17.2–12 SIMPEL 83, A NEW VERSION OF THE SYMBOLIC ADDITION BASED PROGRAM SYSTEM FOR DIRECT METHODS.
By C.Th. Kiers and H. Schenk, Laboratory of Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

The program system SIMPEL is a complete direct-methods system, which starts from |F|-values and may end with an E-map of the structure. The heart of the system is constituted by a series of routines, which successively determine a good starting set, carry out a symbolic addition process, determine the correct numerical values of the phases, and carry out a final phase extension and refinement.

The special features of SIMPEL include the use of quartet relationships for the identification of an optimum starting set, the use of the symbolic addition principle, and the use of many Figures of Merit (FOM's) to determine the correct values of the symbols. In SIMPEL 83 we have extended the number of FOM's, while it is also possible now to calculate FOM's after tangent refinement to compare the extended phase sets of some promising solutions.

The old version of the program was only suitable for CDC computers. The new version is developed to run on various other computers too and is very user friendly. The structure determination package (SDP) of Enraf-Nonius, Delft, contains a centrosymmetric version of the program.

SIMPEL is very fast and has excellent interactive facilities. We intend to show the new version of the programme system on a DEC-professional personal computer.

For a recent survey see H. Schenk in Recl. Trav. Chim. Pays-Bas, 102, 1 (1983).

We are indebted to the Netherlands Foundation of Technical Research (STW) for their financial support of this project.

17.2–13 A HEROIC APPROACH TO THE SOLUTION OF DIFFICULT CENTROSYMMETRIC STRUCTURES
by Eric Stanley, Physics Department, University of New Brunswick, Saint John, N.B.,Canada.

All correct structures have the following characteristics: 1) the electron density never goes very negative, 2) the electron density never rises above that expected at the centre of the atom with the greatest atomic number, 3) the low resolution electron density has all the major features of the fully refined high resolution structure and 4) the atomic bond length and bond angles are within the expected range.

By applying an artificial temperature factor the number of structure factors of significant magnitude is reduced. All possible sign combinations are used to calculate the electron density at one point in the unit cell. All combinations violating the limitations imposed by 1) and 2) above are rejected. The electron density is then calculated for all the remaining sign combinations at a second point in the cell and further sign combinations rejected. In this way, instead of getting the correct set of signs, the incorrect sets are rejected. As the number of remaining combinations gets smaller, the artificial temperature coefficient can be reduced and additional terms added. Eventually sufficiently large numbers of terms will be included to determine the structure. At this stage the sign combinations remaining can be used as the starting point for objective refinement by maximizing the peakiness (Stanley, 1979) and the refined solutions examined for peak heights and bond distances.

Any solution not meeting the chemical criteria is rejected leaving only those solutions which are both physically and chemically plausible. In favourable cases the only solution remaining is the correct solution.

Stanley, E. (1979) Acta Cryst. A 35, 966

17.2–14 ADVANCES IN THE SIR PROGRAM

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The SIR program has proved to be an effective tool for solving difficult structures. One-phase and two-phase, seminvariants, triplet and quartet are used in a cooperative way to overcome the problem arising from few bad estimates.
A new weighting scheme for the tangent formula based on the distribution of α_h has been introduced (Giacovazzo et al. Acta Cryst, A40,000).
The estimates of triplet invariants are made by using their second representation.
At the same time negative triplets are found with sufficient accuracy to be successfully used as a figure of merit together with the one-phase and two-phase seminvariants, the R-karle criterion, the negative quartet figure.
Examples of the application of the SIR will be shown.