Crystal Structures from Powder X-ray Diffraction using Genetic Algorithms

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Contemporary advances of direct space strategies in solving crystal structures directly from powder X-ray diffraction data [1,2], and in particular, the success of the Genetic Algorithm method [3], have opened up a whole area of research which has hitherto been inaccessible even as recent as fifteen years ago. Applications to the study of synthetic products *in situ*, as well as the tackling of structural problems which have the complexity of more than one molecule in the asymmetric unit, are now at the forefront of these techniques. In addition to tackling such new challenges, structure solution strategies employing other analytical or computational methods have become a natural complement alongside the X-ray diffraction data. For example, multi-component molecular co-crystals have been prepared by an *in situ* solid state grinding process, yet have been solved using a combination of powder X-ray diffraction and solid state NMR techniques [4]. Moreover, the collection and assessment of reliable powder diffraction intensity prior to structure solution calculations is an avenue of study that shows considerable promise [5].

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