International Union of Crystallography
World List of Crystallographic Computer Programs
(Third Edition)

Commission on Crystallographic Computing

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          J. S. Rollett
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Ex officio:  F. W. Matthews

General description

1. The format of this list follows the general outline published in Acta Crystallographica (1971) A27, 393–396 and Journal of Applied Crystallography (1971) 4, 264–267. As for the previous lists it is based on the use of standard 80-column punched cards.

2. Normally each program should be a discrete entity capable of being run by itself, even if included in a system. It should have been tested carefully and used successfully under various conditions until the authors are satisfied that maximum debugging has been achieved.

3. Each program is described as follows:
   A. A title line containing the essential information pertaining to the program in a very compressed form. This line has been given an accession number to be used as an index and reference.
   B. Name and source line containing all personal references related to authors and sources.
   C. From 1 to 6 lines of more detailed description giving information which cannot be identified from the title line.

4. The IUCr World List has been organized as follows:
   A. Direct listing of the cards as supplied by the authors:
      * Title line with accession number.
      * Name and source line.
      * Description and general information.
   B. Reference table, made of all the title lines with accession numbers. These are printed in ascending dictionary order of the following three types combined:
      * Machine type.
      * Language.
      * Crystallographic computing system.

5. A dictionary of the abbreviations is printed in alphabetic order of the symbols supplied either by the Editor or by the authors.

6. An index of authors is listed from the author index cards.

Gerard C. Bassi, Editor

C. N. R. S. Laboratoire de rayons X
Cedex No. 166
38-Grenoble-Gare
France
### Formats

**A. Title line**

<table>
<thead>
<tr>
<th>Column</th>
<th>Contents</th>
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<tbody>
<tr>
<td>1-4</td>
<td>* Program accession number, assigned by the Editor.</td>
</tr>
<tr>
<td>6-13</td>
<td>* Machine type, by code name (see Computer abbreviations).</td>
</tr>
<tr>
<td>15-22</td>
<td>* Language in which the program is written (see Programming languages).</td>
</tr>
<tr>
<td>24-31</td>
<td>* Crystallographic computer system, and the program number or identification within the system.</td>
</tr>
<tr>
<td>33-64</td>
<td>* Program name, a comma, and list of functions in coded form (see Function abbreviations).</td>
</tr>
</tbody>
</table>

**B. Name and source line**

<table>
<thead>
<tr>
<th>Column</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>6-40</td>
<td>* Authors, programmers' names. The person to whom technical enquiries should be addressed has an asterisk after his surname if he is not the first author.</td>
</tr>
<tr>
<td>42-75</td>
<td>* Source. If the program happens to be a modification of another program, the original program and authors should be identified; otherwise this space is left blank.</td>
</tr>
</tbody>
</table>

**C. Abstract lines**

<table>
<thead>
<tr>
<th>Column</th>
<th>Contents</th>
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</thead>
<tbody>
<tr>
<td>8-75</td>
<td>* Abstract. It should include the relevant information which cannot be directly identified from the program title line such as special features, speed and generality.</td>
</tr>
</tbody>
</table>

**I Write-up available for input/output only.**

- 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.
List of programs

1 IBM1800 FORTRAN
   PIRUM, POW UCP HKL IND DHK
   WERNER
   ALL SYMMETRIES ARE INCLUDED. DIRECT CELL PARAMETERS WITH STANDARD
   DEVIATIONS ARE CALCULATED. THE PRINCIPLES USED BY THE PROGRAM TO
   CHOOSE SINGLE-INDEXED LINES ARE DESCRIBED IN ARKIV KEMI 31(1969)513.

2 IBM1800 FORTRAN
   PURUM, POW UCP DHK
   WERNER
   ALL SYMMETRIES ARE INCLUDED. DIRECT CELL PARAMETERS WITH STANDARD
   DEVIATIONS ARE CALCULATED FROM LINES INDEXED BY THE USER. THE
   PROGRAM IS A SUPPLEMENT TO PROGRAM PIRUM (BY THE SAME AUTHOR).

3 IBM1800 FORTRAN
   ABSW, ABS WEI ABI LPC SEX
   WERNER, LEIJONMARCK
   IN PROGRAM ABSW THE BOUNDING SURFACES OF THE CRYSTAL ARE GIVEN AS
   EQUATIONS OR, IN THE FORM OF THREE POINTS ON EACH SURFACE. FACTORS
   FOR SECONDARY EXTINCTION ARE CALC. AS DESCRIBED IN ACTA CRYST.

4 IBM1800 FORTRAN
   ABSG, ABS CIR ABI LPC SEX
   WERNER, LEIJONMARCK
   IN PROGRAM ABSG THE BOUNDING SURFACES OF THE CRYSTAL ARE GIVEN AS
   EQUATIONS OR, IN THE FORM OF THREE POINTS ON EACH SURFACE. FACTORS
   FOR SECONDARY EXTINCTION ARE CALC. AS DESCRIBED IN ACTA CRYST.

5 IBM1800 FORTRAN
   PHASE2, DIR ASG S2I SAP PTW MLT
   Koenig
   SAP AND/OR EXPLICIT PHASING AND/OR PTN FOR ANY SPACE GROUP AS SPECIFIED
   BY EQUIVALENT POSITIONS. ONE INDEPENDENT SET UNMODIFIED E USED (MAX 500).
   EXTREMELY FAST. NC TRIPLET TABLES, APPROXIMATIONS, OR REDUNDANCIES.
   USER-SPECIFIED INDEX AND E LIMITS, ACCEPTANCE PARAMETERS. ALLOWS INTER-
   SYMBOL ALGEBRA, WEIGHTED PTN, MLT, MANUAL ON-LINE DATA & CONTROL CHANGES.
   ALL I/O ON ONE TAPE, ANY CAN SERVE AS REINPUT ANYTIME. (E-MAKER GRATIS)

6 IBM36075 FORTRAN
   FALFA, REF FLS FAZ EXT LAD OCC
   Koenig
   USER-DIMENSIONED ATOMIC-PARAMETER AND VARIABLE ARRAYS. FAST. CHANGES OF
   VARIABLES AND CONVERSIONS OF TEMPERATURE FACTORS POSSIBLE BETWEEN CYCLES.
   OTHER OPTIONS BI/BIS ESD FOG LAY LEQ LSP SCL XYZ, GROUP OR OVERALL B,
   NEUTRON CROSS-SECTION REFINEMENT, CORRELATIONS, WEIGHTING ANAYSSES,
   SIM WEIGHTS, c.s.c. OF CALC. PHASE, A0BS-ACALC, B0BS-BCALC.
   ADDITIONAL CORE SIZE (WORDS) 24*ATOMS + VARIABLES*(VARIABLES+7)/2.

7 IBM1800 FORTRAN
   CHOW, GEO MPL SAN SID SBL TOR
   Koenig
   KEYBOARD CONVERSATIONAL VERSION OF HOW, DIMENSIONED FOR 100 ATOMS.
   PRINTS BOTH CRYSTAL AND ORTHOGONAL COORDINATES. ATOMS CHANGEABLE ON-LINE.

8 IBM1800 FORTRAN
   DIR, CSP MLT ORG SAP S11 S21
   NOSTAM
INPUT: TRIPLETS, E'S AND ACCEPTANCE PARAMETERS FROM TAPE AND/OR CARDS. CRG BY USE OF SAP WITH MINIMUM NUMBER OF SYMBOLS INTRODUCED. MLT BY REPLACING SYMBOLS WITH SIGNS. STEPWISE EXPANSION OF ACCEPTED SIGNS BY DECREASING ACCEPTANCE PARAMETERS. FINAL REF OF ALL SIGNS. MANUAL ON-LINE CONTROL CHANGES.

9 IBM1800 FORTRAN4 DIR, TM2 OES S11 S21 10 NSTAM LIA
NORRESTAM
ANALYSIS OF DISTRIBUTION AND SUM OF 1/VAR FOR EACH REF IN TRIPLETS WITH THREE, TWO AND ONE UNKNOWN. A REF IS CONSIDERED UNKNOWN UNTIL ITS SUM OF 1/VAR IS BELOW A GIVEN LIMIT. YIELDED KNOWN REFLS CAN BE USED IN A CYCLIC PROCEDURE AT ANY DESIRED STAGE. BY INTRODUCING THE OES AND THE OTHER NECESSARY REFLS STEPWISE, AN EFFICIENT BUT SMALL BASIS SET IS SELECTED. MANUAL ON-LINE CONTROL CHANGES.

10 IBM1800 FORTRAN4 DIR, TM2 MLT WSM S21 10 NSTAM LIA
NORRESTAM
INPUT: COMPOSITION, E'S, EQUIVALENT POSITIONS, PROPER BASIS SETS AND ACCEPTANCE PARAMETERS. TRIPLETS WITH VAR AND E'S WITH PHASE-RESTRICTIONS ARE STORED ON TAPE. STEPWISE EXPANSION OF ACCEPTED PHASES BY DECREASING ACCEPTANCE PARAMETERS. FINAL REF OF ALL PHASES. WSM IS USED EXCLUSIVELY. MANUAL ON-LINE CONTROL CHANGES.

11 IBM36075 FORTRAN4 DIF, CIR HKL ASG 15 NSTAM LIA
NORRESTAM, KIHLMABERG
GENERATES STEERING TAPE FOR SIEMENS DIF USING OMEGA-TWO(THETA)-SCAN. VARIOUS OPTIONS INCLUDED: LIMIT OF NUMBER OF REFLS, LIMIT OF THETA, INTERVAL BETWEEN STANDARD REFLS, EXTINCTION RULES ETC.

12 IBM1800 FORTRAN4 PRO, NET OUA CMP VAR WTA 5 NSTAM LIA
NORRESTAM
INTERPRETATION OF OUTPUT TAPE FROM SIEMENS DIFFR. CARD OUTPUT.

13 IBM1800 FORTRAN4 DIF, CCD WEI HKL ASG VAR OUA 8 NSTAM LIS
NORRESTAM
PROGRAM SYSTEM FOR ON-LINE CONTROL OF A PAIRED DIFFR IN A TIME-SHARING MODE. INTENSITIES ARE EVALUATED FROM OMEGA-SCAN. VARIOUS OPTIONS INCLUDED, AS PROFILE ANALYSIS OF STEP-SCAN MEASUREMENTS. MINOR PARTS OF PROGRAM SYSTEM CODED IN ASSEMBLER.

14 IBM1800 FORTRAN4 GEO, MPL DIH VAR 8 NSTAM LIA
NORRESTAM, MALMROS
CALCN OF LS-PLANES WITH E.S.D. AND ANGLES WITH E.S.D. BETWEEN THE NORMALS TO DIFFERENT LS-PLANES. WEIGHTING OF ATOMS IS OPTIONAL.

15 IBM1800 FORTRAN4 GEO, TOR PRH 8 NSTAM LIA
NORRESTAM, MALMROS
CALCN OF TORSIONAL ANGLES AND/OR PREDICTION OF HYDROGEN POSITIONS. THE TORSIONAL ANGLES ARE CALCULATED ACCORDING TO IUPAC INFORMATION BULLETIN ON DESCRIPTION OF POLYPEPTIDE CHAINS, 1971.

16 IBM1800 FORTRAN4 SFT, CSF AGR 8 NSTAM LIA
NORRESTAM
INFORMATION OF EIGHT REFLECTIONS IS PRINTED PER LINE (120 CHAR). THE NUMBER OF LINES PER PAGE IS GIVEN AS A PARAMETER.

17 IBM1800 FORTRAN4 REF, BLS BIS LAY XYZ WAV ASG 8 BRANDT LCA
BRANDT, ASBRINK
SFLS, ASBRINK BRANDEN

18 IBM36075 FORTRAN4 FED, ADL FST PRT 13 BRANDT LCA
19 IBM36075 FORTRAN  DRF, ABI CIR WEI LPC PEX SEX  26 BRANDT  LCA
   OLOFSSON, ELFSTRÖM, BRA, ASB, NORD  DATAP2, COPPENS LEI RAB

20 IBM36075 FORTRAN  DRF, ABI CIR LPC PEX SEX  39 BRANDT  LCA
   CARLBOM  DATAPH, COPPENS HAMILTON

21 IBM36075 FORTRAN  FOU, FPD FPS SHF SFC  45 BRANDT  LCA
   LUNDGREN, LIMINGA, LINDGREN, BRA, NORD  DRF, ZALKIN

22 IBM36075 FORTRAN  DRF, PEX SEX  13 BRANDT  LCS
   BRANDT  THE PROGRAM SHALL BE USED IN CONNECTION WITH DATAPH OR DATAP2 BY COPPENS ET AL

23 IBM36075 FORTRAN  REF, BLS BIS LAY XYZ WAN ASG  26 BRANDT  LCA
   BRANDT  SFLS, ASBRINK BRANDEN

24 IBM36075 FORTRAN  REF, FLS LAY BIJ XYZ ESD WAN  39 NORD  LCA
   LIMINGA, LUNDGREN, BRANDEN, NORD, BRA  UCLA LALS1, GANTZEL SPARKS TRUEBLOOD
   USE OF A DYNAMIC FIELD PERMITS A VARIABLE SIZE OF THE MATRIX

25 IBM36075 FORTRAN  REF, FLS LAY BIJ XYZ OCC WAN  52 BRANDT  LCA
   CARLBOM, ASBRINK*  ORFLS, LINUS, BUS MAR LEVY HAM
   REFINEMENT OF EXTINCTION PARAMETERS POSSIBLE

26 IBM36075 FORTRAN  PLT, GDP DRW TEL  43 NORD  LCA
   NORD  SEE J. APP. CRYST. 4 (1971) 196.

27 IBM36075 FORTRAN  DRF, WSN  13 NORD  LCA
   NORD  PERFORMS A WILSON- PLOT FROM 3 OR 2-D DATA

28 IBM36075 FORTRAN  PLT, DRW TEL  30 NORD  LCA
   CARLBOM, NORD*  ORTEP, JOHNSON

29 IBM1800 FORTRAN  POW, CPP BRG DHK  5 NORD  LCA
   NORD  CALCULATES SINSQ(THETA) WITH ESD FROM MEASURED MM VALUES ON GUINIER FILMS

30 IBM36075 FORTRAN  POW, CPP BRG DHK  13 NORD  LCA
   NORD  CALCULATES SINSQ(THETA) WITH ESD FROM MEASURED MM VALUES ON GUINIER FILMS

31 IBM36075 FORTRAN  SFT, CSF  32 BRANDT  LCA
   CARLBOM, NORD*  

32 IBM36075 FORTRAN  PRO, ADL PRT  30 BRANDT  LCA
   BRANDT  TREATS OUTPUT TAPE FROM A PAILRED DIFFRACTOMETER

33 IBM36075 FORTRAN  DRF, HKL NET LPC OUA FOB  26 BRANDT  LCA
   BRANDT  DATARED, GOLDSTEIN LADELL

34 ICL4130 ALGOL  DPS  3 TOLLIN  LIA
   TOLLIN, MUKNS  IMITHP, VMS VOS REC
I(THETA, PHI) FOR PLANAR GROUP ORIENTATION. TOLLIN AND COCHRAN 1964 ACTA CRYST 17, 1322

35 ICL4130 ALGOL DFS DRFLTEA, VMS VOS REC 5 TOLLIN LIA
TOLLIN, MUNNS ROSSMANN, TOLLIN
NON PLANAR GROUP ORIENTATION SEARCH. TOLLIN AND COCHRAN 1964 ACTA CRYST 17, 1322

36 ICL4130 ALGOL DFS DY2DFQ, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO 2-FOLD AXIS BY THE
METHOD OF TOLLIN 1966 ACTA CRYST 21, 613

37 ICL4130 ALGOL DFS KFLTEA, VMS VOS REC RAB 5 TOLLIN LIA
TOLLIN, MUNNS ROSSMANN, TOLLIN
CALCULATES ROSSMANN AND BLOW ROTATION FUNCTION USING THE LARGE TERMS
APPROXIMATION DESCRIBED BY TOLLIN AND ROSSMANN 1966 ACTA CRYST 21, 872

38 ICL4130 ALGOL DFS DY1DFQ, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO SYMMETRY PLANE BY THE
METHOD OF TOLLIN 1966 ACTA CRYST 21, 613

39 ICL4130 FORTRAN DFS EF1DFQ, VMS VOS REC 3 TOLLIN LIA
YOUNG
I(THETA, PHI) FOR PLANAR GROUP ORIENTATION. TOLLIN AND COCHRAN 1964 ACTA CRYST 17, 1322

40 ICL4130 FORTRAN DFS EF2DFQ, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO 2-FOLD AXIS BY THE
METHOD OF TOLLIN 1966 ACTA CRYST 21, 613

41 ICL4130 FORTRAN DFS EF3DFQ, FPD VOS 3 TOLLIN LIA
YOUNG
PATTERSON SECTION IN PLANE GIVEN BY I(THETA, PHI) MAP

42 ICL4130 FORTRAN DFS EF4DFQ, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO SYMMETRY PLANE BY THE
METHOD OF TOLLIN 1966 ACTA CRYST 21, 613

43 UNCII08 FOR IV XATM FOUFL1, FOU FBL FPD FR2 FR3 20 BORGEN LCA
BORGEN, WESTVEDT ORFFE BUSING, MARTIV, LEVY

44 UNCII08 FOR IV XATM FOUFL1, FOU FBL FPD FR2 FR3 20 BORGEN LCA
BORGEN, JINJORD, WESTVEDT GENERAL FOURIER PROGRAM FOR ALL SPACE GROUPS OF ORTHORHOMBIC AND
LOWER SYMMETRY.

