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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