Table 1. *Efficiencies of precession and oscillation cameras without layer-line-screens*

	Precession angle					Oscillation angle				
	1·0°	1·5°	2·0°	2·5°	3·0°	±1·0°	±1·5°	±2·0°	±2·5°	±3·0°
1. Reciprocal lattice points registered on film	1528	2356	3188	3952	4732	1002	1486	2002	2558	2990
2. Rejected because of overlap effects	0	0	127	1300	2716	0	0	192	720	1270
3. Rejected because of edge effects	1020	974	903	506	628	794	830	844	790	728
4. Measurable intensities remaining	562	1382	2158	2166	1386	208	656	966	1048	992
5. Efficiency (ratio of line 4 to line 1)	35%	59%	68%	52%	29%	21%	44%	48%	41%	33%

the X-ray beam, and moved through the indicated precession or oscillation angle. All reflections out to a minimum Bragg spacing of 2·25 Å were indexed. These results show that precession geometry is somewhat superior to oscillation geometry both in the fraction of reflections that are measurable and in the number of these recorded per film. Since exposure time is approximately proportional to the total volume of reciprocal space swept out, or equivalently to the total number of reflections registered on the film, regardless of camera geometry, the precession camera will produce data faster; and since each additional film requires an additional scale constant to be evaluated, the precession camera will yield a full three-dimensional set of data with fewer scale constants.

As a preliminary experimental check, a number of precession films, actually taken without layer-line screens, have been successfully indexed for three different proteins being studied in this laboratory. It has been found that spots may deviate as much as 0·3 mm from their theoretical positions, but this presents no serious problem since the deviation is systematic and may be compensated for by the program. In addition, one set of films, for chymotrypsinogen, has been processed to yield integrated intensities of 1698 reflections. These were found to agree with the corresponding diffractometer measurements to within 6%, on the average.

Finally, let us consider a possible, though not optimum, strategy for collecting a full set of intensity data to 2·25 Å by the method advocated here. In the case of chymotrypsinogen, again, we see from Table 1 that a set of 2° precession films will yield intensity measurements for about 2100 reciprocal lattice points. A sequence of 30 nonoverlapping exposures, at suitable intervals of the spindle dial, will then record $6·3 \times 10^4$ different reciprocal lattice points. This represents 57% of all $1·1 \times 10^5$ reciprocal lattice points under consideration. Three such sequences of exposures,

taken for example in sets about three different crystal axes, would then leave only $(1-0·57)^3$ or 8% of the reciprocal lattice points unrecorded. These may either be ignored, or measured individually with a diffractometer. Note also that each reciprocal lattice point will have been recorded, on the average, $(6·3 \times 10^4 \times 3)/(1·1 \times 10^5) = 1·7$ times, providing a replication number of about 7, on the average, for each unique intensity. We have found, in practice, that exposure times of 8 hours, with 2° precessions, produce spot densities equivalent to those obtained with 40-hour exposures in the conventional 21° precession with layer-line screen. Thus, the total camera time required to obtain the desired 90 exposures should be about one month. Since an automated photometer can easily handle the output of several cameras, it appears that not more than 2 months (instead of 20) should be adequate to accomplish the data acquisition task set out at the beginning of this communication, and in the process almost 4 times as many replications of each unique intensity will be obtained as well. It is also worth noting that the capital outlay required for equipment will be less than half that for an automatic diffractometer, that all intensity data will be obtained with crystals that have been exposed to X-rays for a maximum of 8 hours, and that absorption errors will be minimized because of the small precession angle.

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A graphical aid to indexing of reflections on 3- or 4-circle diffractometers.

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A method is given whereby two- and three-dimensional representations of the reciprocal lattice of a crystal can be derived from measured diffractometer angular coordinates $\varphi, \chi, 2\theta$.

