17.2-11 A RANDOM APPROACH TO CRYSTAL STRUCTURE DETERMINATION. By J. P. Declercq and G. Germain, Laboratoire de Chimie Physique et de Cristallographie, Université de Louvain, Louvain-la-Neuve, Belgium, and M M Woolfson and H Wright, Department of Physics, University of York, Heslington, York YO1 5DD, U K.

It has been found (Baggio, Woolfson, Declercq, Germain, Acta Cryst. (1978). A34, 883) that triple-phase relationships treated as linear equations can be used to refine a set of initially random phases, the 70 - 100 refined phases being used as a starting point for development by the tangent formula. The least-squares method used in refinement is subject to difficulties in weighting the equations and problems arising from the singularity of the matrix can occur. Investigations of alternative methods of refinement show that the method of steepest descents is successful in circumventing these difficulties whilst retaining the advantages of the large starting set method. Novel approaches are made possible by the easier application of weighting schemes and the process is computationally economical. Illustrations are shown using output generated by the distributed program YZARC which optionally uses either method of refinement.

17.2-12 RANTAN - RANDOM MULTAN. By Yao Jia-xing, Department of Physics, University of York, YO1 5DD, England. Permanent address: Institute of Biophysics, Academia Sinica. Peking China.

To overcome the disadvantages of a small starting set in MULTAN a technique called RANTAN is described. A large number of phases are given random values associated with low weights and then refined, together with reflexions fixing origin and enantiomorph, by a weighted tangent formula. An initial random phase is not changed until a phase estimate is obtained with a new weight greater than the initial weight. Then the phase is allowed to vary and to follow its refinement path. In the present method it is possible simultaneously to work with all the reflexions and all the relationships ab initio. More than 20 structures, which represent a wide variety of space groups, structural complexity and difficulty, have been successfully solved by RANTAN. One example is a difficult unknown structure containing 100 atoms in the asymmetric unit with space group $P2_1$. The first E-map, with very good figures of merit, showed 85 atoms. The experimental results have shown that it is possible to use RANTAN to determine more complex structures which contain more than 100 atoms in the asymmetric unit.
Another application of RANTAN is its use with a partial structure, like Karle recycling. The known phases coming from a partial structure are combined with random phases and then RANTAN is run as usual. Normally only 10% of a structure is enough to develop it completely.

17.2-13 MAGEX - A PROCEDURE FOR PHASE DETERMINATION. By S. E. Hull, D. Viterbo, M. M. Woolfson and Zhang Shao-Hui, Department of Physics, University of York, Heslington, York YO1 5DD, U K.

This procedure extends and strengthens the PS method (Declercq, Germain and Woolfson, Acta Cryst. (1979)). Long one-dimensional magic-integer sequences are used to express the phases of from 5 to 20 primary reflexions. A new concept of multiple definition of secondaries is employed and the error involved in their subsequent application in a conventional ψ map is thus much reduced. A parameter-shift process, which is based on one or other of two functions, is used to refine 200 sets of from 40 to 100 phases and a number of the best sets of refined phases is selected. A facility is available for limited multi-pathway phase extension before large-scale phase extension by the controlled use of the tangent formula is undertaken. Examples of successful applications of MAGEX are described.

17.2-14 STRENGTHENED TRANSLATION FUNCTIONS: FINDING THE POSITION OF A SMALL, KNOWN FRAGMENT BY SEARCH METHODS IN DIRDIF-FOURIER SPACE. By H.M. Doesburg and P.T. Beurskens, Crystallography Laboratory, Toernooiveld, 6525 ED Nijmegen, The Netherlands.

A frequently occurring problem in the determination of crystal structures is the positioning of a correctly oriented molecular fragment, relative to the symmetry elements or relative to another known molecular fragment. Knowledge of the orientation of a fragment may be available from:
- Patterson rotation search techniques.
- Direct methods, when a recognizable fragment is found from an otherwise obscure E map.

The present translation method is essentially a convolution of a known, correctly oriented, 'search' fragment with a DIRDIF electron density map
(Van den Hark, Th.E.M., Prick, P. and Beurskens, P.T. Acta Cryst. (1976) A32, 816-821).
Definitions: ρ_p is the electron density of the known fragment and $F_p(\underline{h})$ are the calculated partial structure factors. ρ_r is the electron density of the unknown part of the structure and $F_r(\underline{h})$ are the corresponding structure factors obtained by DIRDIF, using the known fragment as input. ρ_{ps} is a symmetry related image of ρ_p.
The translation function is defined as

$$Q(\underline{q}) = \iiint_{xyz=0}^{1} \rho_{ps}(\underline{r}-\underline{q})\ \rho_r(\underline{r})\ V dx dy dz$$

From convolution theory it follows:

$$Q(\underline{q}) = \frac{1}{V} \sum_{\underline{h}} F^*_{ps}(\underline{h})\ F_r(\underline{h}) \exp -2\pi i\ \underline{h}.\underline{q}$$

The maximum of the Q-function gives the position of ρ_{ps} relative to ρ_r; from this the position of the symmetry element can easily be deduced.