45 UNCII08 FOR IV XATM FOUPLA, FOU FPL FUM SHF 50 BORGEN LCA
BORGEN, WESTVEDT, TIDEMANN CALCULATION OF FOURIER SUMS IN A GENERAL PLANE.

46 UNCII08 FOR V XPRCGF LSFiV4, REF BMIX ESD FLS LAY XYZ 40 BORGEN LIA
BORGEN, WESTVEDT LSFiV3 BORGEN, WESTVEDT
FULL MATRIX LEAST-SQUARES REFINEMENT OF SCALE FACTORS, ATOMIC
COORDINATES, AND MIXED TEMPERATURE FACTORS. SEVERAL VERSIONS.

47 UNCII08 FOR IV XATM DISTAN, GEO SID SBL 10 BORGEN NNS
BORGEN
CALCULATION OF INTERATOMIC DISTANCES AND ANGLES.

48 UNC1108 FOR IV XPROGF PAFIV2, GEO SAN S1D SBL 30 BORGEN LIA
BORGEN, MESTVEDT
BORFPE BUSIN, MARTIN, LEVY
DISTANCES, ANGLES, THERMAL PARAMETERS WITH E.S.D. ARE EVALUATED.

49 UNC1108 NU ALGCL XNTH FOUPL1, PLT FCR 10 BORGEN NCA
BORGEN, SKARSTEN
PLOTTING OF CONTOUR MAPS FOR ANY FUNCTION EVALUATED IN AN OBLIQUE
OR RECTANGULAR PLANE EQUIDISTANT COORDINATE LATTICE.

50 UNC1108 FOR V XNTH PLOSTR, PLT DRW TEL 30 BORGEN LIA
BORGEN, MESTVEDT
EVALUATION AND PRESENTATION OF MOLECULAR GEOMETRY ON KINGMATIC X-Y
PLOTTER.

51 UNC1108 FOR V XNTH TOLLIN, POS', TIMBORN, MESTVEDT 20 BORGEN LCA
BORGEN, MESTVEDT, TIDE MANN
ORIENTATION OF PLANAR MOLECULAR SUBUNITS.

52 UNC1108 FOR V XNTH CNHM, CHF 2 BORGEN MNS
BORGEN
CALCULATION OF REASONABLE COORDINATES FOR HYDROGEN ATOMS WHEN
LOCATION OF HEAVIER ATOMS ARE KNOWN.

53 UNC1108 FOR V XNTH TORCOR, THV RIG 10 BORGEN LIA
BORGEN, MESTVEDT
RIGID BODY ANALYSIS WITH CORRECTION OF COORDINATES.

54 UNC1108 FOR V XNTH BESPLA, GEO MPL 4 BORGEN LCA
BORGEN
'BEST' PLANE THROUGH A NUMBER OF WEIGHTED POINTS.

55 UNC1108 FOR V SYMVEC, THV CSC 65 RA LCS
BORGEN, RA
SYMMETRY TRANSFORMATION PROPERTIES ARE ANALYSED FOR ANY MOLECULE
(REPRESENTED BY ITS ASYMMETRIC SUBUNITS) IN ANY SPACE GROUP. FREE
MOLECULES MAY ALSO BE TREATED AS A SIMPLER SPECIAL CASE.

56 UNC1108 FOR V GRUGEN, MSC REP 20 BORGEN LCS
BORGEN, RA
GENERATION OF FULL REPRESENTATIONS FOR THE NORMAL POINT GROUPS OR
SYMMORPHIC SPACE GROUPS.

57 UNC1108 FOR V XPROGF TAPSII, DRF FOB LPC CIR 4 BORGEN LCS
BORGEN, MESTVEDT
INITIATION OF OR ADDITION TO X-RAY DATA FILE USING INTENSITY DATA,
PAPER TAPE FROM PICKER DIFFRACTOMETER.

58 UNC1108 FOR V XPROGF CARSII, DRF FOB LPC CIR 4 BORGEN LCS
BORGEN, MESTVEDT
INITIATION OF OR ADDITION TO X-RAY DATA FILE USING INTENSITY DATA,
ON PUNCHED CARDS.

59 UNC1108 FOR V XPROGF ABSCO1, DRF ABS 6 BORGEN LCS
BORGEN, MESTVEDT
ABSORPTION CORRECTION FOR CRYSTALS WHOSE SHAPE MAY BE DESCRIBED BY
NOT MORE THAN 25 PLANES.
<table>
<thead>
<tr>
<th>No.</th>
<th>Language</th>
<th>Program Name</th>
<th>Authors</th>
<th>Notes</th>
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</thead>
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<tr>
<td>60</td>
<td>V</td>
<td>XPROGF STABL1, DRF RRA</td>
<td>BORGEN, MESTVEDT</td>
<td>Reference reflection analysis for X-ray diffractometer data.</td>
</tr>
<tr>
<td>61</td>
<td>V</td>
<td>XPROGF SCALE1, PRO SCL</td>
<td>BORGEN, MESTVEDT</td>
<td>Scaling of one or more data sets containing reference reflections.</td>
</tr>
<tr>
<td>62</td>
<td>V</td>
<td>XPROGF LISTF1, FED PRT</td>
<td>BORGEN, MESTVEDT</td>
<td>Documentation routines for X-ray data file.</td>
</tr>
<tr>
<td>63</td>
<td>V</td>
<td>XPROGF FFILE1, FED</td>
<td>BORGEN, MESTVEDT</td>
<td>Generation of working file for structure analysis from observed raw data. Collection of equivalent reflections etc.</td>
</tr>
<tr>
<td>64</td>
<td>V</td>
<td>XRAY*TU COPROI, MSC CCS</td>
<td>BORGEN</td>
<td>Initiation and data collection phase of automatic, 'self-administering' structure analysis file-oriented program system.</td>
</tr>
<tr>
<td>65</td>
<td>CDC 6500</td>
<td>FORTRAN4 DIF, OMC OMR</td>
<td>ELIIS, LIEDL</td>
<td>The program calculates the orientation matrix for two cubic crystals from the measured Eulerian angles and theta for three reflections per crystal. The orientation matrix is refined using Shoemaker's symmetry constraint method (J. Appl. Cryst. (1970), 3, 179). The rotation axis and angle which relates the two crystal orientations is calculated.</td>
</tr>
<tr>
<td>66</td>
<td>IBM36091</td>
<td>FORTRAN4 SPSRM286</td>
<td>BORNE HARDY TOURNARIE*</td>
<td>Protein work, optimal estimates of molecular geometry. Mean plane through a set of atoms, bond lengths. Rotation angles of radicals, torsional angles. Plot of structure drawing (listing, tracing, photography). Optional conversational system for organic structures.</td>
</tr>
<tr>
<td>68</td>
<td>IBM36091</td>
<td>FORTRAN4 SPSRM304 MSC, EDN REN</td>
<td>TOURNARIE</td>
<td>Intensities, moduli, phases of diffracted electron beams. Dynamical effects (extinction, absorption) as function of wavelength, thickness, tilting and structure.</td>
</tr>
<tr>
<td>69</td>
<td>IBM36091</td>
<td>FORTRAN4 SPSRM307 FDW, FPS FR2 SHF</td>
<td>TOURNARIE</td>
<td>Calculation and plot of Fourier or Patterson projection contours for all planar groups. Fourier peaks search. Attenuation of the termination effect.</td>
</tr>
<tr>
<td>Output Cards for Input of SPSRM386</td>
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<tr>
<td><strong>70 IBM36091 FORTRAN SPSRM308</strong>&lt;br&gt;TOURNARIE&lt;br&gt;CONSTRUCTION OF AN APODAL KERNEL&lt;br&gt;WITHOUT DISTORTION OF THE MOMENTS OF FOURIER PEAKS&lt;br&gt;OUTPUT CARDS FOR INPUT OF SPSRM307</td>
<td></td>
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</tr>
<tr>
<td><strong>10 TOURNAR MIA</strong></td>
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<tr>
<th>Output Cards for Input of SPSRM330</th>
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<tr>
<td><strong>71 IBM36091 FORTRAN SPSRM321</strong>&lt;br&gt;TOURNARIE&lt;br&gt;REJECTION OF ERRATIC INTENSITIES&lt;br&gt;OUTPUT CARDS FOR INPUT OF SPSRM330</td>
</tr>
<tr>
<td><strong>40 TOURNAR MIA</strong></td>
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<tr>
<th>Output Cards for Input of SPSRM330</th>
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<tr>
<td><strong>72 IBM36091 FORTRAN SPSRM330</strong>&lt;br&gt;TOURNARIE&lt;br&gt;EXTINCTION AND ABSORPTION CORRECTION&lt;br&gt;ADAPTATION BY A. BERTINOTTI OF THE HAMILTON CODE&lt;br&gt;OUTPUT CARDS FOR INPUT OF SPSRM307, SPSRM321, SPSRM386</td>
</tr>
<tr>
<td><strong>16 TOURNAR MIA</strong></td>
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</tbody>
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<tr>
<th>Output Cards for Input of SPSRM334</th>
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<tr>
<td><strong>73 IBM36091 FORTRAN SPSRM344</strong>&lt;br&gt;TOURNARIE&lt;br&gt;OPTIMAL PLAN THROUGH A SET OF ATOMS&lt;br&gt;OUTPUT CARDS FOR INPUT OF SPSRM307, SPSRM321, SPSRM386</td>
</tr>
<tr>
<td><strong>40 TOURNAR MIA</strong></td>
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</tbody>
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<tr>
<th>Output Cards for Input of SPSRM360</th>
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<tr>
<td><strong>74 IBM36075 FORTRAN SPSRM360</strong>&lt;br&gt;BIBIAN BORNE TOURNARIE*&lt;br&gt;PERFORMS OPTIMAL ESTIMATES OF IMPLICIT PARAMETERS OF ANY FUNCTION&lt;br&gt;DEFINED BY USER'S SUBROUTINE. NO DERIVATIVE FORMULA DEManded.&lt;br&gt;NO INTERNAL LIMITATION ON THE NUMBER OF PARAMETERS OR OBSERVATIONS.&lt;br&gt;ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.&lt;br&gt;QUALITY FACTORS, ERROR SCALE ESTIMATED. WEIGHTING AD LIBITUM.&lt;br&gt;OUTPUT CARDS FOR CURVES AND OBSERVATIONS (LISTING).</td>
</tr>
<tr>
<td><strong>20 TOURNAR MIA</strong></td>
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</tbody>
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<tr>
<th>Output Cards for Input of SPSRM379</th>
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<tbody>
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<td><strong>75 IBM36075 FORTRAN SPSRM379</strong>&lt;br&gt;BIBIAN BORNE TOURNARIE*&lt;br&gt;PERFORMS OPTIMAL ESTIMATES OF IMPLICIT PARAMETERS OF ANY FUNCTION&lt;br&gt;DEFINED BY USER'S SUBROUTINE. NO DERIVATIVE FORMULA DEManded.&lt;br&gt;NO INTERNAL LIMITATION ON THE NUMBER OF PARAMETERS OR OBSERVATIONS.&lt;br&gt;ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.&lt;br&gt;QUALITY FACTORS, ERROR SCALE ESTIMATED. WEIGHTING AD LIBITUM.&lt;br&gt;OUTPUT CARDS FOR CURVES AND OBSERVATIONS (LISTING).</td>
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<tr>
<td><strong>33 TOURNAR MIA</strong></td>
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<th>Output Cards for Input of SPSRM379</th>
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<td><strong>76 IBM36075 FORTRAN SPSRM379</strong>&lt;br&gt;TOURNARIE&lt;br&gt;ALL CRYSTALLOGRAPHIC SYSTEMS, ERRATIC LINES OPTIONALLY REJECTED.&lt;br.EXCENTRICITY CORRECTION (PONDER CAMERA OR GONIOMETER)&lt;br&gt;ASSUMED INDICES CAN BE TESTED WITHOUT PERTURBATION.&lt;br&gt;ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.&lt;br&gt;PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING).&lt;br&gt;CELL VOLUME AND C/A RATIO OUTPUT.</td>
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<td><strong>25 TOURNAR MIA</strong></td>
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<tr>
<td><strong>37 TOURNAR MIA</strong></td>
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CELL VOLUME AND C/A RATIO OUTPUT.

78 IBM36075 FORTRAN4 SPSRM386 REF, BIS EOA ESD LAY XYZ
HARDY TOURNARIE
INTERPOLATION ON SCATTERING FACTOR CURVES, LORENTZ-POLARISATION COR.
WEIGHT ASSIGNMENT
NO INTERNAL LIMITATION ON THE NUMBER OF PARAMETERS OR OBSERVATIONS.
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING)
OUTPUT CARDS FOR INPUT OF SPSRM344

79 IBM36091 FORTRAN4 SPSRM386 REF, BIS EOA ESD LAY XYZ
HARDY TOURNARIE
INTERPOLATION ON SCATTERING FACTOR CURVES, LORENTZ-POLARISATION COR.
WEIGHT ASSIGNMENT
NO INTERNAL LIMITATION ON THE NUMBER OF PARAMETERS OR OBSERVATIONS.
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING, TRACING, PHOTO.)
OUTPUT CARDS FOR INPUT OF SPSRM344

80 IBM36091 FORTRAN4 SPSRM388
TOURNARIE
CALCULATION OF CORRECTED COUNTS
SEPARATION OF THE COMPONENTS OF A MULTIPLET (7 COMPONENTS)
EVALUATION OF THE INTENSITIES, POSITIONS AND WIDTHS
PLOTTING OF CURVES AND OBSERVATIONS (LISTING, TRACING, PHOTO.)
PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING, TRACING, PHOTO.)
OUTPUT CARDS FOR INPUT OF SPSRM330, SPSRM379

81 IBM36091 FORTRAN4 ORDATLIB DRF, ABI FOB LPC CIR ADL SCL
ELLISON, JOHNSON, LEVY
CONVERTS NET COUNTS AND ESD TO F**2, F AND ESD. COMPUTES ABSORPTION
AND MEAN PATHS FOR EXTINCTION CORRECTION FOR ELLIPSOID OR GENERAL
CONVEX POLYHEDRON. OPTIONAL LINEAR INTERPOLATION TO REFERENCE
MEASUREMENTS AND SCALING TO INTENSITY OF STANDARD CRYSTAL. ACCEPTS
ONE OR MORE WAVELENGTHS, XRAY OR NEUTRON OR BOTH. GENERATES INPUT
FOR ORDATSRT, ORXFLS3, OR ORESTES.

