recognition of enantiomorphic solid phases as thermodynamically distinguishable entities and the absence of degrees of freedom when P and T are fixed in the 2-component system (compound and solvent).

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Multialiquot algorithm for the automation of structure determnation from powder

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Recently mentioned [1] inconsistency of figures of merit [2], [3] when indexing high symmetry lattices turned to a conclusion the smaller cells of lower symmetry can be applied as building units when solving a structure by direct space methods. The approach is expected to decrease time necessary for simulated annealing of one structure solution and may appear particularly useful for large organic structures. The poster illustrates the approach based of example compounds with a small pyrochlore structure. The indexing program suggest several possible solutions and the correct solution of highest symmetry among them. The repetition of the same lattice described by different cells should be considered as an indication of the correct indexing solution. From the other hand, that might be random and unfruitful indexing solution if the lattice is non-primitive but is not observed among proposed cells with its primitive representation. The extension to indexing algorithms, eliminating lower symmetry cells for the same lattice described by high-symmetry cell, and the corrected figures of merit taking into account the number of equal proposal cells might be drawn as follows:

$$M'(20) = M(20)_h \cdot N_{ep}$$
$$F'(20) = F(20)_h \cdot N_{ep}$$

where $M(20)_h$ and $F(20)_h$ are $M(20)$ and $F(20)$ for the **h**ighest symmetry cell

N_{ep} is the number of **e**qual **p**roposal cells

Then, one may start to search for the structural model applying a cell of lower/volume symmetry providing it may represent a building unit for the larger cell of higher symmetry or may asssist to find a sublattice.

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Optimizing the input parameters for powder charge flipping

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The charge-flipping structure-solution algorithm [1,2] implemented in the program *Superflip* [3] and adapted to accommodate powder diffraction data [4] is proving to be a powerful one for solving the structures of polycrystalline materials. A variety of structures have been solved, but as the program is relatively new, the selection of the values for the input parameters has been rather arbitrary. Consequently, a systematic study of the effect of the different parameters on the structure solution was undertaken. Several aspects were investigated: (1) the effect of the input parameters themselves, (2) the effect of data resolution, and (3) the effect of including information from other sources. In parallel, criteria for identifying the better solutions were sought.

As it was not considered to be sensible to test all combinations of all parameters, a more pragmatic approach was followed. Combinations of input parameters chosen to fall into what were thought to be sensible ranges were tested. The parameters were: (1) the reflection overlap factor (κ), (2) the isotropic atomic displacement factor (B_{iso}), (3) the cycle for starting the repartitioning of overlapping reflections and the repeat interval, and (4) the threshold value for charge flipping (δ). To investigate possible differences between inorganic and organic materials, the tests were performed on the zirconium phosphate (ZrPOF-Q1) [5] and on D-ribose data [6].

The structure of ZrPOF-Q1 was originally solved using *Superflip*, but the solutions lacked locations of a few of the Zr, P and O atoms in the zirconium phosphate layers and of the quinolinium ions between the layers. Furthermore, the presence of a center of symmetry only became apparent during the refinement. With optimized input parameters, the centro-symmetric space group was recognized by *Superflip* and complete zirconium phosphate layers could be found in the electron density map. Diffuse clouds of electron density between the layers (quinolinium ions) were apparent.

The structure of D-ribose was solved using a combination of simulated annealing and difference Fourier analysis. None of the initial tests of the *Superflip* input parameters yielded a structure solution. Reasoning that starting with more realistic set of phases might help, possible models were generated using the direct-space program FOX [7]. None of these were correct, but by using the phases calculated from a flexible model to generate starting phase sets, and varying the input parameters once again, a set of optimal parameters could be found, and easily interpretable electron density maps with the correct symmetry generated.

In both cases, the optimization procedure was repeated for lower resolution data. For ZrPOF-Q1, the structure could still be solved with 1.8 Å data, and for D-ribose, with 1.18 Å data. Recognizing the best solutions from *Superflip* remains a challenge, but a cluster analysis of the solutions looks promising and is currently being investigated more carefully.

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More reliable intensity extraction from powders using texture

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