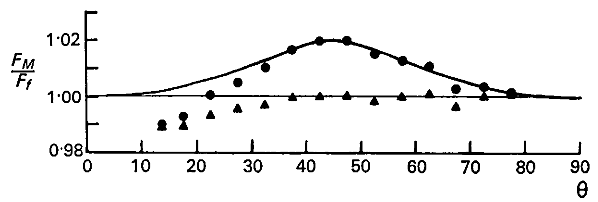

Fig. 1. Ratios F_M/F_f against θ. Dots represent ratios derived by use of p_K, and triangles show ratios resulting from $p = 0{\cdot}65p_D + 0{\cdot}35p_K$. The curve gives $(p_K/(0{\cdot}65p_D + 0{\cdot}35p_K))^{1/2}$ as a function of θ.

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.

This study was supported through a grant from the National Science Foundation. Thanks are due Krista T. Black for help with the calculations.

Reference

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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.

(*b*) An *Author Index* card should be submitted for each author, programmer, and distributor of programs. When one of these names is abbreviated in the Title or Name cards, an additional Author Index card should be supplied, giving the full name as in the following example:

SHMKR, SEE SHØEMAKER, D. P.
SHØEMAKER, D. P., ØREGØN STATE UNIVERSITY, CØRVALLIS, ØREGØN 97331, U.S.A.

(*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

means that the program generates the indices H, calculates the d-spacings, and sorts the reflections in descending order of $d(H)$. The functions may be omitted if desired.

66–67 Core requirement in K words for the program as supplied, where $K=1024$.

69–75 Name of distributor or person in charge of the program to whom enquiries should be addressed.

78 Status of program operability, and availability of program code:
- L well checked out, program code available
- M well checked out, program code not available
- N operable but not well checked out.

79 Status of program write-up:
- C complete write-up available, with the algorithms and the input/output explained.
- I write-up available for input/output only
- N no write-up available

80 Status of availability of program in working form:
- A available on request for no charge
- C available for the charge stated in the abstract.
- N not available at present, probably available at later date.
- S program is of special or local nature, conditionally available.

Name and Source card

1– 4 Program accession number, same as on the Title card.

5 1 (a card sequence number of identification).

6–40 Authors, programmers' names. Only surnames should be given except when use of an initial is necessary to avoid confusion. Surnames should be separated by commas. Where initials are needed they should follow the surname, separated by spaces but no punctuation. The person to whom technical enquiries should be addressed should have an asterisk after his surname if he is not the first author. The name of the distributor should be omitted from this card unless he is one of the authors.

42–75 Source. If the program happens to be a modification of another program, the original program and authors should be identified; otherwise this space should be left blank.

Abstract cards

1– 4 Program accession number, the same as on the Title card.

5 2 ... 7 (a card sequence number for identifica tion).

8–75 Abstract, limited to about 50 words. It should include the relevant information which cannot be directly identified from the program title such as special features, speed, and generality.

Author Index card

1–80 Surname starting in column 1, initials, and mailing address. All name abbreviations should be explained on additional cards.

Definition card

1–10 The abbreviation used, starting in col. 1.

11–80 Full meaning.

PROGRAM AND FUNCTION ABBREVIATIONS

Space group generalities

ASG ALL SPACE GROUPS
CSP CENTROSYMMETRIC SPACE GROUPS ONLY
NSG NON-CENTROSYMMETRIC SPACE GROUPS ONLY
PRI PRIMITIVE UNIT CELLS ONLY
TMO TRICLINIC, MONOCLINIC, AND ORTHORHOMBIC SYSTEMS ONLY

