17.2–7 SATRIX - A COMPUTER PROGRAM FOR THE APPLICATION OF DIRECT METHODS TO STRUCTURES SHOWING SUPERSTRUCTURE EFFECTS. By R. Böhme, Institut für Mineralogie, Ruhr-Universität Bochum, 463o Bochum, West Germany.

Practical experience indicates that at present problems may arise during a 'normal' direct methods procedure, if there are peaks in the Patterson function exceeding 25% of the origin peak. The program SATRIX is a complete system specially developed for the application of direct methods to those structures.

The superstructure effects - i.e. the sets of systematically weak and systematically strong reflexions in reciprocal space - are viewed as pseudotranslations in direct space, which can be obtained directly from a list of the highest peaks of the Patterson function. Up to three independent pseudotranslations of type 1 or 2 can be handled (Böhme, Acta Cryst. (1982), A38, 318) or one pseudotranslation of type 3 (Böhme, Z. Naturforsch. (1983), 38a, 3o4). Triplets containing weak and strong reflexions together can be excluded from the phase determination procedure. Their symmetry-dependent phaseshifts are calculated automatically, when necessary.

The ideas are implemented in a strongly modified direct-methods procedure of the CRYSTAN system (Burzlaff, Böhme, Gomm; Erlangen 1977). SATRIX starts with $|F|$-values and ends up with a list of coordinates, distances and angles. It can be run automatically (e.g.by default value) or interactively on a large or mini computer. The program is being augmented to recognize 'dangerous' pseudotranslations automatically and to be more flexible in handling combinations of pseudotranslations of different type.

17.2–8 MITHRIL - AN INTEGRATED DIRECT-METHODS COMPUTER PROGRAM. By C.J. Gilmore, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland.

MITHRIL (Gilmore, J. Appl. Cryst. (1984) **17**, 42-46) is a direct-methods program written in ANSI 1966 standard FORTRAN IV designed to implement theoretical advances in this field, and exploit, where applicable, the opportunities presented by the new generation of mini- and supermini-computers which can run direct-methods calculations in real time.

The software is built around the MULTAN80 system, but it provides in addition:

(1) The choice of menu-driven, interactive, real-time operations or more traditional batch methods. Three levels of machine-user interaction are provided.
(2) Extensive facilities for editing and checking the raw intensity data.
(3) The MDKS formula, and a related system for estimating and editing triplets.
(4) Quartet and quintet invariants used actively in all phasing procedures, and passively as figures of merit. Quartets are used automatically in symmorphic cases, but quintets, whose use here is experimental, are always invoked explicitly by the user.
(5) Editing facilities at convergence map time. Phase relationships from symbolic addition can be included in the convergence map. The results of the MDKS calculations may also be used to edit the triplets list, and downweight or remove suspect relationships.
(6) YZARC and MAGEX. Quartets are used as well as triplets in YZARC, and there are extra figures of merit
(7) Conventional tangent refinement or random phase tangent refinement. Quartets and quintets may be used here in an active way.
(8) Five figure of merit,including NQEST and an index based on negative quintets.
(9) An integrated E-map package with optional computer graphics for displaying the interpreted maps.
(10) Four types of fragment recycling - Fourier methods, Karle recycling, Karle recycling with random phases for the unknown phases, and the use of groups of known or random position and orientation in the cell.
(11) Sharpened, origin-removed Patterson maps using $E^2 - 1$ as coefficients.

The package is designed for a computer which provides 32-bit FORTRAN words, and a minimum of 1/2 Mbyte of addressable memory.

The software has been designed to be easy to use for the non-expert, and yet provide a wide range of facilities and control for expert users. To this end, it provides suitable defaults for all options . There are three levels of default ranging from the standard to levels which invoke more rigourous demands. These levels may be changed as the user proceeds. The program is split into modules :
NORMAL(normalisation), TRIPLET, QUARTET, QUINTET (which generate triplets, quartets and quintets respectively), CONVERGE (convergence mapping), MAGEX, YZARC, TANG(tangent refinement), RANTAN(random-phase tangent refinement), MAPS, RECYCLE and PATTERSON.

These modules are called automatically in the correct sequence, except QUINTET, MAGEX, YZARC, RANTAN and PATTERSON which need explicit calls. The user need only specify a module directly if:

(a) He wishes to change a default option in it.
(b It is a module that is not called automatically.

17.2–9 AN INVESTIGATION ON THE RELIABILITY OF THE P_7 and P_{13} QUARTET FORMULAE. By A.A. Freer and C.J. Gilmore, Department of Chemistry, The University of Glasgow, Glasgow G12 8QQ, Scotland.

It has been shown, via probability theory, that the more E-magnitudes available for quartet phase estimation, then the more reliable that estimate should be. The two simplest formulae for estimating the sign of a quartet of reflexions and its associated probability in space group $P\bar{1}$ are the 7-magnitude two neighbourhood $P_7^{\pm}$, and the 13-magnitude, three neighbourhood $P_{13}^{\pm}$. The reliability of these sign estimates, and derived probabilities, are investigated for both centrosymmetric formulae. An analysis of the invariant phase estimates gleaned from the non-centrosymmetric $P_{1/7}$ and the $P_{1/13}$ formulae is also carried out.

$P_7^{\pm}$ and $P_{13}^{\pm}$ were studied with a view to resolving the following questions:

(i) The relative reliabilities of the two formulae and which is most applicable to a given situation.
(ii) The limits of structural complexity each is capable of attacking.
(iii) The special problems associated with the third neighbourhood and with negative quartets.

With $P_7^{\pm}$ and $P_{13}^{\pm}$ the calculated invariants may be assigned only one of two values, 0 or π, and therefore appropriate constraints may be applied. In $P_{1/7}$ and $P_{1/13}$, however, there can be no such constraints, and consequently a spread of errors is expected in the final invariant estimates. How these differences in phase errors between calculated and observed phases ($|\phi_{obs}-\phi_{calc}|$) are distributed over different standard deviation intervals was investigated by considering three known structures in space groups P1, $P2_1$ and $P2_12_12_1$.