In addition to structural parameters, the program can refine lattice constants, a linear 20 correction, peak half width and asymmetry, and preferred orientation. It can also handle the broadening of individual lines due to crystallite shape or lattice strain. The data input is kept to a minimum and is partly in free format. At the moment the program requires strictly monochromatic diffractometer data, which are necessary to achieve good resolution. Neutron data can also be employed.

The programs have been successfully tested in a number of different structure refinements including that of zeolite ZSM-5. This zeolite has an orthorhombic structure with a cell of 20x20x13 Å³ and 134 positional parameters. The X-ray data were supplemented with 165 distance and angle constraints.

12.5-03 ANALYSIS OF TIME-OF-FLIGHT DATA FROM A RESOLUTION FOCUSED NEUTRON POWDER DIFRACTOMETER. By B.B. Von Dreile., Department of Chem., Ariz. State Univ., Tempe, Ariz. 85281 and A. R.B. Programming (1975), 9, 1-30. The latter is less sensitive with respect to high correlation since it uses a positive definite matrix with elements converging towards the second order derivatives of the function. This greatly improves the behavior around ill-defined minima, which are frequently encountered in the Rietveld method (R.A. Young (1980), NBS Special Publication 567, 143-162).

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