3. The copper rod *F* which connects the glass hair on which the crystal is mounted with the goniometer head. This rod prevents icing at places where mixing of the cold gas and the outer air can occur, the temperature of the rod being above 0 °C at these places.

Since $\chi \leq 90°$ for the three-circle Nonius diffractometer, for all crystal settings, except those with $\chi \simeq 90°$, the component of the gas stream along the glass hair points to the goniometer head. No icing occurs in the neighbourhood of the crystal for this direction of the gas stream, as it prevents outer air from being sucked along the glass hair towards the crystal. Care must be taken that the crystal does not stay at $\chi \simeq 90°$ for too long during the intensity measurements.

The temperature at the position of the crystal was measured with a very thin Chromel–Alumel thermocouple. Values of 110 (±2) °K or lower can be reached depending on the strength of the current through the electric heater in the evaporation vessel. We usually work at 110 °K. This temperature is obtained with a total consumption of liquid nitrogen of 0·80 litre per hour, 0·35 litre of which is used for the cold gas stream.

The equipment described above has worked well during several long intensity runs. For a recent example, see Koster, van Bolhuis & Visser (1970). The cooling system described above is now commercially available (Enraf–Nonius, Delft, The Netherlands) in a slightly modified form.

The author thanks Dr J. L. de Boer for valuable discussions during the development of the apparatus, and Mr P. Lasker and Mr J. Spoelstra for their technical assistance.

F. VAN BOLHUIS

*Laboratorium voor Structuurchemie*
*Rijksuniversiteit Groningen*
*Bloemsingel* 10
*Groningen*
*The Netherlands*

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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, XRY 70-23, 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 identification).

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 | ABSORPTION 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 |
| | CDC 7600 | 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 |
| | GE 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.

Robert W. Hendricks
Metals and Ceramics Division
Oak Ridge National Laboratory
P.O. Box X
Oak Ridge
Tennessee 37830, U.S.A.

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