axis is calculated by LGT.

2. Search for a "reference" reflection indices. For the reflection given by an experimenter the computer will choose those indices for which $\Delta H^i$ 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 $\pm \Delta H^i$. The indexing is carried out by comparing $H^i_{\text{exp}}$ and $H^i_{\text{calc}}$ with the criteria $\Delta H^i = mH^i$ 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.

3. 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 least squares.

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 "SUN-5" computer of the third generation (~50000 operations/sec).

### 18.5-2 COMPUTER GRAPHICS OF POLYHEDRAL PACKINGS

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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.