MS46-O3 **Advances in TALP, a direct-space LS strategy for solving molecular crystals from powders.** Jordi Rius, Oriol Vallcorba, Carles Frontera, Carles Miravitlles. *Institut de Cičncia de Materials de Barcelona, CSIC, Catalunya (Spain)*.
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Powder diffraction is a powerful tool for solving crystal structures when no single crystals are available. For molecular compounds, direct-space methods are often necessary due to the limited useful *d*-spacing interval and to the severe peak overlap, especially for laboratory X-ray data. Most direct-space strategies are based on Monte Carlo/Simulated Annealing optimization algorithms and have been the subject of recent reviews [1,2].

Here, progress on the application of the direct-space multisolution strategy TALP[3] to powder data of molecular compounds is presented. This strategy involves a search part coupled to fast least-squares (FLS) minimizations of atomic coordinates. The observations are pseudo-integrated intensities extracted from the pattern by a three-step procedure[4] and the molecular model is defined in terms of atomic coordinates, distance restraints and free rotation bonds (FRB). The model can be derived either from calculations or from similar reported structures and, in principle, no conformational information is required. Several independent trials, each one supplying a crystal structure proposal with an associated figure of merit, are developed. Each trial consists of (i) a general scan where random or assisted explorations over the whole unit cell are carried out, and (ii) a sophisticated local refinement around that position, orientation and conformation of the model found in the general scan.

Recently, the assisted exploration mode (AEM) has been implemented. It is intended for large molecules having a known rigid part that can be entered in Patterson search calculations. The AEM is applied during the general scan and uses the rotation function to find the most probable orientations of a model fragment in the unit cell. Also, the search parameters and the overlap prevention system have been optimized resulting in a big performance improvement: Between 2 and 10 times improvement in both speed and success ratio, based on tests with reference crystal structures. The speed and success of the solution process depends on the overall complexity of the structure, i.e. on the number of FRB (conformational freedom), the number of refined parameters (molecular size) and the quality of the diffraction data. Presently, TALP solves structures containing a maximum of 11 torsion angles, 91 refinable parameters and with Z' < 3 from laboratory x-ray diffraction data in reasonable times (from 3 minutes to 1 day).

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Keywords: Powder x-ray diffraction; ab-initio structure determination; molecular compounds

MS46-O4 **Modulation Enchanced Diffraction - from Theory to Experiment.** Dmitry Chernyshov[a] , Wouter van Beek[ab], Hermann Emerich[a], Atsushi Urakawa[c], Luca Palin[b], Marco Milanesio[b], Rocco Caliandro[d], Davide Viterbo[b], *[a]Swiss-Norwegian Beamlines at ESRF, BP 220, Grenoble, 38043, France, [b]Dipartimento di Scienze e Tecnologie Avanzate and NanoSistemi IC, Universita del Piemonte Orientale, Via Michel 11, Alessandria, 15121, Italy, [c]Institute of Chemical Research of Catalonia (ICIQ), Av. Pad'sos Catalans, 16, Tarragona, E-43007, Spain, [d]Institute of rystallography, CNR, via Amendola, 122/o, Bari, 70126, Italy*
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Modulation-enhanced diffraction (MED) is a new method to extract the individual contributions to the diffracted intensity from subsets of atoms of the crystal structure based on a periodic perturbation of the scattering process (Fig. 1). The theory of MED [1] is recalled and discussed in comparison with other methods for untangling the scattered intensity such as MIR and MAD. Simulated results and experimental data collected with help of powder diffraction [2,3] are presented illustrating advantages and drawbacks of the novel modulation technique for structure solution and refinement.

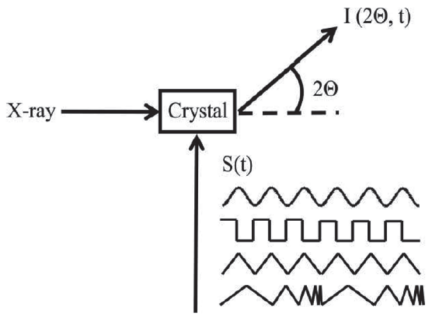

Fig. 1 A scheme of MED experiment. Scattering density is subjected by external periodic modulation, S(t). This modulation is correlated with detected intensity in order to extract structural information on the changing part of scattering density.

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Keywords: Modulation Enhanced Diffraction; powder diffraction; interference