Keywords: computing method, Monte Carlo treatment, molecular replacement

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Optimization of Genetic Algorithm Techniques for Powder Structure Solution

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With advances of direct space strategies for structure solution from powder X-ray diffraction data [1,2], and in particular the success of the Genetic Algorithm method [3], structural problems in a variety of fields are being tackled using information from powder data. Applications to study the structures of increasingly complex molecules present new challenges. Increasing the number of degrees of freedom leads to a concurrent increase in the size of the search space. Implementing a combination of other figures of merit, such as energy together with R-factor, provides an opportunity for optimization of the search space, leading to enhanced rates of success of structure solution. Systematic testing results show that the method is both general and applicable to a number of different problems without a simultaneous increase in computational time required.

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Keywords: powder structure determination, computing in crystallography, crystal structure solution

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Removal of the Phase Problem by the Atomicity Assumption

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In the late twenties Ott[1] showed that, once the atoms are treated as point-like objects, the positions of the atoms present in the unit cell of an ideal crystal are the roots of a set of polynomial equations whose coefficients are determined by a finite set of unitary structure factors. This result was later generalized by Avrami[2] showing that the positions of the peaks of the infinitely resolved Patterson map are the roots of a system of polynomial equations determined from the knowledge of a finite set of reflection intensities. Ott's results were later rediscovered and generalized[3] within the framework of Goedkoop's vectorial formulation of the phase problem. The point missing in these analyses is the algorithm able to select the (smallest) set of the reflections such that the corresponding intensities determine a resolvent system of polynomial equations. This problem was fully solved recently in the case of x-ray scattering[4] and, in this contribution, the proof is extended to the case of neutron scattering.

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