Table 1. *A sample of eligible triple Bragg reflections*

Space group	Crystal system	Known crystals*	Forbidden $\mathbf{h}_4$	Forbidden $\mathbf{h}_3$	Forbidden $\mathbf{h}_4-\mathbf{h}_2$	Allowed $\mathbf{h}_2$	Allowed $\mathbf{h}_3-\mathbf{h}_2$	Allowed $\mathbf{h}_4-\mathbf{h}_3$
*Ia*3*d*	Cubic	52	110	031	222	$\bar{1}\bar{1}\bar{2}$	143	$1\bar{2}\bar{1}$
*Fd*3*c*	Cubic	2	$00\bar{2}$	240	133	$\bar{1}\bar{3}\bar{5}$	375	$\bar{2}\bar{4}\bar{2}$
*Pn*3*m*	Cubic	10	012	201	120	$\bar{1}\bar{1}2$	$31\bar{1}$	$\bar{2}11$
*Pm*3*n*	Cubic	24	111	122	001	110	012	$0\bar{1}\bar{1}$
*Pn*3*n*	Cubic	0	$0\bar{1}4$	100	131	$\bar{1}\bar{4}3$	$24\bar{3}$	$\bar{1}\bar{1}4$
Pnma	Orthorhombic	402	012	021	100	$\bar{1}12$	$11\bar{1}$	$0\bar{1}1$
$P2_1/c$	Monoclinic	279	001	010	101	$\bar{1}00$	110	$0\bar{1}1$

* From Nowacki (1967).

Although no specific examples of potentially useful triple Bragg reflections are presently known, some progress has been made in narrowing the range of possibilities to be considered. The conditions on the structure amplitudes [equation (2)] are quite restrictive. Let us confine our attention to forbidden reflections that are forbidden strictly, that is, by virtue of space-group symmetry (*International Tables for X-ray Crystallography*, 1969). Then it is not difficult to show that only 5 space groups (of unfortunately infrequent occurrence) among the 10 belonging to class *m*3*m* of the cubic system can satisfy equation (2). Similarly, only 2 of the 8 most common (for inorganic crystals) space groups (Nowacki, 1967) are eligible. Unfortunately the cubic diamond structure (space group *Fd*3*m*) and the hexagonal close-packed structure (space group $P6_3/mmc$), both of which are suitable for double Bragg reflection (Kottwitz, 1968), are ruled out by the structure-amplitude conditions. For these 7 eligible space groups a limited amount of trial-and-error calculation has been done to find sets of reflections that satisfy equations (1) and (2). For each space group, a sample set of such reflections is given in Table 1, together with the crystal system and the number of known crystals (Nowacki, 1967).

References

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

JAMES, R. W. (1963). *Solid State Phys.* **15**, 53.

KOTTWITZ, D. A. (1968). *Acta Cryst.* A**24**, 117.

NOWACKI, W. (1967). *Crystal Data, Systematic Tables*, 2nd ed., p. 171. American Crystallographic Association.

Acta Cryst. (1971). A**27**, 392

Polarization factor for graphite X-ray monochromators.

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Comparison of Ni-filtered and graphite-monochromatized Cu $K\alpha$ diffraction data indicates that the 'ideally imperfect' monochromator polarization factor is not applicable.

Since graphite was introduced as an X-ray monochromator the assumption of the polarization factor being that of an ideally imperfect crystal appears to have been tacitly accepted. A communication by Miyake & Togawa (1964), however, clearly points out that for high precision work it becomes necessary to test the validity of this assumption.

After a graphite monochromator had been installed on the Picker diffractometer in this laboratory part of the initial testing consisted of a comparison of a Cu $K\alpha$ (Ni filter) and a Cu $K\alpha$ (graphite monochromator) data set from the same crystal. For the comparison to be valid the specimen crystal must be perfectly stable towards X-ray irradiation, and secondary extinction effects must be small. A filter data set (F_f) satisfying these criteria was available from a reinvestigation of *p,p'*-dichloroazobenzene (initial study by Hope & Victor, 1969.) The structure had been refined to $R=0{\cdot}032$, with $|F_o|$ being about 5% smaller than $|F_c|$ for the most intense reflection. The crystal had been removed from the diffractometer with the goniometer head attached to the mounting base, and when the assembly was remounted on the goniostat it was found that the original setting parameters could be used without change.

The Cu $K\alpha$ (monochromator) data set was collected with exactly the same settings, scan ranges and background-count times as the filter data. About 950 reflections with $I_o > 2\sigma(I_o)$ which were common for the two data sets were used for comparison of polarization factors. The monochromator intensities were first reduced to F's (F_M) by use of the polarization factor for an ideally imperfect monochromator with diffraction vector in a plane normal to the diffractometer equator, given by $p_K=(\cos^2 2\theta+\cos^2 2\theta_M)/(1+\cos^2 2\theta_M)$, where θ is the Bragg angle for the reflection under consideration and θ_M the monochromator Bragg angle (Azároff, 1955). [The corresponding expression for the 'perfect' monochromator is $p_D=(\cos^2 2\theta+|\cos 2\theta_M|)/(1+|\cos 2\theta_M|)$.]

