s10.m1.o1 **New Aspects of Direct Space Structure Solution from Powder Diffraction Data.** K.D.M. Harris, E. Tedesco, R.L. Johnston, G.W. Turner, B.M. Kariuki, *School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT, U.K.*
Keywords: powder diffraction, structure solution, genetic algorithm.

Many solids can be prepared only as microcrystalline powders and are therefore not suitable for structural characterization by conventional single-crystal diffraction methods. For such materials, it is necessary to tackle structure determination using powder diffraction data. Although traditional techniques for structure solution from powder diffraction data have been applied successfully in many cases, organic molecular crystals represent a particularly challenging case. For these reasons, we are focusing on the development, implementation and optimization of new methods for structure solution from powder diffraction data, with particular emphasis on tackling the specific challenges encountered for molecular crystals. Our methods are based on a direct-space strategy in which a hypersurface defined by the profile R-factor (R_{wp}) is searched using Monte Carlo or Genetic Algorithm techniques, with particular recent focus on the Genetic Algorithm technique. In addition to the application of these methods to tackle structure solution problems for a range of materials of academic and industrial interest, we are carrying out systematic explorations to find the optimum ways of implementing the different operations (such as mating, mutation and natural selection) within the Genetic Algorithm technique. Recently, we have also been exploring approaches in which information on the energies of trial crystal structures is blended within our consideration of the powder diffraction data, as well as other developments in the fundamental methodology.

The lecture will provide an overview of the current opportunities for structure solution of molecular crystals from powder diffraction data, with some emphasis on recent developments and optimization of the Genetic Algorithm technique described above. Recent results obtained from the application of this method to solve structures of molecular crystals will be presented, encompassing examples from different areas across the solid state and materials sciences.

s10.m1.o2 **Sructure solution from powder data with accidental overlap.** J. Rius, X. Torrelles, C. Miravitlles. *Institut de Ciència de Materials de Barcelona (CSIC), Campus de la UAB, 08193 Bellaterra, Catalunya, Spain.*
Keywords: direct methods, structure solution, powder data.

Accidental overlap constitutes one of the principal limitations for the solution of crystal structures from powder diffraction data, since it reduces the number of available intensities for the direct methods application. In this contribution, the application field of the direct methods sum function is extended to cope with powder patterns with a relatively large amount of accidental overlap. This is achieved by refining not only the phases of the structure factors but also the estimated intensities of the severely overlapped peaks during the structure solution process. This procedure has been specifically devised for compounds with uncertain cell contents and with probable large atomic disorder, a situation often found when studying complex minerals with limited crystallinity. It has been successfully applied to the solution of the previously unknown crystal structure of the mineral tinticite [1]. Finally, an estimation of the smallest ratio (number of observations-to-number of variables) for the procedure to be successful is also given.

[1] Rius J., Louër D., Louër M., Galí S., Melgarejo J.C., Eur. J. Mineral. 2000,12,000-000: Structure solution from powder data of the phosphate hydrate tinticite.