82 IBM36091 FORTRAN4 ORDATSRT DRF, SRT AVG CMP SCL SCH ASG
ELLISON, JOHNSON, LEVY
CONVERTS HKL TO SYMMETRY-UNIQUE SET, ANY POINTGROUP, FRIEDEL LAW OPTI-
TIONAL. Sorts ON CONVERTED HKL AND SCALE-GROUP. AVERAGES F**2 OVER
REPLICATES AND/OR EQUIVALENTS WITHIN SCALE-GROUPS OR OVER WHOLE SET.
ADJUSTS GROUP SCALE FACTORS TO COMMON REFLECTIONS BY LEAST SQUARES
AND AVERAGES RESCALED ITEMS. 6700 REFLECTIONS, EASILY CHANGED. GEN-
ERATES INPUT FOR ORXFLS3 OR ORESTES.

83 IBM36075 FORTRAN4 ORTEP-2 PLT, DRW TEL STE SBL SAN
JOHNSON, C. K
PLOTS PUBLICATION-QUALITY CRYSTAL-STRUCTURE DRAWINGS INCLUDING
STEREO PAIRS WITH THERMAL ELLIPSOIDS OR SPHERES ON ATOMIC SITES.
USES MECHANICAL PLOTTER OR CRT. TWO MACHINE-LANGUAGE ROUTINES ARE
USED FOR PLOTTING SYMBOLS AND NUMBERS. ORTEP-2 ELIMINATES HIDDEN
PORTIONS OF ATOMS AND BONDS, HOWEVER, THIS FEATURE CAN BE DELETED
EASILY TO OPERATE IN 32K MEMORY. INSTRUCTION MANUAL IS ORNL-3794.

84 IBM36091 FORTRAN4 OR XFLS3 REF, FLS ASG BIJ LAD LAX OCC LAY128 BUSING
LIA
BUSING, JOHNSON, ELLISON, THIessen, LEVY OR FLS, BUSING, MARTIN, LEVY, 1962
STRUCTURE FACTOR LEAST SQUARES BASED ON F OR F**2. ANY SPACE GROUP.
VARIABLES ARE SCALE, ISOTROPIC OR ANISOTROPIC EXTINCTION, NEUTRON
SCATTERING, IMAGINARY PART OF ANOMALOUS SCATTERING, OCCUPANCY, COORDINATES, AND 3RD CUMULANT, ANISOTROPIC, OR ISOTROPIC TEMPERATURE FACTORS INTERMIXED. ARBITRARY CONSTRAINTS EASILY APPLIED. FLEXIBLE WEIGHTING SCHEME. 95 ATOMS, 390 VARIABLES, READILY CHANGED.

85 IBM36091 FORTRAN OR FFE3 GEO, ESD SID SAN DIH TOR TEL CBA128 BUSING LIA BUSING, JOHNSON, THEISSLER, LEVY DRFFE, BUSING, MARTIN, LEVY, 1964 FUNCTIONS OF STRUCTURE PARAMETERS WITH THEIR STANDARD ERRORS. USE INDEPENDENTLY OR WITH COVARIANCE MATRIX FROM XFLS3. DISTANCES, ANGLES, DIHEDRAL ANGLES, SIGNED TORSION ANGLES, DISTANCE OF ATOM FROM PLANE DEFINED BY 3 ATOMS, RMS PRINCIPAL THERMAL DISPLACEMENTS, ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR, DISTANCE CORRECTED FOR THERMAL MOTION. ADDITIONAL FUNCTIONS EASILY PROGRAMMED BY USER.

86 CDC6600 FORTRAN SEARCHER, AHA SIS FPS BLS DRW 96 KОYAMA LCA DR. HIROZO KOYAMA, KENJI OKADA SEARCHER IS A PROGRAM FOR THE AUTOMATIC STRUCTURE ANALYSIS OF ORGANIC COMPOUNDS CONTAINING A HEAVY-ATOM. PROGRAM IS AVAILABLE FOR TRICLINIC, RCMC, AND ORTHORHOMBIC. INPUT IS ONLY HEAVY-ATOM COORDINATES. OUTPUT IS A PROJECTION DIAGRAM (1A#2.5CM) OF THE MOLECULE IN A UNIT CELL. A COMPOUND (P212121) WITH 61 ATOMS SOLVED ABOUT 61 MIN.

87 IBM+UNC FORTRAN FILMDATA MSC, CCS PRO, DRF, PRC WEI LPC FOB 32 PEARSON LCA PEARSON, H. SUSSMAN, J. HYBL, A. FILM DATA REDUCTION SYSTEM OF PROGRAMS. INPUT=MAG. TAPE OF OUTPUT FROM SCANNING DENSITOMETER. OUTPUT=LPC CORRECTED STRUCTURE FACTORS+WEIGHTS. CARD+PRINTER+TAPE DRIVE. IBM360/44PS+DDS, IBM360/91S, UVC1108/EXEC8 FORTRAN IV EXCEPT ASSEMBLY TAPE I/O. SOME ROUTINES AVAILABLE IN BOTH ESPECIALLY DESIGNED FOR SCREENLESS FILM TECHNIQUES. IMPROVED VERSION OF PROGRAM DESCRIBED AT A.C.A. 1970 SPRING MEETING

88 IBM+UNC FORTRAN FILMDATA ICOPAK FED, COMP FORMT 12 PEARSON LCA PEARSON, H. SUSSMAN, J. HYBL, A. FILM DATA REDUCTION SYSTEM OF PROGRAMS. INPUT=MAG. TAPE FROM SCANNING MICRODENSITOMETER. UNPACKS TO A FORMAT ACCEPTABLE TO THE COMPUTER. VOLUME OF DATA REDUCED BY SUMMING ADJACENT DENSITIES WITHIN SCAN (WORDS) AND ACROSS RECORDS. COMP NOT EQUIVALENT TO ENLARGING DENSITOMETER SCAN APERTURE SINCE D=2 LOG(T). REQ. 2 TAPES

89 IBM+UNC FORTRAN FILMDATA 2MAPP FED, PRAT SAMP 32 PEARSON LCA PEARSON, H. SUSSMAN, J. AND BARNHOLDT, R. DUMP OF FILM IMAGE ONTO PRINTER. PRINT DENSITY PROPORTIONAL TO FILM DENSITY. PRINT VOLUME REDUCED BY SAMPLING (MAXIMUM OF ADJACENT DENSITY VALUES SIMILAR TO ICOPAK ROUTINE). SPOT ADDRESSES EASILY FOUND BY NOTING WORD AND RECORD NUMBERS FROM BOX AXES SURROUNDING PRINTOUT.

90 IBM+UNC FORTRAN FILMDATA 3FILM DRF, PRC WEI LPC WTA FOB WC 32 PEARSON LCA PEARSON, H. SUSSMAN, J. 3-OVERLAYS. SCREENLESS (WEI+PRC)+OSC. ALL WEI MU ANGLES+MISALLIGNED GONIOMETER. CALCULATE FILM POSITIONS=X(H,K,L), Y(H,K,L). CALCOMP PLOT (X,Y) FOR FILM OVERLAY. MANY OPTIONS FOR BACKGROUND. FIND CENTROID TO CENTER SPOT. LEAST SQUARES REFINEMENT IN INPUT PARAMETERS. IMPROVED VERSION OF PROGRAM DESCRIBED AT A.C.A. 1970 SPRING MEETING

91 IBM+UNC FORTRAN FILMDATA 4SCALE PRO, LAY AVG CMP JUA SRT 32 PEARSON LCA PEARSON, H. HAMILTON-ROLETT-SPARKS TENTATIVE R CF DATA SET. AVERAGES EQUIVALENT REFLECTIONS. (PRO, CMP) AND MATCHES AGAINST WEIGHT FROM FILM PROGRAM TO CHECK FOR ERRORS. 2 CUTOUTS, (DRF, FOB+WTA) AND THE RATIO (PRO, CMP)/(DRF, WTA)
RATIO OUTPUT CAN BE USED FOR SUBSEQUENT STATISTICAL ANALYSIS.

92 IBM36065 PL/I
FOU, FCT ASG FPD FR3
32 JACOBSN LCA
HUBBARD, QUICKSALL, JACOBSON*
ALFF* AMES LAB FAST FOURIER PROGRAM EMPLOYING THE COOLEY-TUKEY ALGORITHM
FOR ANY SPACE GROUP, ANY AXIS ORIENTATION. AXIS LENGTHS RESTRICTED TO
2**N. FRIEDEL'S LAW IS IMPLICITLY ASSUMED TO HOLD. ONE HEMISPHERE OF
DATA REQUIRED*SEE PROGRAM FRIEDEL. RELATED PROGRAMS ARE ALFF, ALFFDP AND
ALFFPROJ. WRITEUP IS2625 AVAILABLE.

93 IBM36065 PL/I
FOU, FCT FTM FR3
32 JACOBSN LCA
HUBBARD, QUICKSALL, JACOBSON*
ALFFT* AMES LAB FAST FOURIER TRANSFORM FOR CALCULATION OF FOURIER COE
FROM A REAL MAP. AXIS LENGTHS MUST BE 2**N. LOGICAL INVERSE OF THE
PROGRAM ALFF. WRITEUP IS2625 AVAILABLE.

94 IBM36065 PL/I
MSC, FCT FR3 VVR TMO
32 JACOBSN LCA
HUBBARD, QUICKSALL, JACOBSON*
ALFFDP* AMES LAB FAST FOURIER DIFFERENCE PATTERSON PROGRAM FOR CALC.
OF THE DISCRIMINATOR INDEX OF THE DIFFERENCE PATTERSON. SEE ACTA CRYST
B26(1970), 1682 FOR DETAILS OF THIS STRUCTURE SOLUTION METHOD. ALFFDP
USES THE SAME ALGORITHMS AS DOES ALFF. WRITEUP IS2625 AVAILABLE.

95 IBM36065 PL/I
FOU, FCT FPD FRI FR2
32 JACOBSN LCA
HUBBARD, QUICKSALL, JACOBSON*
ALFFPROJ * AMES LAB FAST FOURIER PROJECTION PROGRAM FOR CALCULATION OF
ONE AND TWO DIMENSIONAL FOURIER MAPS. WRITEUP IS2625 AVAILABLE.

96 IBM36065 PL/I
FED, ASG GRT
32 JACOBSN LCA
HUBBARD, QUICKSALL, JACOBSON*
FRIEDEL GENERATES ONE HEMISPHERE OF DATA USING SYMMETRY OPERATIONS ON THE
UNIQUE DATA. COMPATIBLE WITH THE FAST FOURIER PROGRAMS ALFF AND ALFFPROJ
WRITEUP IS2625 AVAILABLE.

97 IBM36065 FORTRAN
VMS, VMF TMO
32 JACOBSN LCA
HUBBARD, JACOBSON*
ALS * AMES LAB SUPERPOSITION PROGRAM FOR CALCULATION OF MULTIPLE
SUPERPOSITIONS OF THE PATTERSON ON ANY BASE MAP (E.G. SYMMETRY, E,
SUPERPOSITION OR PATTERSON MAP) USING THE MINIMUM FUNCTION. ORIGIN SHIFTS
AND WEIGHTING ARE POSSIBLE. ALS MAY USE THE OUTPUT OF THE VECTOR
VERIFICATION PROGRAM SYMM AS THE BASE MAP. A USER PROGRAM CREATES THE
DIRECT ACCESS MAP AS DEFINED IN THE WRITEUP IS2210.

98 IBM36065 FORTRAN
VMS, VVR
32 JACOBSN LCA
HUBBARD, JACOBSON*
SYMM IS USED IN CONJUNCTION WITH THE PROGRAM ALS. SYMM CALCULATES A
SYMMETRY MAP FROM THE PATTERSON AND SYMMETRY VECTORS. THE PATTERSON MUST
BE WRITTEN AS A DIRECT ACCESS MAP AS DEFINED IN THE WRITEUP IS2210.

99 CDC
FTN IV ETHOS DLS, FLS
33 MEIER LCA
VILLIGER, MEIER*
PROGRAM FOR ADJUSTING INTERATOMIC DISTANCES TO PRESCRIBED VALUES BY
LEAST SQUARES. THE VARIABLES CAN BE CHOSEN FROM ATOMIC COORDINATES,
CELL PARAMETERS AND GROUPS OF INTERATOMIC DISTANCES. DIMENSIONED FOR
200 INTERATOMIC DISTANCES AND 150 VARIABLES. AN EXTENDED VERSION
DLSR WITH SUBSIDIARY LINEAR RESTRICTIONS IS AVAILABLE.

100 CDC
FTN IV SCOPECUCFIT, FLS DLS
32 THOENI LIA
THOENI
FLS PROGRAM TO ADJUST A SYSTEM OF ANALYTIC FUNCTIONS TO A GIVEN
PROFIL. MAIN APPLICATIONS - POWDER DIFFRACTION (XDN,NDN), SPECTROSCOPY. DIMENSIONED FOR 3000 PROFIL POINTS AND 310 VARIABLES. THE FUNCTION OF A SINGLE PEAK CAN BE COMPOSED OF TWO INDEPENDENT FUNCTIONS (LEFT PART, RIGHT PART) TO CORRECT PEAK ASYMMETRY.

101 CDC6600 FORTRAN4 BCSU,ASG BRG DHK DST HKL GSC 28 WOLTEN LIA
   WOLTEN
   INPUT LAT. PAR., LAMBDA, CRYST. SYST., CALC. MANY FUNCT. OF HKL AND D,
   ORIENTER SETTINGS, VECTORS, NORMALS.

102 CDC6600 FORTRAN4 SPHERE,ASG GSC HKL GRT DST STE 28 WOLTEN LIA
   WOLTEN
   FULL SPHERE ORIENTER SETTINGS, CALC. STEREOGRAPHIC PROJ. AND
   PLOTS IT (PLOT LOCAL CODE).

103 CDC6600 FORTRAN4 CELFIX, 17 WOLTEN LIA
   WOLTEN
   TRANSFORMS MONOCLINIC CELLS TO I.U.C.R. STANDARD SETTING.

104 CDC6600 FORTRAN4 LIM, WOLTEN LIA
   WOLTEN
   TABLE, LARGEST MONOCLINIC BETA POSSIBLE AS FUNCTION OF C/A IF

105 CDC6600 FORTRAN4 TWIN,TMO WOLTEN LIA
   WOLTEN
   TWIN INDICES, OBLIQUITIES. WOLTEN, ACTA CRYST. 21, 450, 1966.

106 CDC6600 FORTRAN4 ANGLES, 17 WOLTEN LIA
   WOLTEN
   HEMISPHERE OF INTERPLANAR ANGLES FOR MORPHOLOGY.

107 CDC6600 FORTRAN4 PRECES,PRC WOLTEN LIA
   WOLTEN
   TABLE, PRECESSION CAMERA SETTINGS.

108 CDC6600 FORTRAN4 BRAGG WOLTEN LIA
   WOLTEN
   TABLES OF 2 THETA VS. D IN STEPS OF 0.01, ANY 2 LAMBdas.

109 CDC6600 FORTRAN4 STACK 20 WOLTEN LIA
   WOLTEN
   PROGRAM IMPLEMENTS ALGORITHM BY GRUBER, ACTA CRYST. A26, 622, 1971.

