HUNTER: A Package of small Tools to Manipulate FOX

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The HUNTER package consists of a number of small programs for handling the .xml-input files of the simulated annealing program FOX [1]. By use of simple scripts HUNTER allows to set up genetic algorithm techniques [2] for crystal structure determination. In this context the simulated annealing serves as Lamarckian [3] component of the evolution process. The package can also be used to explore possible neighboring minima to a current local minimum of the structure cost function. This is accomplished by sophisticated application of reorientations of randomly chosen molecules or building groups.

The individual tools currently available are: MATE, which produces a new file from two parent files by choosing randomly position, orientation and content of each molecule (or atom) from one of the parent files. ORIENTATION locates the main axes of a random molecule and applies a randomly chosen reorientation of twofold symmetry. DEFORMATION applies a rotation to a randomly chosen group of atoms using a user-defined list of groups and rotation axes. FITNESS extracts the cost function from the files written by FOX and stores it into the .xml-file, using either the current cost minimum or an exponentially extrapolated value. SELECTION sorts structure files by their fitness. Additional programs will complement the package.

[1] Favre-Nicolin V., Černý R., *Z. Krist.*, 2004, **219**, 847. [2] Harris K.D.M., Habershon S., Cheung E.Y., Johnston R.L., *Z. Krist.*, 2004, **219**, 838. [3] Turner G.W., et al., *Chem. Phys. Lett.*, 2000, **321**, 183. **Keywords: structure solution, software, powder diffraction**