Busing & Levy (1967) have recently presented equations for angle calculations related to the operation of 3- and 4-circle diffractometers. They indicated numerical methods for initial determination of orientation parameters and cell dimensions. In connection with these initial steps a technique using a graphical interpretation of some of the procedures has been found to be useful, particularly in cases where accurate reciprocal cell dimensions have not been
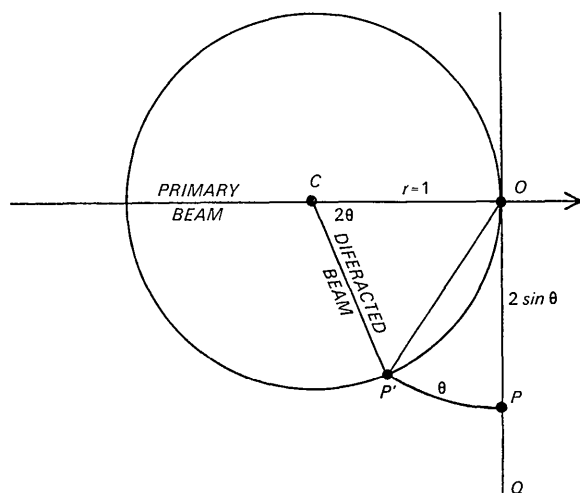
Fig. 1. Representation of the equatorial plane of the diffractometer. *C* is a crystal at the center of the instrument; *O* is the origin of the reciprocal lattice.
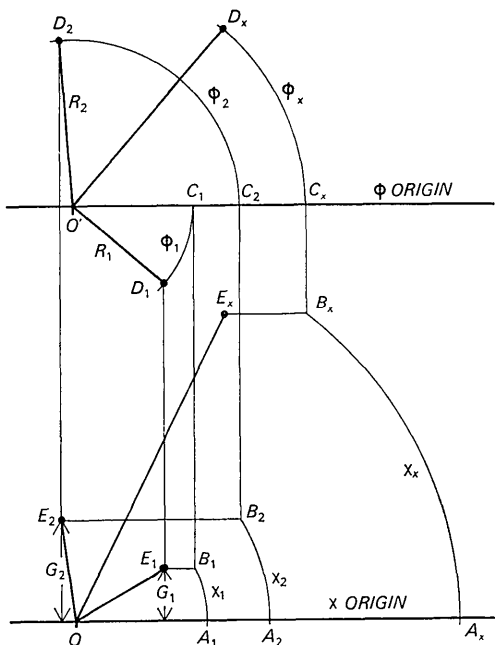

Fig. 2. Graphical representation of the φ and χ setting operations. Points D_x and E_x result from the vector operations $2(O'D_1+O'D_2)$ and $2(OE_1+OE_2)$ respectively. [Clearly, another lattice point is defined by $(O'D_1+O'D_2)$ and (OE_1+OE_2).]

determined and where the shape of the crystal does not reveal any crystallographically important direction.

The purpose of our graphical representation is to obtain two projections showing the positions of reciprocal lattice points when all instrument angles are at their zero points, and from projections of 'derived' points (*vide infra*) to determine their φ, χ and 2θ coordinates.

A brief review of some geometrical characteristics of the 3-circle diffractometer is appropriate. Let Fig. 1 represent the equatorial plane of the diffractometer. A reciprocal lattice point P is situated on the line OQ when the detector arm is at $2\theta=0°$. For an instrument with the usual $2\theta-\theta$ coupling the point P will move to the position P' on the reflecting sphere as the detector arm is moved to the appropriate 2θ position. Positioning of the crystal to give a desired reflection can therefore be accomplished by (1) rotation of the φ axis to bring the corresponding reciprocal lattice point into the plane perpendicular to the primary beam and passing through the point O, (2) rotation of the χ axis to place the point on OQ, and (3) setting of 2θ.

The graphical representation of steps (1) and (2) is shown in Fig. 2 for two 'observed' points and one 'derived'. The line marked 'χ origin' corresponds to OQ in Fig. 1. The upper part of Fig. 2 ('top view') corresponds to Fig. 1 after a 90° rotation, while the lower part ('front view') corresponds to a view along OC of Fig. 1. Assume that angular coordinates φ_1, χ_1 and $2\theta_1$ have been obtained for a reciprocal lattice point (1). To find the two projections D_1 and E_1 of point (1) when the instrument angles are at their origins, the distance OA_1 is first laid off proportional to $2\sin\theta_1$, and the operations indicated by the sequence $A_1B_1C_1D_1E_1$ are then carried out. (A three-dimensional representation can also be constructed by use of cylindrical coordinates φ_1, R_1, G_1). Similar treatment of a point (2) with coordinates $\varphi_2, \chi_2, 2\theta_2$ yields points D_2 and E_2.

Determination of $\varphi, \chi, 2\theta$ coordinates for a 'derived' point (x) can be accomplished by following a reverse path $D_xC_xB_x$ and $E_xB_xA_x$. By combination of all possible vectors between three linearly independent points (and the origin) it is possible to construct a complete reciprocal lattice from which indexing, and subsequently extinction rules *etc.* can be readily derived (due consideration being given the possibility of having found multiples of reciprocal lattice vectors). A three-dimensional representation is particularly useful for indexing purposes.

The success of the technique to some extent depends on the care with which the graphs are prepared. We have found it convenient to use a scale where one $2\sin\theta$ unit corresponds to 400 mm, and have also prepared a table giving OA in mm *versus* 2θ in degrees.

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