

## INDEXING POWDER DIFFRACTION PATTERNS WITH THE DICHOTOMY ALGORITHM

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The objective of pattern indexing is the determination of dimensions and symmetry of the unit cell from the one-dimensional data available in a powder diffraction pattern. It is a basic requirement in most applications of the powder diffraction method, such as *ab initio* structure determination from powder diffraction data of varied kinds of materials, including pharmaceutical compounds. A representative example was the structure determination of a metastable polymorph of piracetam (Louër *et al.*, *Acta Cryst.* B51, 182, 1995). The pattern indexing approach discussed here is the successive dichotomy method (Louër & Louër, *J. Appl. Cryst.* **5** 271, 1972), for which the currently used computer program is DICVOL91 (Boultif & Louër, *J. Appl. Cryst.* **24**, 987, 1991). The method is based on the variation, in direct space, of the lengths of cell edges and inter-axial angles by finite ranges, which are progressively reduced according to a dichotomy algorithm. The absolute error on peak measurements is incorporated in the procedure. With this strategy, solutions are searched exhaustively in a  $n$ -dimensional space (from  $n = 1$  for cubic to  $n = 6$  for triclinic). In a new version of the program additional facilities have been implemented. They include (i) a tolerance with respect to spurious lines, (ii) a refinement of the zero-point position, (iii) a reviewing of all input lines from the solution found from, generally, the first 20 lines, (iv) a cell analysis based on the concept of reduced cell and (v) an optional analysis of input data to detect the presence of a zero-point error in data collection, to be used prior the indexing procedure. With the increasing performances of PCs, new strategies have also been implemented to limit the risk to miss a solution, e.g. each lattice symmetry is analyzed independently using a volume partition extended up to the input volume limit (default value: 2500 Å). With such a strategy the lattice metric singularity occurring with hexagonal lattices is more clearly pointed out. The introduction of the automated reviewing of all available powder data is an aid to space groups derivation. These improvements will be presented and illustrated by examples. Problems and limits encountered with some pharmaceutical compounds (e.g. short or long axis, intrinsic diffraction line broadening) will be discussed.