LAT **Lattice constants**

LCD LATTICE CONSTANTS DETERMINATION
LCR LATTICE CONSTANTS REFINEMENT
RUC REDUCTION OF UNIT CELL

DIF **Diffractometer control**

CCD COMPUTER CONTROLLED DIFFRACTOMETER
CIR 3 OR 4 CIRCLE GEOMETRY
GSC GONIOSTAT SETTINGS CALCULATION
HKL GENERATE THE INDICES
OMC ORIENTATION MATRIX CALCULATION
OMR ORIENTATION MATRIX REFINEMENT
WEI WEISSENBERG GEOMETRY

PRO **Processing of raw intensity data**

AVG AVERAGING OF INTENSITIES
CMP COMPARISON OF MULTIPLE MEASUREMENTS
OUA OBS/UNOBS ASSIGNMENT
LAY SCALING ACCORDING TO LAYERS
NET CALCULATION OF NET COUNTS
SCH SEARCH FOR UNMEASURED REFLEXIONS
SCL SCALING OF THE INTENSITIES
SRT SORT ON THE INDICES

DRF **Data reduction and generation of data file**

ABS ABSORPTION CORRECTIONS
ACT ACENTRIC–CENTRIC TEST
CIR 3 OR 4 CIRCLE GONIOSTAT GEOMETRY
FOB F OBS CALCULATION
ISC INTERPOLATION ON SCATTERING FACTOR CURVES
LPC LORENTZ AND POLARIZATION CORRECTIONS
PRC PRECESSION GEOMETRY
SHF SHARPENING FUNCTION APPLICATION
WEI WEISSENBERG GEOMETRY
WSN WILSON STATISTICS
WTA WEIGHT ASSIGNMENT

DIR **Direct phasing**

EHS NORMALIZED STRUCTURE FACTORS AND STATISTICS
MLT MULTISOLUTION PROCEDURE
OES ORIGIN AND ENANTIOMORPH SELECTION
ORG ORIGIN SELECTION
PAS PHASE ESTIMATION FROM ANOMALOUS SCATTERING
PIA PHASE ESTIMATION FROM ISOM. REPL. AND ANOM. SCAT.