110 CDC6600 FORTRAN4 ASTM7,SCH WOLTEN NIA
   WOLTEN
   CONVERSION TO CDC OF G. JOHNSON'S PROG. VERSION 12, RECENT.

111 IBM1130 FORTRAN X-ARC-00 X-RAYARC, MSC CCS XDN TRUTER LCA
   VICKERY, BRIGHT, MALLINSON*
   PROGRAM SYSTEM FOR X-RAY CRYSTALLOGRAPHY, DESIGNED FOR OPERATION
   UNDER IBM 1130 DISK MONITOR SYSTEM VERSION 2, WITH 16K CORE AND TWO
   DISK DRIVES. ALL DATA FILES REQUIRED FOR TWO AVERAGE-SIZE STRUCTURES
   MAY USUALLY BE ACCOMMODATED ON ONE DISK CARTRIDGE. MONITOR AND X-RAY
   SYSTEM PROGRAMS IN OBJECT FORM OCCUPY SYSTEM CARTRIDGE, WITH SCRATCH
   FILE SPACE. X-RAY ARC IS AVAILABLE ON DISK IN SOURCE-CARD IMAGE FORM.

112 IBM1130 FORTRAN X-ARC-19 DEES, POW HKL DHK BRG DST 16 TRUTER LCA
   RHONE, NAVE*
   NRC-21 M.E. PIPPY
   RECIPROCAL SPACE IS SCANNED FOR ALL NON-EQUIVALENT REFLECTIONS
   WITHIN A SELECTED SPHERE OR PART-SPHERE, LIMITED BY THE MINIMUM
VALUE OF D SET BY THE USER. CONDITIONS FOR SPACE GROUP ABSENCES MAY BE SUPPLIED, TO OBTAIN RESULTS FOR PERMISSIBLE REFLECTIONS AND ABSENCES SEPARATELY. 100 REFLECTIONS COMPUTED WITH D AND THEETA VALUES IN 5 MINUTES.

113 IBM1130 FORTRAN X-ARC-02 PICK3, DIF HKL OMC OMR LCR GSC 16 TRUTER LIA BRIGHT
SPECIALIZED PROGRAM FOR PICKER 4 CIRCLE CARD-CONTROLLED DIFFRACTOMETER, INCORPORATES ORDERING OF REFLECTIONS SO AS TO MINIMIZE SLEWING TIME. 500 REFLECTIONS GENERATED IN 30 MINUTES.

114 IBM1130 FORTRAN X-ARC-13 ABSEP, COR ABI 16 TRUTER NIS VICKERY
ABSORPTION CORRECTION IS PUNCHED ON OUTPUT CARDS FROM PICKER 4 CIRCLE DIFFRACTOMETER, FOR SUBSEQUENT APPLICATION BY DATA REDUCTION PROGRAM. REQUIRE ORDERING MATRIX FROM PICKER SETTING PROGRAM BY R.H.B.MAIS AND D.G.WATSON. SPEED APPROX. 1 REFLECTION/ MINUTE, DEPENDING ON SIZE OF DIVISIONS.

115 IBM1130 FORTRAN X-ARC-03 PRED,PRO DRF NET OUA LPC FOB WTA 8 TRUTER LIA VICKERY,RHONE
INPUT IS FROM CARDS OUTPUT BY PICKER 4 CIRCLE DIFFRACTOMETER IN 2-THETA SCAN MODE WITH OR WITHOUT ATTENUATORS. STANDARD REFLECTION COUNTS MAY BE USED TO SCALE INTENSITIES. OBSERVED STRUCTURE AMPLITUDES WITH STANDARD DEVIATIONS ARE OUTPUT ON DISK. SPEED 100 REFLECTIONS/MINUTE WITH PRINTING SUPPRESSED.

116 IBM1130 FORTRAN X-ARC-24 FSORT, FED FST 5 TRUTER LIA MALLINSON
DISK FILE CONTAINING PROCESSED DATA IS SORTED ON INDICES WITH ANY OF H, K, L VARYING MOST RAPIDLY AND/OR FILE IS PUNCHED ON CARDS. RUN TIME 30 MIN FOR 3000 REFLECTIONS, EXCLUDING PUNCHING.

117 IBM1130 FORTRAN X-ARC-04 DATAR, SCF ISC 7 TRUTER LCA VICKERY
DISK FILE CONTAINING PROCESSED DATA AND UP TO 11 INTERPOLATED SCATTERING FACTORS FOR EACH REFLECTION IS GENERATED. SPEED 200 REFLECTIONS/ MIN.

118 IBM1130 FORTRAN X-ARC-05 FODAP, FOU FBL FPD FR3 FPS ASG 16 TRUTER LIA BRIGHT,FITZGERALD.
3-D FOURIER SUMMATION FOR ANY SPACE GROUP. INCORPORATES OPTIONAL AUTOMATIC SCALING, CONTOURED LINE PRINTER OUTPUT, PEAK SEARCH AND RE-START FACILITIES. RUN TIME 2 HOURS FOR 7000 GRID POINTS WITH 1500 REFLECTIONS.

119 IBM1130 FORTRAN X-ARC-07 SAPI-4B, DIR EHS STF S2I SAP SCP 16 TRUTER NCA VICKERY
FIVE PROGRAMS COVERING SIGN DETERMINATION BY SYMBOLIC ADDITION PROCEDURE APPLIED TO CENTROSYMMETRIC SPACE GROUPS, INCLUDING WILSON PLOT, E VALUE CALCULATION, GENERATION OF SIGMA2 TRIPLETS AND SELECTION OF ORIGIN DEFINING REFLECTIONS. SIGMA2 RUN TIME APPROX. 15 HOURS FOR 400 REFLECTIONS.

120 IBM1130 FORTRAN X-ARC-06 MAMIE,REF BIS XYZ OGC LAY FLS 15 TRUTER LCA VICKERY,MALLINSON*
FULL MATRIX LEAST-SQUARES REFINEMENT OF ATOMIC POSITIONAL AND ISOTROPIC THERMAL PARAMETERS, LAYER SCALE FACTORS AND, OPTIONALLY, OVERALL ANISOTROPIC TEMPERATURE FACTOR, UP TO 70 ATOMS AND 81 VARIABLES. DERIVATIVES FOR EQUIVALENT PARAMETERS OF ATOMS IN SPECIAL
POSITIONS MAY BE SET BY USER SUBROUTINE. SPEED 3 HOURS PER CYCLE WITH 20 ATOMS, 80 VARIABLES, 1500 REFLECTIONS.

121 IBM1130 FORTRAN X-ARC-20 BLOK, REF BLS LAD B1J SCH OCC XYZ 16 TRUTER LIA VICKERY, MALLINSON

BLOCK DIAGONAL LEAST-SQUARES REFINEMENT 5X5 OR 10X10 FOR ISOPTROPIC OR ANISOTROPIC THERMAL PARAMETERS, OVERALL SCALE FACTOR, TEMPERATURE FACTOR BACK-SHIFT CORRECTION, UP TO 60 ATOMS AND 400 VARIABLES, WITH PROVISION FOR ANOMALOUS DISPERSION. DERIVATIVES FOR EQUIVALENT PARAMETERS OF ATOMS IN SPECIAL POSITIONS MAY BE SET BY USER SUBROUTINE. SPEED 5 HR/CYCLE WITH 40 ATOMS, 160 VARIABLES, 1500 REF.

122 IBM1130 FORTRAN X-ARC-11 HGEn, GEO 9 TRUTER LIA VICKERY

GENERATION OF CC-ORDINATES FOR TETRAHEDRAL OR TRIGONAL POSITIONS RELATIVE TO GIVEN ATOMIC POSITIONS.

123 IBM1130 FORTRAN X-ARC-27 BOND, SBL SAN 10 TRUTER LCA MALLINSON

SCANS ASYMMETRIC UNIT FOR BONDS AND ANGLES WITH OPTIONAL CALCULATION OF E.S.D., ASSUMING UNCORRELATED CO-ORDINATE ERRORS. SPECIFIC DISTANCES AND ANGLES MAY ALSO BE CALCULATED. ORTHOGONALIZED CO-ORDINATES AND BOND DIRECTION COSINES ARE OUTPUT.

124 IBM1130 FORTRAN X-ARC-10 MPLN, GEO MPL D1H 11 TRUTER LCA VICKERY, NRC-22 M.E. PIPPY AND F.R. AHMED

CALCULATION OF MEAN PLANES THROUGH GROUPS OF ATOMS WITH CHI SQUARED VALUES. DISTANCES OF OTHER ATOMS FROM THE MEAN PLANE, WITH E.S.D.

125 IBM1130 FORTRAN X-ARC-14 TORSN, GEO TOR 7 TRUTER LCA VICKERY

TORSIONAL ANGLE CALCULATION FOR RING SYSTEMS OR CHAINS OF ATOMS.

126 IBM1130 FORTRAN X-ARC-12 INIAx, PLT DRW 16 TRUTER LIA BRIGHT

CALCULATES PRINCIPAL MOMENTS OF INERTIA AND INERTIAL AXES FOR A GROUP OF ATOMS. THE MINIMAL INERTIAL AXIS IS THE NORMAL TO THE MEAN PLANE THROUGH THE ATOMS. THE COORDINATES OF A SECOND SET OF ATOMS WITH RESPECT TO THE INERTIAL AXES OF A FIRST SET MAY BE CALCULATED AND USED TO OBTAIN BALL AND STICK DRAWINGS ON THE PLOTTER.

127 IBM1130 FORTRAN X-ARC-22 FTAB, SFT CSF 16 TRUTER LIA MALLINSON

PRINTS STRUCTURE FACTOR TABLE IN COMPRESSED FORM FOR PUBLICATION, Optionally with phase angles for non-centrosymmetric structures. Alternatively SIGMA F(OBS) MAY BE PRINTED. SEVERAL COPIES OF THE TABLE MAY BE OBTAINED IN ONE RUN OF THE PROGRAM.

128 IBM1130 FORTRAN X-ARC-23 RCELL, POW UCP 9 TRUTER NNN MALLINSON, NAVe

REFINES UNIT CELL PARAMETERS BY LEAST SQUARES GIVEN FILM SPACINGS OF INDEXED POWDER DIFFRACTION LINES. THE E.S.D.S OF THE CELL PARAMETERS ARE ALSO OBTAINED.

129 IBM1130 FORTRAN X-ARC-26 ECALC, DIR EHS 16 TRUTER LCA MALLINSON

NORMALISED STRUCTURE FACTORS ARE OBTAINED FROM A PLOT OF RECIPROCAL AVERAGE INTENSITY AGAINST (SINE THETA)/LAMBDA FOR OVERLAPPING RANGES OF (SINE THETA)/LAMBDA. A POLYNOMIAL UP TO FOURTH ORDER IS FITTED TO THE EXPERIMENTAL CURVE, WHICH IS DISPLAYED ON PRINT-OUT TOGETHER.

JAC 6-5
WITH FITTED CURVE AND E VALUE STATISTICS. REQUIREMENTS OF LAUE SYMMETRY AND SPACE GROUP PROVIDED BY USER SUBROUTINES. 30 MIN/2000 REF.

130 IBM 1130 FORTRAN X-ARC-29 ELIPS, THV TEL MALLINSON
CALCULATION OF L(I,J) AND E.S.D. FROM BETA(I,J) AND E.S.D. WITH DIRECTIONS OF PRINCIPAL AXES OF THERMAL ELLIPSOIDS AND PRINCIPAL VIBRATION AMPLITUDES.

131 IBM 1130 FORTRAN X-ARC-21 RANGE, REF 13 TRUTER LIA VICKERY
ANALYSIS OF WEIGHTING SCHEME FOR LEAST-SQUARES STRUCTURE REFINEMENT. VALUES OF AVERAGE \( \sigma^2 (\Delta \text{SQUARED}) \) ARE OUTPUT FOR CONSECUTIVE RANGES OF F(OBS) AND OF (SINE THETA)/LAMBDA. THE DISTRIBUTION OF F(OBS) AS A FUNCTION OF THE INDICES AND EVEN/ODD COMBINATIONS OF THE INDICES IS ALSO EXAMINED. RUN TIME 20 MIN FOR 1500 REFLECTIONS, INCLUDING SORT CN F(OBS) TO CONSTRUCT EQUALLY POPULATED RANGES.

132 IBM 1130 FORTRAN X-ARC-08 BANGL, GEO SBL SID SAN 9 TRUTER LIA BRIGHT
INTERMOLECULAR CONTACT AND ANGLE SEARCH OVER 27 UNIT CELL TRANSLATIONS WITH UP TO 24 SYMMETRY OPERATIONS. RUN TIME 3 HR WITH 40 ATOMS AND 4 SYMMETRY OPERATIONS.

133 IBM 36050 FORTRAN NRC-1 DIF, GSC CIR HKL ASG LPC 4 AHMED LCA PIPPY, AHMED*
GONIOSTAT SETTINGS FOR FOR 3 OR 4 CIRCLE DIFFRACTOMETERS. ASSUMES TWO RECIPROCAL AXES IN EQUATORIAL PLANE, OR OVO AXIS AT CHI=90. COMPUTES SETTINGS GIVEN THE STARTING INDICES, THEIR INCREMENTS, AND 2 THETA MAX. OMITS PROHIBITED REFLEXIONS. OUTPUT IS ON PRINTER, AND PUNCH CARDS FOR PICKER DIFFRACTOMETER.

134 IBM 36050 FORTRAN NRC-2A PRD, AVG CMP OUA NET SCH SCL SRT 22 AHMED LCA AHMED
PROCESSING OF PICKER DIFFRACTOMETER RAW DATA. DATA CARDS MAY BE IN ANY ORDER WITH OR WITHOUT REPETITIONS. SETTING CARDS MAY BE LEFT IN DECK. AVERAGES MEASUREMENTS, SortS, IDENTIFIES MISSING REFLEXIONS, AND PRODUCES TAPE ACCEPTABLE TO NRC-2.

135 IBM 36050 FORTRAN NRC-2 DRF, FOB ISC CIR WEI LPC SHF WTA 8 AHMED LCA AHMED, HUBER
DATA REDUCTION AND GENERATION OF STANDARD LISTS FILE. INPUT REFLEXIONS MUST BE IN SORTED ORDER OF INDICES. CALCULATES NET COUNTS, F(OBS), SCATTERING FACTORS, WEIGHTS. CAN APPLY ABSORPTION CORRECTIONS FOR SPHERE OR CYLINDER. GENERATES STANDARD DATA FILE NEEDED FOR INPUT TO ALL NRC PROGRAMS.

136 IBM 36050 FORTRAN NRC-3 COR, ABS ABI CIR 9 AHMED LCA AHMED, SINGH
ABSORPTION CORRECTION FOR 3 CIRCLE GONIOSTAT GEOMETRY. Applicable only to crystals with planar faces. Uses Gaussian integration. The number of grid points may be different in the 3 directions.

137 IBM 36050 FORTRAN NRC-4 DIR, SAP CSP TMO STF EHS ORG S21 22 AHMED LCA HALL, AHMED*
DIRECT PHASING BY THE SYMBOLIC ADDITION PROCEDURE. APPLICABLE TO CENTROSYMMETRIC SPACE GROUPS ONLY. CONSISTS OF FIVE SEPARATE PROGRAMS WHICH PERFORM THE BASIC SAP OPERATIONS AUTOMATICALLY, BUT PERMIT HUMAN INTERVENTION. HAS AN EXCELLENT RECORD OF SUCCESS.
138 IBM36050 FORTRAN4 NRC-5  DIR, TMD STF EHS PTN S21  25 AHMED  LCA
huber, briesse  pdp-6 programs by s r hall
direct phasing for centric and noncentric space groups. consists
of five separate programs. has optional methods of normalization,
including overall anisotropic temperature factor corrections.
applies the tangent formula of phase refinement.

