axis is calculated by LST.
2. Search for a "reference" reflection indices. For the reflection given by an experimentor the computer will choose those indices for which $\Delta H_{\perp}^{i}$ has the least value. Considering this reflection to be situated on the Ewald sphere, we find the coordinates of the centre point of the sphere and respectively, the coordinates of spheres separated by $\pm\Delta\varphi$.
3. Indexing is carried out by comparing $H_{\perp}^{exp}$ and $H_{\perp}^{calc}$ with the criteria $\Delta H_{\perp} = min$, and the signs of indices do not contravene those of X and Y in the X-ray photograph with due regard for the position of the Ewald spheres in the reciprocal space.
4. Computations of the coordinates X_i and Y_i of the computer-simulated X-ray photograph and the discrepancy factor.
5. Results of computations can be plotted or displayed and compared with experimental ones. The lattice parameters are refined by LST. The following information can be presented on the "TV" screen in one of its quadrants or on the whole of the screen: the view of the experimental or model X-ray photograph, the reciprocal lattice net of any layer line with the Ewald sphere position and that of the reflections on the given net.

The program contains 1500 statements. The time needed for the computation of an index is 1 sec using a "SM-3" computer of the third generation (~150000 operations/sec).

18.4–4 A MINICOMPUTER PROGRAM FOR THE AUTOMATIC ANALYSIS OF PATTERSON FUNCTIONS. By T.I. Malinovsky, I.F. Burshtein, and V.S. Fundamensky, Institute of Applied Physics, Academy of Sciences MSSR, Kishinev NPO "Burevestnic", Leningrad, USSR

Nearly all crystallographic program systems for use on minicomputers include programs for structure analysis by the direct method, but lack a program to analyse the Patterson function. To eliminate this deficiency, we have written a program for automatic interpretation of the interatomic vectors, compatible with the program systems XTL (NOVA-1200) and RESTAN (SM-4 and M-6000). The program algorithm is applicable to the symmetries of Patterson functions in the triclinic, monoclinic and orthorhombic systems. Essential information about the space group symmetry, unit cell parameters, and the coordinates of the peaks in the Patterson function are read automatically from the appropriate files created by the other programs in the system. Based on this information, the present program produces the atomic coordinates and interatomic distances of a molecular fragment, which in some cases may comprise more than 50% of the structure. It is possible to proceed automatically from this stage to calculation of an electron density map. Such a program may be included in any program system for structure analysis on minicomputers. Some examples of different complexity will be demonstrated.

18.5–1 USE OF THE SERC INTERACTIVE COMPUTING FACILITY FOR MOLECULAR GRAPHICS AND MINERALOGICAL STUDIES

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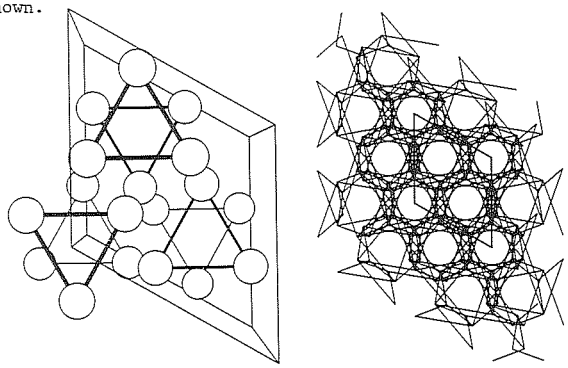
Members of the Computing Division of the Rutherford Appleton Laboratory set up and maintain a network of multi-user minicomputers for interactive working. Users of the network have access to many different types of output device, including local pen plotters and the precision III FR80 microfilm recorder. The molecular drawing program PLUTO78 has been mounted on the network, and many enhancements made in order to bring a powerful tool for molecular and mineral display to a large, geographically widely distributed research community. Several other display programs are currently being prepared, and sample output from these will be shown.



18.5–2 COMPUTER GRAPHICS OF POLYHEDRAL PACKINGS. By R. Norrestam, Chemistry Dept. B, Technical University of Denmark, DK-2800 Lyngby, Denmark.

The packing of coordination polyhedra is often used to visualize inorganic crystal structures. Frequently, pictures of such packings are simply photographs of models constructed by assembling idealized colored plastic polyhedra (see e.g. S.Andersson, Acta Cryst. (1980) B36, 2513). With the use of a high resolution raster display it is possible to obtain such pictures of comparable quality and showing the correct polyhedral geometry.
A computer program, POLY, for applying color raster graphics has been developed and some examples of the results from this program will be described. POLY is written in standard FORTRAN language, with a few supplementary color plotting routines from the UNIRAS software system.