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Highly pathogenic avian influenza A virus strains with H5N1 subtype are entrenched in poultry worldwide and pose a growing threat to human health. Of the 382 reported human cases of avian influenza since 2003, 241 have been fatal. The development of novel anti-influenza therapeutics is vital in order to increase preparedness against a global influenza pandemic. To this end, we initiated a structural biology program in China to systematically study the proteins from the avian H5N1 influenza A virus (A/goose/Guangdong/1/96). Our aims are to understand the underlying mechanisms of viral replication and the interaction of the virus with host cell factors. Here I will report some exciting recent progress in our efforts.

Keywords: avian influenze H5N1, crystal structure, drug target

KN11

Acta Cryst. (2008). A**64**, C5-6

The crystallochemical basis of synthetic mineral immobilisation technologies

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The selection of synthetic mineral immobilisation matrices for the treatment of inorganic pollutants is governed by several considerations. First, toxic metals should be incorporated in their least harmful chemical states. For example, As^{3+} and Cr^{6+} are less poisonous than As^{5+} and Cr^{3+}. Second, as it may be necessary to simultaneously accommodate the oxidized and reduced species of different metals, the suite of mutually compatible minerals that can be selected is restricted. Third, structures with multiple cation and/or anion acceptor sites minimize the number of phases required to crystallise simultaneously, and allows greater flexibility to respond to variations in waste stream composition. This, in turn, limits the chance of undesirable compounds forming. Finally, phases with the highest proportions of appropriate cation acceptor sites are advantageous, to achieve high waste loadings with less 'bulking' through the introduction of inert additives. Within these constraints, a subset of structural families - perovskite, spinel, apatite, zirconolite, zeolites, clays - form the basis of many synthetic mineral immobilisation technologies. The crystallochemical properties of these waste forms are complex and remain the subject wide investigation. The final products are usually far from thermodynamic