139 IBM36050 FORTRAN4 NRC-8  FOU, FPD FR3 FUM SHF ASG  23 AHMED  LCA
ahmed
three dimensional fourier. produces properly scaled, undistorted
fourier maps for direct plotting, or the usual distorted maps.

140 IBM36050 FORTRAN4 NRC-9  REF, DFS XYZ ESD  27 AHMED  LCA
ahmed, pippy
refinement of atomic coordinates by differential syntheses.
limit is 30 atoms per run. calculates and applies the back-shift
correction for finite summation errors.

141 IBM36050 FORTRAN4 NRC-10  REF, BLS XYZ BIJ BIS OCC SCL ESD 22 AHMED  LCA
ahmed
block-diagonal least-squares. block sizes are 4x4, 5x5, 9x9, 10x10,
or 3x3 & 6x6 per atom, or a mixture of these. features include
anomalous dispersion, special positions and fractional occupancy,
anisotropic and isotropic temperature factors, overall scale
refinement, and schomaker's correction. limit 90 atoms.

142 IBM36050 FORTRAN4 NRC-12  GEO, SBL SAN SID ESD POL  23 AHMED  LCA
pippy, ahmed*
scan of interatomic distances and valence angles. can produce the
coordination table for each atom. calculates the e.s.d.'s ignoring
errors in unit-cell parameters and the covariances. limit 150
atoms and 1000 distances.

143 IBM36050 FORTRAN4 NRC-14  AGA  4 AHMED  LCA
huber
analysis of agreement between fo and fc in terms of fo amplitudes,
sin(theta), or layer. prints outstanding discrepancies between obs
and calc data.

144 IBM36050 FORTRAN4 NRC-21  POW, DHK DST HKL ASG  10 AHMED  LCA
pippy
interplanar spacings. sorts in order of d(hkl), and prints separate
lists for permissible and prohibited reflections.

145 IBM36050 FORTRAN4 NRC-22  GEO, MPL DIH  6 AHMED  LCA
pippy, ahmed*
mean planes. calculates the least squares plane through a group of
atoms, and the deviations of other atoms from the plane. tests the
planarity by the chi-squared test. limit 150 atoms.

146 IBM36050 FORTRAN4 NRC-23  SFT, CSF  13 AHMED  LCA
pippy
structure factor tables. can pack over 2500 reflexions on one page
in the proper dimension ratio for pages of acta cryst.

147 IBM36050 FORTRAN4 NRC-24  PRJ, ORT  4 AHMED  LCA
singh, ahmed*
projection of atoms onto a plane. produces three cartesian
coordinates per atom, including distance from plane of projection.
limit 150 atoms.
148 ICL 4120 NEAT RFL 226 ALGCON ST08 pow 2? F UKAEA LNA
CONNOLLY
CONVERTS MERCURY 5 HOLE TAPE TO 8 HOLE ISO 7 EVEN PARITY CODED TAPE

149 ICL 4120 FORTRAN4 RFL 336 FIRESCALP 18TD17 POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
CONVERSION OF FIELD WIDTH 18 TO FIELD WIDTH 17

150 ICL 4120 FORTRAN4 RFL 337 FIREPAIR TOTAL POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
COUNTS NUMBER OF ANGLE/COUNT PAIRS ON A TAPE

151 ICL 4120 FORTRAN4 RFL 292 FIRETWIST INVERT POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
INVERTS THE SEQUENCE OF ANGLE/COUNT PAIRS ON A TAPE

152 ICL 4120 ALGOL RFL 297 FIREPLOT PLT C POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
PLOTS COUNTS VS TIMES AS A FUNCTION OF ANGLE USING A PLOTTER

153 ICL4120 FORTRAN4 RFL 330 FIREPJP EDIT POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
EDITS OUT PARTITIONS OF A LARGE TAPE BEARING ANGLE/COUNT PAIRS

154 ICL4120 ALGOL RFL 334 FIRESPLARK EDITS POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREBRAND2 OR FIRESTREAK

155 ICL4120 FORTRAN4 RFL 333 FIREGLOW EDITS POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREBRAND2 OR FIRESTREAK

156 ICL4120 ALGOL RFL 357 FIREBRAND2 PLT MAX POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
PLOTS COUNTS AS FUNCTION OF ANGLE AND LOCATES ANGLE OF MAX COUNT

157 ICL4120 ALGOL RFL 335 FIRESTREAK FMAX POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
FINDS POSITIONS OF MAXIMUM IN A SEQUENCE OF COUNTS BY FOURIER METHOD

158 ICL4120 ALGOL RFL 7083 FIRESTAR LCD T POW UCP 9 F UKAEA LNA
ASTELE G FERGUSC I F*
DETERMINES UNIT CELL FROM INDEXED POWDER PATTERN TRG REPORT 1812(S)

159 ICL4120 ALGOL RFL 7069 FIRESTAR LCD MO POW UCP 10 F UKAEA LCA
ASTELE G FERGUSC I F*
DETERMINES UNIT CELL FROM INDEXED POWDER PATTERN TRG REPORT 1812(S)

160 ICL4120 ALGOL RFL 7072 FIRESTAR LCD TEHR POW UCP 9 F UKAEA LCA
ASTELE G FERGUSC I F*
DETERMINES UNIT CELL FROM INDEXED POWDER PATTERN TRG REPORT 1812(S)

161 ICL4120 ALGOL RFL 7037 FIRESTAR LCD C POW 7 F UKAEA LCA
ASTELE G FERGUSC I F*
DETERMINES UNIT CELL FROM INDEXED POWDER PATTERN TRG REPORT 1812(S)

162 ICL4120 ALGOL RFL 7062 FIRECRACKER CAL POW 1 F UKAEA LCA
ASTELE G FERGUSC I F*
DETERMINES Y=M*X+C CALIBRATION FOR 2CIRCLE DIFFRACTOMETER WITH STANDARD
163 ICL4120 ALGCL RFL 331 FIREDAWG EDITW POW
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREWOLF

164 ICL4120 FORTRAN4 RFL 332 FIREDOG EDITW POW
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREWOLF

165 ICL4120 FORTRAN4 RFL 359 FIREADD EDITF POW
FERGUSON I F HUGHES T E
ADDS THE CORRESPONDING ANGLES TO A SEQUENTIAL LIST OF COUNTS

166 ICL4120 FORTRAN4 RFL 360 FIRECOP EDITG POW
FERGUSON I F HUGHES T E
ALTERS THE ANGLES ON A SEQUENTIAL LIST OF ANGLES AND COUNTS

167 ICL4120 ALGOL RFL 267 FIREWOLF INT POW LB
FERGUSON I F HUGHES T E
INTEGRATES THE INTENSITY OF A BRAGG REFLEXION AND FINDS ITS BREADTH

168 ICL4120 ALGOL RFL 231 FIREDRAKE POW BRG DHK DST
FERGUSON I F HUGHES T E STOCKS C
CALCULATES POSITIONS OF BRAGG REFLEXIONS FOR ANY UNIT CELL

169 ICL4120 ALGOL RFL SS FIREBALL POW INT
FERGUSON I F HUGHES T E STOCKS C
CALCULATES INTERPLANAR ANGLES BETWEEN A GIVEN AKL AND ALL OTHERS

170 ICL 4120 FORTRAN4 RFL 347 FIRECUB POW SKH LB
FERGUSON I F TSEUNG G C Y
CALCULATES SCHERRER CONSTANTS FOR ANY HKL FOR ANY CUBOID

171 ICL 4120 FORTRAN4 RFL 350 FIREPRISM POW SKH LB
FERGUSON I F TSEUNG G C Y
CALCULATES SCHERRER CONSTANTS FOR ANY HKL FOR ANY TRIANGULAR PRISM

172 ICL 4120 FORTRAN4 RFL 348 FIREHEX POW SKH LB
FERGUSON I F TSEUNG G C Y
CALCULATES SCHERRER CONSTANTS FOR ANY HKL FOR ANY HEXAGONAL PRISM

173 ICL 4120 FORTRAN4 RFL 349 FIRETANGLE POW SKH LB
FERGUSON I F TSEUNG G C Y
CALCULATES SCHERRER CONSTANTS FOR ANY HKL FOR ANY RECTANGULAR CUBOID

174 ICL 4120 FORTRAN4 RFL 352 FIRERICE POW LB
FERGUSON I F TSEUNG G C Y
USED IN CONJUNCTION WITH FIRECHOP

175 ICL 4120 FORTRAN4 RFL 340 FIRERICE POW LB
FERGUSON I F TSEUNG G C Y
WITH FIRECHOP REMOVES ALPHA2 COMPONENT OF DOUBLET BY RACHINGERS METHOD

176 ICL 4120 ALGCL RFL 254 FAIRFAX POW
FERGUSON I F HUGHES T E
INTERCONVERSION OF THETA D SIN2THETA AND TWOthETA

177 ICL 4-70 FORTRAN4 HMJSRO03 FIREFLY POW BRG CPP DHK DST ASG 136 F UKAEA LCA
FERGUSON I F KIRKAN J E
GIVEN HKL, DETAILS OF THE UNIT CELL AND THE EQUIPMENT THIS PROGRAM
WILL CALCULATE THE INTENSITIES OF UP TO 100 BRAGG REFLECTIONS AND,
AS OPTIONS, INTRATOMIC DISTANCES AND ANGLES IN THE UNIT CELL. THE
PROGRAM WILL MAKE FULL ALLOWANCE FOR MULTIPLICITIES GIVEN A SPACE
GROUP AND WILL COMPARE CALCULATED AND OBSERVED INTENSITIES

178 ICL 4-70 FORTRAN HMJSR002 FENRIS POW LB DST
FERGUSON I F KIRWAN J E
GIVEN THE AREAS AND PEAK HEIGHTS OF BRAGG REFLECTIONS THIS PROGRAM
DERIVES THE INTEGRAL BREADTHS OF BRAGG REFLECTIONS THEN AFTER
CORRECTION FOR ALPHA1/ALPHA2 AND INSTRUMENTAL BROADENING THE
CRYSTALLITE SIZE FOR EACH REFLEXION IS CALCULATED. THEN USING
A LEAST SQUARES TREATMENT OF A HALL PLOT THE TRUE CRYSTALLITE
SIZE, LATTICE STRAIN, CORRESPONDING SURFACE AREAS AND ENERGIES ARE CALC.

179 IBM1130 FORTRAN DRF, LPC PRC WEI
EQUI-INCLINATION, NORMAL BEAM WEISSENBERG, EXTENDED SPOT CORRECTION
HIGHER LEVEL PRECESSION

180 IBM1130 FORTRAN PRO, AVG CMP SCL SRT
INDEX TRANSFORMATION, SORTING, SCALING, DETERMINATION OF SCALES
BETWEEN SETS (UP TO 8), AVERAGING

181 IBM1130 FORTRAN DIR, SCL WSN EHS
SCALE AND TEMP. FACTORS BY WILSON PLOT, NORMALIZED SF, SORTED IN DE-
CREASING ORDER OF MAGNITUDE (UP TO 7000 REF.). MAY BE RENORMALIZED
IN TERMS OF DIFFERENT CATEGORIES

182 IBM1130 FORTRAN SFC, ASG SAN SFO
UP TO 100 ATOMS IN ONE RUN, NO LIMIT IN MULTIPLE RUNS

183 IBM1130 FORTRAN REF, ASG SCL XYZ BLS ESD BIJ
50 ATOMS MAX., 29 ATOMS FOR 8K VERSION. UP TO 5000 REFLEXIONS WITH
THE SINGLE DISK SYSTEM.

184 IBM1130 FORTRAN FOU, TMO FBL FPD FR3
1/1000 TH OF CELL OR ITS MULTIPLE.

185 IBM1130 FORTRAN SCF, ISC
N-POINT INTERPOLATION BY AITKEN (N: 2-9)

186 IBM1130 FORTRAN LAT, LCR ASG
LEAST-SQUARES REFINEMENT OF THE APPROXIMATE VALUES WITH THE OBSERVED
SINE THETA VALUES.

187 IBM1130 FORTRAN MSC, ASG HKL BRG DHK DST
GENERATES INDEPENDENT OR ALL POSSIBLE REFLEXIONS WITH A GIVEN SPACE
GROUP. SORTED OUTPUT.

188 IBM1130 FORTRAN DIF, CIR HKL GSC
FOR CARD CONTROLLED PICKER, SETTING ARE SORTED TO OPTIMIZE DIFFRACTO
**METER MOVEMENT**

189 IBM 1130 FORTRAN

DRF, LPC, CIR, SCL

16 SHIONO LCA

FOR FACS-I, CAD-3 ETC. SCALES THE INTENSITIES WITH STANDARDS BY N-POINT INTERPOLATION

190 IBM 1130 FORTRAN

GEO, ASG, SBL, SID, SAN

16 SHIONO LCA

SHIONO, CHU S C
SCAN ALL POSSIBLE INTER AND INTRA MOLECULAR DISTANCES. SORTED DISTANCES OUTPUT.

191 IBM 1130 FORTRAN

GEO, TOR

16 SHIONO LCA

GARDLAND, SHIONO
ALL TORSION ANGLES WITH DISTANCES LESS THAN A LIMIT.

192 POP 10 FORTRAN

SFT, CSF

32 SHIONO LCA

SHIONO, SAX
PACKS UP TO 2800 REFLECTIONS PER PAGE, PRINTS ONLY RUNNING INDEX EVERY TIME. THE LENGTH OF EACH COLUMN IS AUTOMATICALLY ADJUSTED.

193 CDC 3600 FORTRAN

CEL PAR, LCR, XDN, WEI, ASG

20 WADHWAAN LIA

WADHWAAN
LEAST-SQUARES REFINEMENT ON BRAGG THETA OBTAINED FROM ZERO-LAYER WEISSENBERG PHOTOCCopy, PROVISION FOR UPTO FOUR CORRECTION TERMS FOR SYSTEMATIC ERRORS, USER-DEFINED CORRECTION FUNCTIONS. ANY NUMBER OF PARAMETER SELECTIONS POSSIBLE IN THE SAME RUN. PLOTS THETA(OBS) - THETA(CAL) VERSUS THETA(CAL) FOR EACH PARAMETER SELECTION CARD. CONVERTS REFINED PARAMETERS TO DIRECT SPACE, WITH STANDARD DEVIATIONS.

194 ICL 4130 FORTRAN CRYSTAL I PRO, AVG OUA, SRT, DRF, LPC, PRC, WEI

15 CROSS LCA

A PHOTOGRAPHIC DATA REDUCTION PROGRAM. PARTS REQUIRED ARE USER DETERMINED. INTENSITIES FROM PACKS OF FILMS PUT ON COMMON SCALE, LP CORRECTIONS FOR WEISSENBERG AND PRECESSION CAMERAS, W-FACTOR, EQUVALENT REFLECTIONS AVERAGED, UNOBSERVEDS INSERTED AT ZERO INTENSITY, REFLECTIONS SORTED IN EACH LAYER. O/P IS HKL F**2 SINE SQUARED THETA.

195 ICL 4130 FORTRAN CRYSTAL II DRF, CIR, LPC, WTA

32 POWELL LCA

GRiffiths, Powell
A DATA REDUCTION PROGRAM FOR FOUR CIRCLE DIFRACTOMETER DATA. CORRECTIONS APPLIED FOR COUNTING LOSSES DUE TO RESOLVING TIME OF COUNTER, BACKGROUND RADIATION, LOST OR EXCESS COUNTS CAUSED BY DRIFT OF ELECTRONICS AND LORENTZ-POLARISATION FACTORS. IN ADDITION TESTS ARE INCLUDED TO DETECT CRYSTAL MOVEMENT OR EXCESSIVE ELECTRONIC DRIFT. THE E.S.D. OF EACH INTENSITY IS CALCULATED.

