(9) A high-speed peak intensity measurement procedure, which is valuable in space-group determination and in selecting suitable reflections for cell refinement before data collection; in some cases, it can also serve as a means of collecting a rough preliminary data set.
(10) Intensity data collection by a profile-fitting technique (W.Clegg, Acta Cryst.(1981) A37, 22) to give high precision at high speed.
(11) Variation of counting times to give approximately constant-precision intensity measurements.
(12) Special optional routines, integrated into the data collection, for azimuthal scans and Friedel pair measurements.
(13) Monitoring of crystal orientation, with automatic corrective action if it changes significantly.
(14) Flexible handling of a multi-purpose reflection list.

Local computing considerations dictated the use of BASIC as the program language on a Data General Eclipse S/250 mini-computer, diffractometer operation being time-shared with structure determination (Fortran programs), plotting, and other BASIC users.
The total diffractometer time required for a crystal, including setting up for data collection, is about 1.5 hours per independent non-H atom, giving a turnround of 2-3 medium-sized structures per week. Final R indices for crystals of medium to high quality are typically 0.03-0.06.

16.2-02   RUBY SPHERES FOR ALIGNING SINGLE-CRYSTAL DIFFRACTOMETERS. By L.D. Calvert, E.J. Gabe and Y. Le Page, Chemistry Division, N.R.C., Ottawa, Canada, K1A 0R6.

A standard crystal for the calibration of single-crystal diffractometers should ideally have the following properties. It should have long-term chemical stability and no phase transition over a wide range of temperature. It should be insoluble in most solvents and not be subject to radiation damage. It should have high diffracting power, even at high 2θ angles and have many symmetrically equivalent reflections. It is most important that the material should be readily available as single-crystal spheres of suitable diameter. Pure α-Al_2O_3 (corundum) satisfies all these criteria except its availability as spherical crystals. However, synthetic ruby spheres (α-Al_2O_3 with small amounts of Cr) are commercially available.

The organizing committee of the present Congress has obtained a supply of such spheres (0.15 mm diameter) to distribute to participants at the Congress and thereafter on receipt of written requests. The cell data for corundum are well known (N.B.S. (U.S.) Circ. 539, 9, 3 (1960)). Cell and structural data relevant to the particular ruby spheres will be given at the Congress and distributed with the spheres.

16.2-03   A NEW MICROPROCESSOR-BASED AXIS POSITIONER. By Kenneth Baldwin, William Huebsch, and Charles Prewitt, Dept. Earth & Space Sci., SUNY at Stony Brook N.Y. 11794, USA

A new, general-purpose, programmable axis positioner suitable for use in x-ray diffractometry is under development. The positioner makes use of a commercially-available Z80A-based single card computer with programmable ROM firmware for long range versatility and adaptability.
An external clock and associated circuitry will be added to provide programmable speeds ranging from 0.1°/min to 6.0°/sec and ramped slew. The positioner is capable of performing incremental and absolute positioning up to a maximum rotation of 360 degrees. When used with a five-phase stepping motor in half-step mode, the resolution for a conventional diffractometer axis is 0.001 degrees.
Communication to and from the positioner is in ASCII via an RS232 serial line at programmable speeds of 110 to 9600 baud. A simple command string structure has been implemented to allow off-line control from a terminal as well as on-line control from a host computer.
By clustering multiple positioners with a communications priority, only a single RS232 serial line is needed to control all axes simultaneously. In addition to conventional diffractometry, this axis positioner concept can be used in any application requiring control of stepping motors, such as for equipment on a synchrotron beam line.

16.2-04   EFFECT OF SCAN TYPE ON INTEGRATED INTENSITY. By. R.G. Hazell, F.K. Larsen, S. Kræmmer, Department of Chemistry, Aarhus University, DK-8000 Aarhus C, and B. Lebech, Physics Department, Risø National Laboratory, DK-4000 Roskilde, Denmark.

For a crystal with large mosaic spread an ω-scan gives a higher integrated intensity than a θ-2θ scan at moderate θ. This has in some cases led us to collect data using the ω-scan technique. In neutron diffraction where the collimation before and after the monochromator allows a fairly large wave length spread the counter aperture is only wide enough to accept all of the diffracted beam at low θ-values. Comparison of ω and θ-2θ data from the same crystal collected at Risø, DK, shows a constant ratio between the two data sets for $0<\theta\leq30°$ but for $\theta>30$ the ratio falls, and our data in the range $30<\theta<55°$ show a linear fall off with θ or with $\tan\theta$. The point where the cut off starts and its slope depend on the apparatus, the size of the sample and possibly its mosaicity. A least-squares refinement with two extra parameters to describe this permitted a satisfactory refinement using the ω-data. Sequeira (Acta Cryst. (1974) A30, 839) gives formulae which, if all collimations and mosaicities are known, allow the calculation of the intensity loss for any scan type. The collimators are, however, assumed to give Gaussian intensity distributions which is not fulfilled by our open tubes and only a qualitative agreement with the experiment is obtained. We attempt to use the resolution ellipsoid approach of Lebech and Nielsen (Abstracts, Petten, 1975, p. 467) to illustrate the problem and calculate numerically the loss for non-Gaussian collimators for different scan directions. Failure to take the loss of intensity into account leads to incorrect thermal parameters, unless the θ-2θ scan technique is used and the mosaicity is small or isotropic. The error is worst for neutron data but can also be important in the X-ray case.