PIR	PHASE ESTIMATION FROM ISOMORPHOUS REPLACEMENT
PLS	PHASE ESTIMATION BY LEAST SQUARES
PST	PHASE REFINEMENT BY THE SQUARED TANGENT FORMULA
PTN	PHASE REFINEMENT BY THE TANGENT FORMULA
SAP	SYMBOLIC ADDITION PROCEDURE
SIC	STRUCTURE INVARIANT CALCULATION
STF	SCALE AND TEMPERATURE FACTOR ESTIMATION
SYR	SAYRE'S EQUATION APPLICATION
S1I	SIGMA 1 INTERACTIONS SEARCH
S2I	SIGMA 2 INTERACTIONS SEARCH
USF	UNITARY STRUCTURE FACTORS
SCF	**Scattering factor determination**
ISC	INTERPOLATION ON SCATTERING FACTOR CURVES
NSC	NEUTRON SCATTERING FACTOR DETERMINATION
XSC	X-RAY SCATTERING FACTOR DETERMINATION
SFC	**Structure factor calculation**
AGA	AGREEMENT ANALYSIS OF OBS & CALC DATA
SAD	STRUCTURE FACTORS WITH ANOMALOUS DISPERSION
SAN	STRUCTURE FACTORS WITH ANISOTROPIC THERMAL PARAMETERS
SIS	STRUCTURE FACTORS WITH ISOTROPIC THERMAL PARAMETERS
SFO	S.F. WITH FRACTIONAL OCCUPANCIES
SFT	S.F. TRIALS BY ADDITION OR SUBTRACTION OF ATOMS
SRG	CONTRIBUTION OF RIGID GROUP
FOU	**Fourier type calculation**
FBL	FOURIER WITH BEEVERS–LIPSON TYPE CALCULATION
FCT	FOURIER BY COOLEY–TUKEY ALGORITHM
FPD	FOURIER, PATTERSON & DIFFERENCE SYNTHESES
FPS	FOURIER PEAK SEARCH
FR1	ONE-DIMENSIONAL FOURIER
FR2	TWO-DIMENSIONAL FOURIER
FR3	THREE-DIMENSIONAL FOURIER
FTM	FOURIER TRANSFORM
FUM	FOURIER PRODUCING UNDISTORTED MAPS
SHF	SHARPENING FUCTION APPLIED
VMS	**Vector map solving and manipulation**
VHA	VECTOR HEAVY ATOM ANALYSIS
VMF	VECTOR MINIMUM FUNCTION
VOS	VECTOR ORIENTATION SEARCH
VPS	VECTOR POSITION SEARCH
VVR	VECTOR VERIFICATION
COR	**Corrections to observed data**
ABA	APSORPTION CORRECTION BY ANALYTICAL METHOD
ABI	ABSORPTION CORRECTION BY GAUSSIAN INTEGRATION
ABE	ABSORPTION CORRECTION BY EXPERIMENTAL METHOD
LPC	LORENTZ AND POLARIZATION CORRECTIONS
MPD	CORRECTION FOR MULTIPLE DIFFRACTION
PEX	CORRECTION FOR PRIMARY EXTINCTION
SEX	CORRECTION FOR SECONDARY EXTINCTION
FED	**File editing and manipulation**
ADL	ADD TO OR DELETE FROM FILE
FST	FILE SORT ON THE INDICES
GRT	GENERATE EQUIVALENT REFLEXIONS IN HIGH SYMMETRY SPACE GROUPS
PRT	PRINT FILE CONTENTS
REF	**Refinement of atomic parameters**
BIJ	REFINEMENT OF ANISOTROPIC THERMAL PARAMETERS
BIS	REFINEMENT OF ISOTROPIC THERMAL PARAMETERS
BLS	BLOCK DIAGONAL LEAST SQUARES
DFS	REFINEMENT BY DIFFERENTIAL SYNTHESES
DLS	DIAGONAL LEAST SQUARES
ESD	CALCULATION OF THE ESTIMATED STANDARD DEVIATIONS
FDG	APPLICATION OF FUDGE OR RELAXATION FACTORS
FLS	FULL MATRIX LEAST SQUARES
LAD	LEAST SQUARES WITH ANOMALOUS DISPERSION
LAY	REFINEMENT OF LAYER SCALE FACTORS
LEQ	LEAST SQUARES FOR ATOMS WITH EQUIVALENT COORDINATES
LSP	LEAST SQUARES WITH ALLOWANCE FOR ATOMS IN SPECIAL POSITIONS
OCC	REFINEMENT OF OCCUPANCY FACTORS
RBL	RIGID BODY LEAST SQUARES
SCH	SCHOMAKER'S CORRECTION OF THERMAL PARAMETER SHIFTS
SCL	REFINEMENT OF OVERALL SCALE FACTOR
XYZ	REFINEMENT OF POSITIONAL PARAMETERS
GEO	**Molecular geometry calculations**
DIH	DIHEDRAL ANGLE BETWEEN PLANES
MPL	MEAN PLANE THROUGH A SET OF ATOMS BY LEAST SQUARES
POL	COORDINATION POLYHEDRA
ROT	ROTATION ANGLES
SAN	SCAN OF ANGLES
SID	SCAN OF INTERMOLECULAR DISTANCES
SBL	SCAN OF BOND LENGTHS
TOR	TORSIONAL ANGLES
THV	**Thermal vibration analysis**
ACC	ACCUMULANTS
CBA	CORRECTIONS OF BOND LENGTHS AND ANGLES