196 ICL 4130 FORTRAN CRYSTAL II PRO/DRF, AVG CMP OUA, SCHR SRT

32 POWELL LCA

POWELL
A UNIQUE SET OF REDUCED DATA ARE EXTRACTED FROM OUTPUT OF CRYSTAL-I. DEALS WITH SPACEGROUPS 1-141, DATA ARE SORTED IN RUNNING L,K,H. TESTS ARE MADE FOR UNOBSERVED REFLECTIONS AND THESE ARE INSERTED WITH ZERO INTENSITY AND MARKED.

197 ICL 4130 FORTRAN CRYSTAL III PRO/DRF, LAY, SCL, ISC, WSN, FOB

32 POWELL LCA

POWELL
A PROGRAM WHICH ACCEPTS PROCESSED INTENSITY DATA AND PLACES THEM ON THE SAME OVERALL ABSOLUTE SCALE USING AN ADAPTATION OF WILSON
STATISTICS. AN OVERALL ISOTROPIC TEMPERATURE FACTOR IS DEDUCED AND THE PROGRAM CALCulates THE PREDICTED ACCURACY OF ATOMIC POSITIONS FOR THE AMOUNT OF DATA COLLECTED (CRUICKSHANK ACTA 13, 774).

198 ICL 4130 FORTRAN CRYSTL-4 FOU, FR3 FBL FPD SHF TMD 32 POWELL LCA
GRiffiths, Powell
PROGRAM DEALS WITH SPACEGROUPS 1 TO 74 EXCLUDING FDD2 AND FDD4. DATA MAY BE INPUT IN ANY FORM SINCE A FAST SORTING ROUTINE IS INCLUDED. OUTPUT CAN BE ADJUSTED APPROXIMATELY TO SCALE AND INCORPORATES A BETA ANGLE.

199 ICL 4130 FORTRAN CRYSTL-5 REF, HLS XYZ BIJ FDG LAY LSP SCH 32 POWELL LCA
GRiffiths, Powell
A BLOCK-DIAGONAL STRUCTURE FACTOR/LEAST SQUARES PROGRAM. POSITIONS ARE REFINED FROM 3X3 MATRICES, ANISOTROPIC TEMP. FACTORS FROM 6X6 MATRICES, AND ISOTROPIC TEMP. FACTORS FROM A 1X1 MATRIX WITH SCHOMAKER CORRECTION. AN OVERALL SCALE FACTOR IS OBTAINED FROM A 2X2 MATRIX WITH DUMMY OVERALL B-FACTOR. LAYER SCALES ARE OBTAINED FROM A SET OF NORMAL EQUATIONS WITH THE DUMMY OVERALL B-FACTOR SHIFT.

200 ICL 4130 FORTRAN CRYSTL-6 GEO, SAN SBL SID ESD MPL DIH TEL 32 POWELL LCA
GRiffiths, Powell
MOLECULAR GEOMETRY PROGRAM INTENDED TO LINK WITH THE CCS STRUCTURE FACTOR/LEAST SQUARES PROGRAM CRYSTL-5.

201 IBM36065 FORTRAN4 FOU, FBL ASG FR3 FUM SHF SAN SAD ARAKI MCA
ARAKI FINGER
A GENERALIZED FOURIER PROGRAM. PARAMETER LIMITS ARE FAR BEYOND PRACTICAL USE, EXCEPT POINTS ON LINE DUE TO PRINTER. ALL KINDS OF FOURIER TYPE MAP, WEIGHT ON COEFFICIENTS. OPTIONS FOR SECTION MAP PRINTED FORM INCLUDING TRIANGLE SHAPE DUE TO DIAGONAL MIRROR. DENSITY BY TWO LETTERS. TESTED FOR CDC6600.

202 360/370 FORTRAN4 SADIAN69, GEO SAN SBL DRW PRJ 32 BAUR LI
BAUR, Wenninger
ASG, STANDARD DEVIATIONS ACCORDING TO DARLOW AND AHMED & CRUICKSHANK PREPARES PRINTER PLOTS OF THE THREE MAIN PROJECTIONS OF THE CRYSTAL STRUCTURE AND PRESENTS SCALED ORTHOGONAL COORDINATES FOR THE EXECUTION OF STRUCTURE DRAWINGS.

203 IBM7094 FORTRAN2 MANI2C, EST ASG 32 BAUR LIA
BAUR
ELECTROSTATIC ENERGY CALCULATIONS BASED ON BERTAUT AND EWALD FORMULAS, INVERSE POWER REPULSION AND VAN DER WAALS TERMS CAN BE PROVIDED FOR. CONTAINS A SET OF SUBROUTINES FOR PERFORMING SOLID ANALYTICAL GEOMETRY AND SUBROUTINES FOR CALCULATING WATER MOLECULE ORIENTATIONS IN HYDRATES.

204 360/370 FORTRAN4 CALHPO, GEO ASG 32 BAUR LIA
BAUR
CALCULATES HYDROGEN ATOM POSITIONS IN CRYSTALLINE SOLIDS, BASED ON GEOMETRIC CRITERIA. THE HYDROGEN ATOMS CAN BE PLACED ALONG SPECIFIED LINES OR PLANES IN THE STRUCTURE, OR AT SPECIFIED ANGLES OFF THESE LINES OR PLANES, WHICH ARE DEFINED BY INDICATING THE COORDINATES OF POINTS THROUGH WHICH THEY GO.

205 360/370 FORTRAN4 LPFPRE, COR LPC PRC ASG 32 BAUR LIA
BAUR
COMPLETELY GENERAL, ANY ORIENTATION OF THE CRYSTAL RELATIVE TO THE CAMERA IS ALLOWED.
206 360/370 FORTRAN4 OUTPICK, PRO DRF ASG 64 BAUR LIS
BAUR IBERS & DOEDENS PICKOUT,CDC3400 AVG CMP OUA NET SCL SRT CIR LPC hTA

207 IBM36091 FORTRAN4 DR012 FIGATOM, DRW PLT STE ASG SPL 400 LANGLET LIS
LANGLET
VERY FEW INPUT C. NEC. ; NO FORMAT NEC. FOR DATA; NO SYMMETRY C. NEC.
STEREO DRAWINGS OBTAINED ON BENSON PLOTTER OR IBM 2250 UNIT;
MAY CONSIDER 1000 ATOMS OR MORE (ADJUSTABLE DIMENSIONS);
AUT. OVERLAPPING FOR SPHERICAL ATOMS : NO HAND CORRECTIONS NEC.:
AUT. BOND & COORDINATION POLYHEDRON DRAWING; CAL. BOND LENGTH & COMP.
100 ATOMS:15 SEC.; 400 ATOMS:80 SEC. (LOWER CORE REQ. WITH OVERLAY).

208 ICLKDF9 ALGOL JYQ6160 MSC, POW DEC CLARKE LIC
CLARKE
DECONVOLUTION OF CURVES BY CONSTRAINED LEAST SQUARES.FOR SIZE AND STRAIN
ANALYSIS ETC.,WHERE FOURIER TECHNIQUES INAPPLICABLE DUE TO SIMILARITY OF
CURVES OR PCCR QUALITY DATA.CYCLIC CASES AS FOR ORIENTATION DISTRIBUTIONS
HANDLED AS WELL AS NON CYCLIC-INSTRUMENTAL AND OBSERVED CURVES NEED EQUAL
NUMBERS OF POINTS N. STORE APPROXIMATELY (8+NXNX0.002)K.
SPEED (10+ 0.00004NXNXN) SECS.CHARGE NEGOTIATED FOR COMMERCIAL USE.

209 ICLKDF9 ALGOL JYQ4445 PLT, HKL STE LAU CLARKE LIC
CLARKE, WOOLF
CALCULATES FROM CELL DIMENSIONS AND PROJECTION AXIS ONLY,PRINTS AND/OR
PLOTS COORDINATES OF POLES FOR STEREOGRAPHIC AND/OR LAUE PATTERNS
AS RECORDED ON FLAT PLATE FRONT OR BACK REFLECTION,OR CYLINDRICAL CAMERAS.
STORAGE DYNAMIC APPROXIMATELY (6+0.013N)K FOR N POLES.SPEED APPROX.
(6+0.001NXN) SECONDS.CHARGE NEGOTIATED FOR COMMERCIAL USE.

210 ICLKDF9 ALGOL JYQ8484 MSC, XDN KOS DHK LNM CLARKE LIC
CLARKE
CALCULATES PATTERN CENTRE SPACING AND DIRECTION COSINES OF POLE FOR
SINGLE WAVELENGTH KOSSEL PATTERNS WITHOUT INFORMATION ON LOCATION OF
SOURCE.DETECTS SLIGHTLY ERRONEOUS COORDINATE DATA.DYNAMIC STORAGE.
MINIMUM USEFUL ABOUT 10K.SPEED APPROX. (10+SIGMA0.0001NXNXN) SECONDS.
N:NUMBER OF POINTS PER CONIC.CHARGE NEGOTIATED FOR COMMERCIAL USE.

211 HONTS ALGCL JYQ021 POW, HKL DHK DST CLARKE LIC
CLARKE
ALL CRYSTAL CLASSES DISTINGUISHABLE BY POWDER DIFFRACTION,CENTRED
ABSENCES OMITTED.FOR HONEYWELL-FORMERLY BULL-GE COMMERCIAL TS TERMINAL.
INSTRUCTIONS SUPPLIED AT RUN TIME,DATA SUPPLIED INTERACTIVELY,DESIGNED
FOR PERSONNEL WITH NO PROGRAMMING EXPERIENCE AND LITTLE CRYSTALLOGRAPHIC
KNOWLEDGE. SPEED FOR N REFLECTIONS (6+ 0.002NXV) SECONDS.
CHARGE NEGOTIATED FOR COMMERCIAL USE.

212 IBM36044 FORTRAN LAT, RJC LAWTON LIC
LAWTON
TRACER II. COMPUTES REDUCED UNIT CELL OF ANY INPUT CELL AND FROM IT
DETERMINES THE UNIT CELL OF HIGHEST POSSIBLE SYMMETRY (i.e., CRYSTAL
SYSTEM, BRAVAIS LATTICE, AND CELL PARAMETERS). TRANSFORMATION
MATRICES ARE ALSO OUTPUT. MATHEMATICAL PROCEDURE BASED ON CH. 11 IN
'THE POWDER METHOD IN X-RAY CRYSTALLOGRAPHY' BY AZAROFF AND BUERGER,
1958. PROGRAM IS AVAILABLE IN EITHER BCD OR EBCDIC CODE.

213 ICL4130 FORTRAN XRAY63 ABS,ABA ALCOCK LIC
ALCOCK
VERY GENERAL IN ATLAS VERSION, INCLUDING MANY RECORDING GEOMETRIES
AND CALCULATION OF EXTINCTION COEFFICIENT. 4130 VERSION IS STAND-
ALONE.

214 ICI1905 FORTRAN PLT, POL
ROTHWELL
CONSTRUCTION OF POLE FIGURES DRAWN ON A DIGITAL PLOTTER. REFERENCES
LEWIS, D. ET AL. STUDY OF TWINSING IN HEAVILY-DRAWN HIGH-DENSITY
POLYETHYLENE (1971) J. APPL. CRYST. 4, 1
ROTHWELL, M. A. COMPUTER PROGRAM FOR THE CONSTRUCTION OF POLE FIGURES
(1971) J. APPL. CRYST. TO BE PUBLISHED.

215 CI1510 ASLOGA S24K AFI, BIS ESD FLS LAD LAY LSP XYZ 12 BASSI
BASSI G C
REFINEMENT ON SINGLE REFLECTIONS. MULTIPLICITY IS ALLOWED. SPACE GROUP
IS DESCRIBED AS PRINTED IN THE INTERNATIONAL TABLES.

216 CI1510 ASLOGA S24K AFI, BIS ESD FLS LAD LAY LSP XYZ 12 BASSI
BASSI G C
SAME AS AFI PLUS: REFINEMENT ON MULTIPLE REFLECTIONS AS IN POWDER
TECHNIQUE AND POSSIBILITY OF USING ONE GROUP OF X-RAYS INTENSITIES
AND ONE GROUP OF NEUTRONS INTENSITIES.

217 CI1510 ASLOGA S24K INS, ASG SAD SIS 12 BASSI
BASSI G C
GENERAL PROGRAM GIVING INTENSITY WITH MULTIPLICITY, STRUCTURE FACTOR
WITH SIGN OR PHASE.

218 CI1510 ASLOGA S24K IND, HKL DST 12 BASSI
BASSI G C
IND TAKES ACCOUNT OF GENERAL CONDITIONS ON (HKL).

219 CI1510 ASLOGA S24K DII, ASG BOL 12 BASSI
BASSI G C, GEYNET M
PRINTS ALL DISTANCES LESS THAN ONE LIMIT PER PAIR OF SITES.

220 CI1510 ASLOGA S24K FOU, FR3 FPD 12 BASSI
BASSI G C, GEYNET M
GIVES A MAP IN REC FOR NEGATIVE PARTS AND BLACK FOR POSITIVE REGIONS
USING A SET OF 34 DIFFERENT ALPHANUMERIC CHARACTERS.

221 CI1510 ASLOGA S24K GOU, FR3 FPD 12 BASSI
BASSI G C, GEYNET M
SAME AS FOU BUT PERMITS A LOCAL DISTORTION TO INCREASE THE RESOLUTION
POWER OF THE MAP.

222 CI1510 ALGOL S24K AFFIMAILLE, LCR 12 BASSI
BASSI G C, ROUDALT M
CELL REFINEMENT FROM POWDER DIFFRACTION PATTERNS. SIX SEPARATE PRO-
GRAMS, ONE PER SYSTEM.