Average normalized F_M/F_f ratios were calculated for 5° ranges in θ with the results plotted in Fig. 1. Although small, the hump centered at $\theta=45°$ clearly points to a systematic, angle dependent error.

Following the procedure suggested by Miyake & Togawa (1964) the monochromator polarization factor was then expressed as $p=cp_D+(1-c)p_K$. From the shape of the initial F_M/F_f curve a value of $c=0{\cdot}65$ was estimated, and a new set of F_M was calculated. The average ratio was plotted as before, with the result also shown in Fig. 1. We see that above $\theta \sim 35°$ the observed ratios very closely approach unity. At lower θ values there is a gradual drop to a ratio of 0·99 at 15°, pointing to some other systematic error. Inspection of the raw filter data revealed some degree of

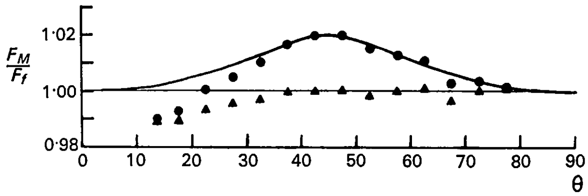

Fig. 1. Ratios F_M/F_f against θ. Dots represent ratios derived by use of p_K, and triangles show ratios resulting from $p=0{\cdot}65p_D+0{\cdot}35p_K$. The curve gives $(p_K/(0{\cdot}65p_D+0{\cdot}35p_K))^{1/2}$ as a function of θ.

skewness in background at lower θ angles, in part resulting from background measurements being made at points where 'white' radiation is strongly absorbed by the filter, giving rise to underestimated background values.

The possibility of an intensity-related error was ruled out by comparing F_M with F_f as a function of F, with no systematic trend apparent. An R index of 0·010 ($R=2(\Sigma\,|F_M-F_f|)/\Sigma\,(F_M+F_f)$) calculated for the reflections used indicates a very satisfactory overall agreement between the two data sets.

The results obtained in this study show that commercially available graphite monochromators can behave quite differently from 'ideally imperfect' crystals, and that allowance should be made for any departure from ideal behavior. Each monochromator must of course be calibrated; it is also conceivable that the calibration might change as a result of irradiation.

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Reference

Azároff, L. V. (1955). *Acta Cryst.* **8**, 701.
Hope, H. & Victor, D. (1969). *Acta Cryst.* **B25**, 1849.
Miyake, S. & Togawa, S. (1964). *Acta Cryst.* **17**, 1083.

International Union of Crystallography

Commission on Crystallographic Computing

Call for material for the third edition of the *World List of Cryrstallographic Computer Programs*

The Commission on Crystallographic Computing of the International Union of Crystallography wishes to announce its decision to prepare a third edition of the *World List of Crystallographic Computer Programs*. The Editor in charge of this edition is

Dr G. C. Bassi
C.N.R.S., Laboratoire d'Electrostatique et de Physique du Métal
Cedex no. 166, 38-Grenoble–Gare, France.

Suitable publication of the *List* will be arranged. The *Journal of Applied Crystallography* is being considered as a possible publication medium. Authors and/or distributors of crystallographic computer programs or systems are invited to submit the necessary information about their programs to the Editor, G. C. Bassi, by 1 November 1971, or earlier if possible. Formats for the submission cards are described below; if punched-card equipment is not available the information may be presented on sheets in the prescribed formats.

All material to be included in the third edition will be based only on the newly submitted cards (or sheets), regardless of whether or not the programs are included in the second edition. It is hoped that this will encourage programmers to eliminate any programs which are out of date, or of very limited interest. In general, only programs that are well checked and in good running order will be accepted. Proper documentation is essential, and the Editor urges those submitting programs to ensure that they will be well documented by the time of publication of the *World List*.

Required information

(*a*) A *Title* card, a *Name and Source* card, and six or less *Abstract cards* are needed for each program.

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(*c*) A *Definition* card should be included for each abbreviated function, machine, language, or system that has been used but is not already included in the list of abbreviations supplied.

Formats

Title card

Card columns	*Contents*
1– 4	Program accession number, to be assigned by the Editor. Programs are numbered serially in chronological order of receipt by the Editor.
6–13	Machine type, by code name or number.
15–22	Language in which the program is written.
24–31	Crystallographic computer system, and the program number or identification within the system, as for example XRAY-23, XRY70-23, or NRC-10.
33–64	Program name, and functions in coded form chosen from the supplied abbreviation list. If necessary only use new symbols defined in a Definition card. The name should be followed by a comma, and the functions should be separated by a blank space. The functions should serve as identification of the types of calculation included in the program. Example:

POW, HKL DHK DST