PLT AUTOMATIC PLOTTING OF THERMAL ELLIPSOIDS
RID RIDING MOTION
RIG RIGID BODY MOTION
TEL THERMAL ELLIPSOIDS CALCULATION

SFT **Structure factor tables for publication**

AGR AGREEMENT ANALYSIS OF THE OBS & CALC STRUCTURE FACTORS
CSF COMPRESSED STRUCTURE FACTOR TABLES FOR PUBLICATION

PLT **Plotter programs**

FCR FOURIER CONTOURS
DRW STRUCTURE DRAWING
TEL THERMAL ELLIPSOIDS

POW **Powder diffraction**

BRG CALCULATION OF BRAGG ANGLES
CPP CALCULATION OF POWDER PATTERN
DHK CALCULATION OF INTERPLANAR SPACINGS
DST SORTING IN DESCENDING ORDER OF INTERPLANAR SPACINGS
HKL GENERATE THE INDICES
IND INDEXING OF POWDER PATTERN
LCD LATTICE CONSTANTS DETERMINATION FROM POWDER PATTERN
SCH SEARCH OF THE ASTM POWDER FILE
STP STRUCTURE REFINEMENT FROM POWDER PATTERN BY LEAST SQUARES
UCP UNIT CELL REFINEMENT FROM POWDER PATTERN BY LEAST SQUARES

PRJ **Projections of the structures**

ORT ORTHOGONAL PROJECTION
STE STEREOSCOPIC PROJECTION

MSC **Miscellaneous**

ASD ATOMIC STRUCTURE DETERMINATION
ATR ATOMIC RADII
CCS CRYSTALLOGRAPHIC COMPUTER SYSTEM
EDN ELECTRON DIFFRACTION
MFF MAGNETIC FORM FACTOR DETERMINATION
MSD MAGNETIC STRUCTURE DETERMINATION
NDN NEUTRON DIFFRACTION
PRT PROTEIN WORK
REN RENNINGER EFFECT
RTS REAL TIME SYSTEM
SPW SIMPLEX METHOD
TDS THERMAL DIFFUSE SCATTERING
VAR VARIANCE
XDN X-RAY DIFFRACTION

COMPUTER ABREVIATIONS

Name	Type	Abbreviation
BURROUGHS	B 500	B 500
	B 6500	B 6500
CONTROL DATA	CDC 3300	CDC3300
	CDC 3500	CDC3500
	CDC 6600	CDC6600
	CDC7600	CDC7600
DIGITAL EQUIPMENT	PDP 7	PDP7
	PDP 8	PDP8
	PDP 8/I	PDP8I
	PDP 8/E	PDP8E
	PDP 9	PDP9
GENERAL ELECTRIC	GE 615	GE615
	FE 635	GE635
	GE 655	GE655
HEWLETT PACKARD	HP 2114 A	HP2114A
	HP 2115 A	HP2115A
	HP 2116 B	HP2116B
HONEYWELL	200/1200	H2001200
	200/1250	H2001250
	200/2200	H2002200
	H 632	H632
IBM	360/65	IBM36065
	360/50	IBM36050
	360/44	IBM36044
	360/40	IBM36040
	1130	IBM1130
	1800	IBM1800
NCR	CENTURY 100	NCRC100
	CENTURY 200	NCRC200
UNIVAC	1106	UNC1106
	1108	UNC1108
XEROX DATA SYSTEMS	SIGMA 3	XDSSIG3
	SIGMA 5	XDSSIG5
	SIGMA 6	XDSSIG6
	SIGMA 7	XDSSIG7
ICL	1901	ICL1901
	1901 A	ICL1901A
	1902 A	ICL1902A
	1903 A	ICL1903A
	1904 A	ICL1904A
	1906 A	ICL1906A
	KDF 9	ICLKDF9
BULL-GE	415	BGE415
	425	BGE425
	435	BGE435
C.I.I.	510	CII510
	90/10	CII0910
	90/40	CII9040
	90/80	CII9080
	10020	CII10020
	10070	CII10070
SIEMENS	4004/35	SI400435
	4004/45	SI400445
TELEFUNKEN	TR 4	TR4
	TR 86	TR86
	TR 440	TR440

Commission on Crystallographic Apparatus

An international project for the calibration of absolute intensities in small-angle X-ray scattering