223 CI1510 ALGOL S24K TRACE, PLT DRW 12 BASSI
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224 CI1510 ALGOL S24K SEPARRAIES, PRS 12 BASSI
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225 CI1510 ALGOL S24K ABSORPLAQUES, ABS
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226 CI1510 ALGOL S24K DIAGNEUTRONS, FOB LPC
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227 CI1510 ALGOL S24K ANGLES, DIF GSC
BASSI G C, GUITEL J C
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228 CI1510 ALGOL S24K GENERATEJR, DIF HKL
BASSI G C
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229 CI1510 ALGOL S24K SIMPLEXE, SPW ASD
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230 CI1510 ASLOGA S24K LAMI, DIF CCD CIR GSC OMC QMR RTS 12 BASSI
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231 CDC6600 FORTRAN FLETCHER, STEPHENS
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232 CDC6600 FORTRAN STEPHENS
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CORRECTED FOR LORENTZ AND POLARISATION FACTORS

233 NEAC2200 FORTRAN ASHIDA
ASHIDA 'SIGMA' PERFORMS WILSON STATISTICS AND SIGMA 2 INTERACTIONS SEARCH

234 NEAC2200 FORTRAN ASHIDA
ASHIDA

235 NEAC2200 FORTRAN ASHIDA
ASHIDA 'HBL5-IV' PERFORMS REF, GEO, SFT AND FOU IN A SINGLE PROGRAM
REF, BLS XYZ BIJ SCL ESD FDG LAD LSP (ASG)
GEO, SBL SAN (ASG)
SFT, CSF AGR (ASG)
FOU, FBL (TMC)
236 NEAC2200 FORTRAN UNICS GEO, DIH MPL ROT SAN SID SBL ASG 16 ASHIDA LIA ASHIDA

237 ICL1905E FORTRAN HURAY-05 CINTER,ISC 05 CMORGAN LIA HALL, MORGAN*
THIS PROGRAM CONSTRUCTS THE DATA FILE NECESSARY TO USE CIS0SF AND CANILS, IN THE HURAY SYSTEM.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

238 ICL1905E FORTRAN HURAY-10 CANILS, TMO BIJ BLSE ESD FDG LSP 20 CMORGAN LIA HALL, MORGAN*
REFINES POSITIONAL, ISOTROPIC AND ANISOTROPIC THERMAL PARAMETERS;
OVERALL SCALE FACTOR, UP TO 60 ATOMS IN STANDARD FORM, FUDGE FACTORS.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

239 ICL1905E FORTRAN HURAY-11 CIS0SF, SIS TMO 16 CMORGAN LIA HALL, MORGAN*
FAST STRUCTURE FACTOR CALCULATION FOR EARLY STAGES OF SOLUTION.
RESCALES OBSERVED AMPLITUDES ON BASIC OF OBSERVED AND CALCULATED
SUMS IF REQUIRED.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

240 ICL1905E FORTRAN HURAY-20 CF0U R, TMO FPD FRS 29 CMORGAN LIA HALL, MORGAN*
DOES NOT ACCEPT FC02 OR FDDD. REQUIRES SEPARATE OUTPUT PROGRAM CFOUT.
LIMIT OF 3000 INDEPENDENT REFLEXIONS.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

241 ICL1905E FORTRAN HURAY-21 CFOUT 21 CMORGAN LIA HALL, MORGAN*
OUTPUTS RESULTS OF CF0U R IN ANY OF 6 POSSIBLE ORIENTATIONS ON
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PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

242 ICL1905E FORTRAN HURAY-40 CMOLGY, MPL 17 CMORGAN LIA HALL, MORGAN*
CALCULATES SPECIFIED ANGLES AND BONDS, AND MEAN PLANES. ALSO SPECIFIED
INTERMOLECULAR DISTANCES.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

243 UNC1105 FORTRAN FFOCUS1, SAXS DESM 16 VONK LIA VONK
SAXS DESMEARING PROCEDURE. SEE J. APPL. CRYST. (1971) 4, 340

244 IBM36065 ALGOL60 LSP, POW UCP (HKL IND DHK DST) 24 VISSER LIA VISSE R J W
INPUT: LINE POSITIONS (2THETA, D OR Q) + APPROXIMATE CELL CONSTANTS
OUTPUT: REFINED CELL CONSTANTS+STAND. DEV., ORDERED LIST OF
2THETA-D-HKL-Q. USES SPACEGROUP RESTRICTIONS.
TWO VERSIONS, ONE FOR 2-PARAMETER PROBLEMS, ONE FOR TMO.

245 IBM36065 ALGOL60 ITO-ALG, POW LCD 32 VISSER LIA VISSE R J W
FINDS UNIT CELL FROM POWDER PATTERN. NEEDS AT LEAST 20 LINES,
MEASURED AS ACCURATELY AS POSSIBLE; A FEW IMPURITY LINES DO
NOT MATTER.

246 IBM36065 PL/1 ITO-PL/1, POW LCD 32 VISSER LIA VISSE R J W
FINDS UNIT CELL FROM POWDER PATTERN. NEEDS AT LEAST 20 LINES,
MEASURED AS ACCURATELY AS POSSIBLE, A FEW IMPURITY LINES DO NOT MATTER.

247 IBM36091 FORTRAN4 ORESTES DIR, EHS STF BIJ ASG ACT WSN WTA 25 THIessen LEVY
ESTIMATES OVERALL SCALE AND THERMAL PARAMETERS (ISOTROPIC OR ANISOTROPIC) FROM SINGLE-CRYSTAL X-RAY OR NEUTRON DIFFRACTION DATA, CALCULATES AND SORTS A SET OF NORMALIZED STRUCTURE-FACTOR MAGNITUDES, AND COMPUTES RELEVANT STATISTICS OF THE SET.
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338 WORLD LIST OF COMPUTER PROGRAMS

96 IBM36065 PL/1  FED, ASG GRT  32 JACOBSN LCA
92 IBM36065 PL/1  FOU, FCI ASG FPD FR3  32 JACOBSN LCA
95 IBM36065 PL/1  FOU, FCI FPD TRI FR2  32 JACOBSN LCA
93 IBM36065 PL/1  FOU, FCI FTM FR3  32 JACOBSN LCA

246 IBM36065 PL/1  ITO-PL/1, POW LCD  32 VISSER LCA
94 IBM36065 PL/1  MSG, FCT FR3 VVR TMO  32 JACOBSN LCA
20 IBM36075 FORTRAN  DRF, ABI CIR LPC PEX SEX  39 BRANDT LCA
19 IBM36075 FORTRAN  DRF, ABI CIR &EI LPC PEX SEX  26 BRANDT LCA
33 IBM36075 FORTRAN  DRF, HKL NET LPC DUQ FOB  26 BRANDT LCA
22 IBM36075 FORTRAN  DRF, PEX SEX  13 BRANDT LCA
27 IBM36075 FORTRAN  DRF, WSN  13 NORD LCA
18 IBM36075 FORTRAN  FED, ADL FST PRT  13 BRANDT LCA
21 IBM36075 FORTRAN  FOU, FPD FPS SHF SFC  45 BRANDT LCA
28 IBM36075 FORTRAN  PLT, DRW TEL  .6 NORD LCA
26 IBM36075 FORTRAN  PLT, GDP DRW TEL  43 NORD LCA
30 IBM36075 FORTRAN  POW, CPP BRG DHK  13 NORD LCA
32 IBM36075 FORTRAN  PRO, ADL PRT  30 BRANDT LCA
25 IBM36075 FORTRAN  REF, FLS LAY BIJ XYZ OCC WAN  52 BRANDT LCA
23 IBM36075 FORTRAN  REF, HLS BIS LAY XYZ WAN ASG  26 BRANDT LCA
24 IBM36075 FORTRAN  REF, FLS LAY BIJ XYZ ESD WAN  39 NORD LCA
31 IBM36075 FORTRAN  SFT, CSF  32 BRANDT LCA
11 IBM36075 FORTRAN  SFT, CIR HKL ASG  15 NORD LIA
6 IBM36075 FORTRAN  SFT, CIR HKL ASG  20 KOENIG LIA
83 IBM36075 FORTRAN  ORTEP-2 PLT, DRW TEL STE SBL SAN  50 JOHNSON LCA
74 IBM36075 FORTRAN  ORTEP-3 PLT, DRW TEL STE SBL SAN  20 TOURNAR MIA
76 IBM36075 FORTRAN  ORTEP-7 PLT, DRW TEL STE SBL SAN  25 TOURNAR MIA
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85 IBM36091 FORTRAN  ORTEP-3 PLT, DRW TEL STE SBL SAN  20 TOURNAR MIA
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78 IBM36091 FORTRAN  ORTEP-20 PLT, DRW TEL STE SBL SAN  20 TOURNAR MIA
79 IBM36091 FORTRAN  ORTEP-21 PLT, DRW TEL STE SBL SAN  20 TOURNAR MIA
80 IBM36091 FORTRAN  ORTEP-22 PLT, DRW TEL STE SBL SAN  20 TOURNAR MIA
203 IBM7094 FORTRAN 2 MANIOC, EST ASG  32 BAUR LIA
209 ICL7069 ALGCL JQY4445 PLT, HKL STE LAU  32 BAUR LIA
208 ICL7069 ALGCL JQY6160 MSC, KDN DEC  32 BAUR LIA
210 ICL7069 ALGCL JQY9484 MSC, XDN KOS DHK LMN  32 BAUR LIA
214 ICL7105 FORTRAN 2 PLT, POL  16 ROTHW LCA
213 ICL7105E FORTRAN 4 HWAY-05 CINTER, SMC  16 ROTHW LCA
238 ICL7105E FORTRAN 4 HWAY-10 CANILS, TM0 BIJ BLS ESD FGW LSP  16 ROTHW LCA
239 ICL7105E FORTRAN 4 HWAY-11 CISOFO, TM0 BIJ BLS ESD FGW LSP  16 ROTHW LCA
240 ICL7105E FORTRAN 4 HWAY-20 CF DURR, TM0 BIJ BLS ESD FGW LSP  16 ROTHW LCA
241 ICL7105E FORTRAN 4 HWAY-21 CF DURR, TM0 BIJ BLS ESD FGW LSP  16 ROTHW LCA
242 ICL7105E FORTRAN 4 HWAY-40 CMOLGY, MPL  16 ROTHW LCA
178 ICL4-70 FORTRAN 4 HWAY-002 NENRIS POW LB DST  16 ROTHW LCA
177 ICL4-70 FORTRAN 4 HWAY-003 EWYRI POW LB DST  16 ROTHW LCA
169 ICL4120 ALGCL RFL 55 FIREBALL POW INT  16 TOURNAR LCA
176 ICL4120 ALGCL RFL 254 FAIRFAX POW  16 TOURNAR LCA
152 ICL4120 ALGOL RFL 297 FIREPLOT PLT C POW 1 F UKAEA LNA
154 ICL4120 ALGOL RFL 334 FIRESPARK EDITS POW 1 F UKAEA LNA
157 ICL4120 ALGOL RFL 335 FIRESTREAK FMAX POW 1 F UKAEA LNA
156 ICL4120 ALGOL RFL 357 FIREBRAND2 PLT MAX POW 1 F UKAEA LNA
168 ICL4120 ALGOL RFL 231 FIREDRAKE POW BRG DHK DST 8 F UKAEA LNN
167 ICL4120 ALGOL RFL 267 FIREWOLF INTF POW LB 4 2 F UKAEA LNA
163 ICL4120 ALGOL RFL 7037 FIRESTAR LGD C POW 7 F UKAEA LCA
162 ICL4120 ALGOL RFL 7062 FIRECRACKER CAL POW 1 F UKAEA LCA
159 ICL4120 ALGOL RFL 7069 FIRESTAR LGD MO POW UCP 10 F UKAEA LCA
160 ICL4120 ALGOL RFL 7072 FIRESTAR LGD TEHR POW UCP 9 F UKAEA LCA
158 ICL4120 ALGOL RFL 7083 FIRESTAR LGD T POW UCP 9 F UKAEA LNA
151 ICL4120 FORTRAN RFL 292 FIRETWIST INVERT POW 1 F UKAEA LNA
153 ICL4120 FORTRAN RFL 330 FIREPUP EDIT POW 1 F UKAEA LNA
155 ICL4120 FORTRAN RFL 333 FIREGLOW EDITS POW 1 F UKAEA LNA
149 ICL4120 FORTRAN RFL 336 FIRESCALP TOW17 POW 1 F UKAEA LNA
148 ICL4120 ALGOL RFL 226 ALGCON 5T08 POW
38 ICL4130 ALGOL DFS DYIDQF, VMS VPS REC
36 ICL4130 ALGOL DFS DY2DQF, VMS VPS REC
34 ICL4130 ALGOL DPS IMITHP, VMS VOS REC
35 ICL4130 ALGOL DPS IMRFNIA, VMS VOS REC
195 ICL4130 ALGOL DFS
41 ICL4130 ALGOL DPS
213 ICL4130 FORTRAN XRAY63
234 NEAC2200 FORTRAN UNICS
233 NEAC2200 FORTRAN UNICS
236 NEAC2200 FORTRAN UNICS
235 NEAC2200 FORTRAN UNICS
192 PDPATH FORTRAN
47 UNC1108 FOR IV XNTH DISTAN, GEO SID SBL 10 BORGEN NNS
43 UNC1108 FOR IV XNTH FOFU1, Fou FBL FPD FR2 FR3 20 BORGEN LCA
44 UNC1108 FOR IV XNTH FOFU1, Fou FBL FPD FR2 FR3 20 BORGEN LCA
45 UNC1108 FOR IV XNTH FOUPA1, Fou FPL FUM SHF 50 BORGEN LCA
48 UNC1108 FOR IV XPORG F PAVF,2, GEO SAN SID SBL 30 BORGEN LIA
56 UNC1108 FOR V GRUGEN, MSG REP 20 BORGEN LCS
55 UNC1108 FOR V SYMVAC, THV CSC 65 RA LCS
51 UNC1108 FOR V SCALE1, PRP SCL 1 BORGEN LCS
54 UNC1108 FOR V XNTH BESPLA, GEO MPL 3 BORGEN LCA
52 UNC1108 FOR V XNTH CNMM, CHP 2 BORGEN MNS
50 UNC1108 FOR V XNTH PLOSTR, PLT DRW TEL 30 BORGEN LIA
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<td>SADIAN69, GEO SAN SBL DRW PRJ</td>
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Dictionary of Abbreviations

Programming languages

ALGOL ALGORITHMIC LANGUAGE
ASLOGA C. I. L. 510 ASSEMBLER
ASM IBM/360 ASSEMBLY+DOS AND OS MACROS, UNIVAC ASSEMBLY WITH EXEC8 REQUESTS
FORTRAN FORMULA TRANSLATOR
PL/I PROGRAMMING LANGUAGE NUMBER 1