The importance of absolute intensity measurements in small-angle X-ray experiments has been recognized for many years, and a wide variety of methods have been reported for achieving such calibrations (Luzzati, 1960; Gerold, 1961; Kratky & Wawra, 1963; Damaschun & Müller, 1965; Kratky, Pilz & Schmitz, 1966). Apart from a comparison by Weinberg (1963) of the foil-attenuation method with the gas-scattering method and a comparison by Shaffer (1964) and Shaffer & Beeman (1970) of the data for zero-angle scattering for several gases, there has been no attempt to compare the many techniques. The problem of precision in measurements of absolute intensity, and the need for a comparison of the different techniques for a common standard sample, were discussed at the recent Second International Conference on Small-Angle Scattering of X-rays held in Graz, Austria, in August, 1970. The results of these discussions may be summarized as follows:

I. An international project should be established with the aims of (1) testing the precision of reproducibility and the comparative accuracy of the various calibration techniques in current use, and (2) clarifying the areas of difficulty in absolute intensity calibration.

II. There shall be no attempt to nominate a single absolute intensity calibration technique. Each participating laboratory will use its own preferred technique to carry out measurements on a set of standard specimens to be provided by the project organizer.

III. The secondary standards would be (1) chemically, thermally, and physically stable, (2) unaffected by long exposures to X-rays, (3) easily transported, and (4) easily handled. On the basis of these criteria, liquid samples were eliminated from consideration. Three solid samples were agreed upon as suitable standards: (1) glassy carbon, (2) polyethylene, and (3) cellulose acetate. Each specimen would be mounted in a specimen holder suitable for use in almost all small-angle scattering geometries.

IV. The project organizer would have the responsibility for (1) designing the specimen holders, (2) preparing the instructions to participants, (3) maintaining and distributing the standards, and (4) collecting and comparing the data.

Each participating laboratory will receive for calibration one of each of the three standard samples from the project organizer. The same three samples will be destributed sequentially to all participants in order to assist in separating technique errors from specimen errors. Detailed instructions regarding the kind and quantity of data required to make the comparison of results from different laboratories meaningful will be provided. Basically, data will be required that fully characterize (1) the geometry of the small-angle collimation system, (2) the X-ray generator and the focal spot, (3) the X-ray wavelength and monochromatization, and (4) the X-ray detection system. These data will be recorded on forms provided. Detailed descriptions of the calibration techniques and all raw data will be recorded. Equations and sample calculations for the data reduction must be shown, including the method of collimation corrections if any is used. The final result – the absolute differential X-ray scattering cross section for each sample – will be used to compare the results from the different laboratories. The data from participants will be analyzed with the assistance of L. B. Shaffer and a report prepared for publication. Complete anonymity of all participants will be maintained.

The standard samples and their mounts and the detailed instructions for participation are now being prepared and checked. All interested researchers are encouraged to communicate with the project organizer (address below) for further details.

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Tennessee 37830, U.S.A.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 *White Friars, Chester CH*1 1*NZ, England).*

Conference on Frameword Silicates and Metals Cambridge (England), 10 December 1971

The Crystallography Group of The Institute of Physics and The Physical Society and The Mineralogical Society are jointly holding a one-day meeting at the Cavendish Laboratory, Cambridge, in honour of Dr W. H. Taylor, who will retire from the position of Reader in Crystallography in September 1971. The meeting will have two sessions on topics which have been of particular interest to Dr Taylor; in the morning the session will be devoted to *Framework Silicates* and in the afternoon the topic will be *Metals*. A Conference Dinner will be held in St John's College on the evening of 10 December.

Further information and registration forms will be available through the two societies. Accommodation for the nights of 9 and 10 December (if required) will be provided in a College. The Local Secretary (Dr P. Gay, Department of Mineralogy and Petrology, Downing Place, Cambridge, England) will be pleased to give advice to prospective participants.