** MODIFIERS **

FIN IV FORTRAN IV
FORTRAN2 FORTRAN II
FORTRAN4 FORTRAN IV
FORT FORTRAN IV AND FORTRAN V
FOR V FORTRAN V

Function abbreviations

ABA ABSORPTION CORRECTION BY ANALYTICAL METHOD
ABE ABSORPTION CORRECTION BY EXPERIMENTAL METHOD
ABI ABSORPTION CORRECTION BY GAUSSIAN INTEGRATION
ABS ABSORPTION CORRECTIONS
ABSG PROGRAM FOR ABSORPTION CORRECTION OF DIFFRACTOMETER (GONIOSTAT) DATA
ABSW PROGRAM FOR ABSORPTION CORRECTION OF WEISSENBERG DATA
ACC ACCUMULANTS
ACT ACENTRIC-CENTRIC TEST
ADL ADD TO OR DELETE FROM FILE
AGA AGREEMENT ANALYSIS OF OBS & CALC DATA
AGR AGREEMENT ANALYSIS OF THE OBS & CALC STRUCTURE FACTORS
AHA AUTOMATIC HEAVY-ATOM ANALYSIS OF ORGANIC COMPOUNDS
ARC AGRICULTURAL RESEARCH COUNCIL
ASD ATOMIC STRUCTURE DETERMINATION
ASG ALL SPACE GROUPS
ATR ATOMIC RADII
AUT. AUTOMATIC
AVG AVERAGING OF INTENSITIES
BIJ REFINEMENT OF ANISOTROPIC THERMAL PARAMETERS
BIS REFINEMENT OF ISOTROPIC THERMAL PARAMETERS
BLS BLOCK DIAGONAL LEAST SQUARES
BMIX REFINEMENT OF MIXED ISOTROPIC AND ANISOTROPIC THERMAL PARAMETERS
BOL BOND LENGTHS
BRG CALCULATION OF BRAGG ANGLES
C CUBIC ONLY
CAL POWDER DIFFRACTOMETER CALIBRATION SEE TRG REPORT 1812(S)
CAL. CALCULATE(S)
CBA CORRECTIONS OF BOND LENGTHS AND ANGLES
CCD COMPUTER CONTROLLED DIFFRACTOMETER
CCS CRYSTALLOGRAPHIC COMPUTER SYSTEM
CHP CALCULATION OF REASONABLE HYDROGEN COORDINATES
CIR 3 OR 4 CIRCLE GONIOSTAT GEOMETRY
CMP COMPARISON OF MULTIPLE MEASUREMENTS
COMP COMPACTION OF VOLUME OF DATA BY SUMMING
COMP. COMPACITY
COR CORRECTIONS TO OBSERVED DATA
CPP CALCULATION OF POWDER PATTERN
CRYSCCM CRYSTALLOGRAPHIC COMPUTING, 1970, MUNKSGAARD, PAGE 90.
CRYST CRYSTALLOGraphy
CSC CRYSTAL SYMMETRY COORDINATES
CSF COMPRESSED STRUCTURE FACTOR TABLES FOR PUBLICATION
CSP CENTROSYMMETRIC SPACE GROUPS ONLY
DEC DECONVOLUTION, SOLUTION OF FREDHOLM INTEGRAL EQUATION OF FIRST KIND.
DESM DESMEARING OF SLIT-SMEARED SAXS-PATTERNS
DFS REFINEMENT BY DIFFERENTIAL SYNTHESSES
DHK CALCULATION OF INTERPLANAR SPACINGS
DIF DIFFRACTOMETER CONTROL
DIH DIHEDRAL ANGLE BETWEEN PLANES
DIR DIRECT PHASING
DLS DIAGONAL LEAST SQUARES
DLS INTERATOMIC DISTANCES LEAST SQUARES PROGRAM
DPS PROGRAM SYSTEM DESCRIBED BY TOLLIN IN CRYSCOM
DRF DATA REDUCTION AND GENERATION OF DATA FILE
DRW STRUCTURE DRAWING
DST SORTING IN DESCENDING ORDER OF INTERPLANAR SPACINGS
DY DYNAMIC LIMITATION OF STORAGE
EDIT EDITS OUT SELECTED PORTIONS OF A LARGE TAPE OF ANGLE/COUNT PAIRS
EDITF EDITS TAPE WITH COUNTS ONLY SO AS TO ADD CORRESPONDING COUNTS
EDITG EDITS THE COUNTS ON A SEQUENTIAL LIST OF ANGLES AND COUNTS
EDITS EDITS TAPE TO GIVE INPUT FOR FIREBRAND2 OR FIRESTREAK
EDITW EDITS TAPE TO GIVE INPUT FOR FIREWOLF
EDN ELECTRON DIFFRACTION
EHS NORMALIZED STRUCTURE FACTORS AND STATISTICS
EOA BEST ESTIMATES BY OPTIMAL ALGORITHM (TOURNARIE, J. PHYS., P737, 1969)
ESD CALCULATION OF THE ESTIMATED STANDARD DEVIATIONS
EST ELECTROSTATIC LATTICE SUMS
EXT CAN REFINE EXTINCTION PARAMETERS, ISOTROPIC, ANISOTROPIC TYPE 1 OR 2.
FAZ CAN REFINE VERSUS OBSERVED OR ASSIGNED PHASES AS WELL AS /F/ OR 1.
FBL FOURIER WITH BEEVERS-LIPSON TYPE CALCULATION
FCR FOURIER CONTOURS
FCT FOURIER BY COOLEY-TUKEY ALGORITHM
FDG APPLICATION OF FUDGE OR RELAXATION FACTORS
FED FILE EDITING AND MANIPULATION
FLS FULL MATRIX LEAST SQUARES
FMAX LOCATION OF A MAXIMUM IN A SEQUENCE OF COUNTS BY A FOURIER METHOD
FOB F OBS CALCULATION
FORMT REFORMAT BIT UNPACKING THEN REPACKING, I.E. BYTES TO WORDS
FOU FOURIER TYPE CALCULATION
FPD FOURIER, PATTERSON & DIFFERENCE SYNTHESSES
FPL FOURIER IN A GENERAL PLANE
FPS FOURIER PEAK SEARCH
FR1 ONE-DIMENSIONAL FOURIER
FR2 TWO-DIMENSIONAL FOURIER
FR3 THREE-DIMENSIONAL FOURIER
FST FILE SORT ON THE INDICES
FTM FOURIER TRANSFORM
FUM FOURIER PRODUCING UNDISTORTED MAPS
GDP OUTPUT ON GRAPHIC DISPLAY
GEO MOLECULAR GEOMETRY CALCULATIONS
GRT GENERATE EQUIVALENT REFLEXIONS IN HIGH SYMMETRY SPACE GROUPS
GSC GONIOSTAT SETTINGS CALCULATION
HKL GENERATE THE INDICES
HONTS HONEYWELL, FORMERLY BULL-GE, COMMERCIAL TS SYSTEM.
IBM IBM360/44PS-DOS, AND IBM360/910S
IND INDEXING OF POWDER PATTERN
INT CALC OF ALL INTERPLANAR ANGLES FOR ANY UNIT CELL AND A GIVEN HKL
INTC INTEGRATES AND FINDS THE BREADTH OF A BRAGG REFLEXION
INVERT INVERTS THE SEQUENCE OF ANGLE/COUNT PAIRS ON A TAPE
ISC INTERPOLATION ON SCATTERING FACTOR CURVES
KOS KOSSEL LINES
LAD LEAST SQUARES WITH ANOMALOUS DISPERSION
LAT LATTICE CONSTANTS
LAU LAUE PATTERN
LAX LEAST-SQUARES REFINEMENT OF ANISOTROPIC EXTINCTION PARAMETERS
LAY SCALING ACCORDING TO LAYERS
LAY REFINEMENT OF LAYER SCALE FACTORS
LB LINE BROADENING
LCD LATTICE CONSTANTS DETERMINATION
LCD LATTICE CONSTANTS DETERMINATION FROM POWDER PATTERN
LCR LATTICE CONSTANTS REFINEMENT
LEQ LEAST SQUARES FOR ATOMS WITH EQUIVALENT COORDINATES
LMN DIRECTION COSINES
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<th>Description</th>
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<tr>
<td>LPC</td>
<td>Lorentz and Polarization Corrections</td>
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<tr>
<td>LSP</td>
<td>Least Squares with Allowance for Atoms in Special Positions</td>
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<tr>
<td>MD.</td>
<td>Maryland</td>
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<tr>
<td>MFF</td>
<td>Magnetic Form Factor Determination</td>
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<tr>
<td>MLT</td>
<td>Multisolution Procedure</td>
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<tr>
<td>MO</td>
<td>Monoclinic and Orthorhombic Only</td>
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<tr>
<td>MPD</td>
<td>Correction for Multiple Diffraction</td>
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<tr>
<td>MPL</td>
<td>Mean Plane Through a Set of Atoms by Least Squares</td>
</tr>
<tr>
<td>MSC</td>
<td>Miscellaneous</td>
</tr>
<tr>
<td>MSD</td>
<td>Magnetic Structure Determination</td>
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<tr>
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<td>Neutron Diffraction</td>
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<td>NET</td>
<td>Calculation of Net Counts</td>
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<tr>
<td>NSC</td>
<td>Neutron Scattering Factor Determination</td>
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<tr>
<td>NSG</td>
<td>Non-Centrosymmetric Space Groups Only</td>
</tr>
<tr>
<td>OCC</td>
<td>Refinement of Occupancy Factors</td>
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<td>OES</td>
<td>Origin and Enantiomorph Selection</td>
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<tr>
<td>OMC</td>
<td>Orientation Matrix Calculation</td>
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<tr>
<td>OMR</td>
<td>Orientation Matrix Refinement</td>
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<td>ORG</td>
<td>Origin Selection</td>
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<tr>
<td>ORT</td>
<td>Orthogonal Projection</td>
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<tr>
<td>OSC</td>
<td>Oscillation Films in Weissenberg Geometry, Any Mu Angle</td>
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<td>OSA</td>
<td>Obs/Unobs Assignment</td>
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<tr>
<td>PAS</td>
<td>Phase Estimation from Anomalous Scattering</td>
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<tr>
<td>PEX</td>
<td>Correction for Primary Extinction</td>
</tr>
<tr>
<td>PIA</td>
<td>Phase Estimation from Isom. Repl. and Anom. Scat.</td>
</tr>
<tr>
<td>PIR</td>
<td>Phase Estimation from Isomorphous Replacement</td>
</tr>
<tr>
<td>PIRUM</td>
<td>Program for Indexing and Refinement of Unit Cell Matrix</td>
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<td>PLS</td>
<td>Phase Estimation by Least Squares</td>
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<td>PLT</td>
<td>Plotter Programs</td>
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<tr>
<td>PLT C</td>
<td>Automatic Plotting of Thermal Ellipsoids</td>
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<td>PLT MAX</td>
<td>Plots Counts or Times as a Function of Angle</td>
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<tr>
<td>POL</td>
<td>Construction of Pole Figures</td>
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<td>POL</td>
<td>Coordination Polyhedra</td>
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<td>POS</td>
<td>Plane Orientation Search</td>
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<td>POW</td>
<td>Powder Diffraction</td>
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<td>PRC</td>
<td>Precession Geometry</td>
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<td>PRH</td>
<td>Prediction of Hydrogen Positions from Geometrical Considerations</td>
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<tr>
<td>PRI</td>
<td>Primitive Unit Cells Only</td>
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<td>PRJ</td>
<td>Projections of the Structures</td>
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<td>PRO</td>
<td>Processing of Raw Intensity Data</td>
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<td>Powder Peaks Separation</td>
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<td>PST</td>
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<td>Phase Refinement by the Tangent Formula</td>
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<tr>
<td>PURUM</td>
<td>Program for Refinement of Unit Cell Matrix</td>
</tr>
<tr>
<td>RAB</td>
<td>Reference Rossmann and Blow 1962 Acta Cryst, 15, 24</td>
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<tr>
<td>RBL</td>
<td>Rigid Body Least Squares</td>
</tr>
<tr>
<td>REC</td>
<td>Calculation Performed in Reciprocal Space</td>
</tr>
<tr>
<td>REF</td>
<td>Refinement of Atomic Parameters</td>
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<tr>
<td>REN</td>
<td>Renninger Effect</td>
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<tr>
<td>REP</td>
<td>Generation of Operators, and Representations for Point Groups</td>
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<tr>
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<tr>
<td>RIG</td>
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<td>Rotation Angles</td>
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<td>RRA</td>
<td>Reference Reflexion Analysis</td>
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<tr>
<td>RTS</td>
<td>Real Time System</td>
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<tr>
<td>RUC</td>
<td>Reduction of Unit Cell</td>
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<tr>
<td>SAD</td>
<td>Structure Factors with Anomalous Dispersion</td>
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<tr>
<td>SAMP</td>
<td>Compaction of Volume of Data by Using Maximum Value of Group</td>
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<tr>
<td>SAN</td>
<td>Structure Factors with Anisotropic Thermal Parameters</td>
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<tr>
<td>SAN</td>
<td>Scan of Angles</td>
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<td>SAP</td>
<td>Symbolic Addition Procedure</td>
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<td>SAXS</td>
<td>Small Angle X-Ray Scattering</td>
</tr>
<tr>
<td>Abbreviation</td>
<td>Description</td>
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<tr>
<td>SBL</td>
<td>Scan of Bond Lengths</td>
</tr>
<tr>
<td>SC</td>
<td>Screenless Film Technique</td>
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<tr>
<td>SCF</td>
<td>Scattering Factor Determination</td>
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<tr>
<td>SCH</td>
<td>Schomaker's Correction of Thermal Parameter Shifts</td>
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<tr>
<td>SCH</td>
<td>Search of the ASTM Powder File</td>
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<tr>
<td>SCH</td>
<td>Search for Unmeasured Reflexions</td>
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<td>SCL</td>
<td>Scaling of the Intensities</td>
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<td>SEX</td>
<td>Refinement of Overall Scale Factor</td>
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<tr>
<td>SFC</td>
<td>Correction for Secondary Extinction</td>
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<td>SFT</td>
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<tr>
<td>SFC</td>
<td>Scale with Fractional Occupancies</td>
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<td>SFO</td>
<td>S.F. Trials by Addition or Subtraction of Atoms</td>
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<tr>
<td>SFT</td>
<td>Structure Factor Tables for Publication</td>
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<tr>
<td>SGG</td>
<td>Space Group Generalities</td>
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<tr>
<td>SHF</td>
<td>Sharpening Function Application</td>
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<tr>
<td>SID</td>
<td>Scan of Intermolecular Distances</td>
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<td>SIS</td>
<td>Structure Factors with Isotropic Thermal Parameters</td>
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<td>SKH</td>
<td>Calculation of Scherrer Constants</td>
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<td>Simplex Method</td>
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<td>Contribution of Rigid Group</td>
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<td>Sort on the Indices</td>
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<td>STE</td>
<td>Stereoscopic Projection</td>
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<td>Stereogram</td>
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<td>Scale and Temperature Factor Estimation</td>
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<td>SII</td>
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</tr>
<tr>
<td>S2I</td>
<td>Sigma 2 Interactions Search</td>
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<tr>
<td>T</td>
<td>Triclinic Only</td>
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<tr>
<td>TDS</td>
<td>Thermal Diffuse Scattering</td>
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<tr>
<td>TEHR</td>
<td>Tetragonal Hexagonal and Rhombohedral Only</td>
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<tr>
<td>TEL</td>
<td>Thermal Ellipsoids</td>
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<tr>
<td>TEL</td>
<td>Thermal Ellipsoids Calculation</td>
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<tr>
<td>THV</td>
<td>Thermal Vibration Analysis</td>
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<tr>
<td>TMO</td>
<td>Triclinic, Monoclinic, and Orthorhombic Systems Only</td>
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<tr>
<td>TOR</td>
<td>Torsional Angles</td>
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<tr>
<td>TOTAL</td>
<td>Counts the Number of Angle/Count Pairs on a Tape</td>
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<td>UCP</td>
<td>Unit Cell Refinement from Powder Pattern by Least Squares</td>
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<td>Unitary Structure Factors</td>
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<td>VAR</td>
<td>Variance</td>
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<td>Vector Minimum Function</td>
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<td>VMS</td>
<td>Vector Map Solving and Manipulation</td>
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<td>Vector Position Search</td>
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<tr>
<td>VVR</td>
<td>Vector Verification</td>
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<td>WAN</td>
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<td>WEI</td>
<td>Weissenberg Geometry</td>
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<tr>
<td>WSM</td>
<td>Weighted Sum Formula. WTA used is Estimate of 1/VAR</td>
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<td>WSN</td>
<td>Wilson Statistics</td>
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<td>WTA</td>
<td>Weight Assignment</td>
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<td>X-Ray Arc</td>
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<td>XDN</td>
<td>X-Ray Diffraction</td>
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<tr>
<td>XSC</td>
<td>X-Ray Scattering Factor Determination</td>
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<tr>
<td>XYZ</td>
<td>Refinement of Positional Parameters</td>
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<td>18TO17</td>
<td>Converts Angle/Count Data from Field Width 18 to 17</td>
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<tr>
<td>360/370</td>
<td>IBM 360 and IBM 370 Systems</td>
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<tr>
<td>5TO8</td>
<td>Converts Mercury 5-Hole Tape to 8-Hole ISO 7 Even Parity Tape</td>
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**Computer abbreviations**

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<thead>
<tr>
<th>Abbreviation</th>
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<td>CDC 3600</td>
<td>CDC 3600</td>
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<td>CDC 6500</td>
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</table>
WORLD LIST OF COMPUTER PROGRAMS

CDC 6600
CDC 6400/6500
CDC 3600
CDC 36091
CDC 36075
CDC 36065
CDC 36050
CDC 36044
CDC 36043

DIGITAL EQUIPMENT
PDP 10
PDP10

GENERAL ELECTRIC
T. S. SYST.
HONTS

IBM
360/91
IBM36091
360/75
IBM36075
360/65
IBM36065
360/50
IBM36050
360/44
IBM36044
1130
IBM1130
1800
IBM1800
7094/90
IBM7094

UNIVAC
1108
UNC1108
1108
UNC

ICL
1905
ICL1905
1905 E
ICL1905E
KDF 9
ICLKDF9
4-70
ICL4-70
4120
ICL4120
4130
ICL4130

C. I. I.
510
CI510

NEAC
2200
NEAC2200

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