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

Commission on Crystallographic Computing

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General description

1. The format of this list follows the general outline published in *Acta Crystallographica* (1971) **A**27, 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

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Formats

A. Title line

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

B. Name and source line

Column		Contents
6–40	*	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.
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 is left blank.

C. Abstract lines

Column		Contents
8–75	*	Abstract. It should include the relevant information which cannot be directly identified from the program title line such as special features, speed and generality.

List of programs

1 IBM1800 FORTRAN PIRUM, POW UCP HKL IND DHK 13 PEW LIA
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 13 PEW LIA
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 9 PEW LIA
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. 16(1963)1141 SEE ALSO ACTA CRYST. 20(1966)407.

4 IBM1800 FORTRAN ABSG, ABS CIR ABI LPC SEX 13 PEW LIA
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. 16(1963)1141 SEE ALSO ACTA CRYST. 20(1966)407.

5 IBM1800 FORTRAN2 PHASE2, DIR ASG S2I SAP PTN MLT 10 KOENIG LIA
KOENIG PHASE 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. NO 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 FORTRAN4 FALFA, REF FLS FAZ EXT LAD OCC 20 KOENIG LIA
KOENIG ORFLS BUSING, MARTIN, LEVY
USER-DIMENSIONED ATOMIC-PARAMETER AND VARIABLE ARRAYS. FAST. CHANGES OF VARIABLES AND CONVERSIONS OF TEMPERATURE FACTORS POSSIBLE BETWEEN CYCLES. OTHER OPTIONS BIJ BIS ESD FOG LAY LEQ LSP SCL XYZ, GROUP OR OVERALL B, NEUTRON CROSS-SECTION REFINEMENT, CORRELATIONS, WEIGHTING ANALYSES, SIM WEIGHTS, E.S.D. OF CALC. PHASE, AOBS-ACALC, BOBS-BCALC.
ADDITIONAL CORE SIZE (WORDS) 24*ATOMS + VARIABLES*(VARIABLES+7)/2 .

7 IBM1800 FORTRAN2 CHOW, GEO MPL SAN SID SBL TOR 10 KOENIG LIA
KOENIG HOW DUNITZ ET AL
KEYBOARD CONVERSATIONAL VERSION OF HOW, DIMENSIONED FOR 100 ATOMS. PRINTS BOTH CRYSTAL AND ORTHOGONAL COORDINATES. ATOMS CHANGEABLE ON-LINE.

8 IBM1800 FORTRAN4 DIR, CSP MLT ORG SAP S1I S2I 10 NSTAM LIA
NORRESTAM

INPUT: TRIPLETS, E'S AND ACCEPTANCE PARAMETERS FROM TAPE AND/OR CARDS. ORG 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, TMO OES S1I S2I 10 NSTAM LIA
NORRESTAM
ANALYSIS OF DISTRIBUTION AND SUM OF 1/VAR FOR EACH REFL IN TRIPLETS WITH THREE, TWO AND ONE UNKNOWN. A REFL 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, TMO MLT WSM S2I 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, KIHLBORG
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 FORTRAN DIF, CCD WEI HKL ASG VAR OUA 8 NSTAM LIS
NORRESTAM
PROGRAM SYSTEM FOR ON-LINE CONTROL OF A PAILRED 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 CALCD IN ACCORDANCE WITH 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 FORTRAN REF, BLS BIS LAY XYZ WAV ASG 8 BRANDT LCA
BRANDT,ASBRINK SFLS, ASBRINK BRANDEN

18 IBM36075 FORTRAN FED, ADL FST PRT 13 BRANDT LCA

BRANDT

19 IBM36075 FORTRAN DRF, ABI CIR WEI LPC PEX SEX 26 BRANDT LCA
OLOFSSON,ELFSTROM,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 UCLALS1, 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 ORTEP, JOHNSON
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 IMITHP, VMS VOS REC 3 TOLLIN LIA
TOLLIN,MUNNS

I(THETA,PHI) FOR PLANAR GROUP ORIENTATION.TOLLIN AND COCHRAN1964ACTA CRYST17,1322

35 ICL4130 ALGOL DPS IMRENIA, VMS VOS REC 5 TOLLIN LIA
TOLLIN,MUNNS ROSSMANN,TOLLIN
NON PLANAR GROUP ORIENTATION SEARCH.TOLLIN AND COCHRAN1964ACTA CRYST 17,1322

36 ICL4130 ALGOL DPS DY2DQF, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO 2-FOLD AXIS BY THE METHOD OF TOLLIN1966ACTA CRYST,21,613

37 ICL4130 ALGOL DPS RFLTEA, 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 ROSSMANN1966ACTA CRYST21,872

38 ICL4130 ALGOL DPS DY1DQF, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO SYMMETRY PLANE BY THE METHOD OF TOLLIN1966ACTA CRYST,21,613

39 ICL4130 FORTRAN DPS EFITF , VMS VOS REC 3 TOLLIN LIA
YOUNG
I(THETA,PHI) FOR PLANAR GROUP ORIENTATION.TOLLIN AND COCHRAN1964ACTA CRYST17,1322

40 ICL4130 FORTRAN DPS EF2DQF, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO 2-FOLD AXIS BY THE METHOD OF TOLLIN1966ACTA CRYST,21,613

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

42 ICL4130 FORTRAN DPS EF1DQF, VMS VPS REC 5 TOLLIN LIA
YOUNG
DETERMINATION OF GROUP POSITION RELATIVE TO SYMMETRY PLANE BY THE METHOD OF TOLLIN1966ACTA CRYST,21,613

43 UNC1108 FOR IV XNTH FOUFU1, FOU FBL FPD FR2 FR3 20 BORGEN LCA
BORGEN,MESTVEDT ORFFE BUSING,MARTIN,LEVY

44 UNC1108 FOR IV XNTH FOUFU1, FOU FBL FPD FR2 FR3 20 BORGEN LCA
BORGEN,FINJORD,MESTVEDT
GENERAL FOURIER PROGRAM FOR ALL SPACE GROUPS OF ORTHORHOMBIC AND LOWER SYMMETRY.

45 UNC1108 FOR IV XNTH FOUPLA, FOU FPL FUM SHF 50 BORGEN LCA
BORGEN,MESTVEDT,TIDEMANN
CALCULATION OF FOURIER SUMS IN A GENERAL PLANE.

46 UNC1108 FOR V XPROGF LSFIV4, REF BMIX ESD FLS LAY XYZ 40 BORGEN LIA
BORGEN,MESTVEDT LSFIV3 BORGEN,MESTVEDT
FULL MATRIX LEAST-SQUARES REFINEMENT OF SCALE FACTORS,ATOMIC COORDINATES,AND MIXED TEMPERATURE FACTORS.SEVERAL VERSIONS.

47 UNC1108 FOR IV XNTH DISTAN, GEO SID SBL 10 BORGEN NNS

BORGEN
CALCULATION OF INTERATOMIC DISTANCES AND ANGLES.

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

49 UNC1108 NU ALGOL XNTH FOUPL1, PLT FOR 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 ORTEP JOHNSON
EVALUATION AND PRESENTATION OF MOLECULAR GEOMETRY ON KINGMATIC X-Y PLOTTER.

51 UNC1108 FOR V XNTH TOLLIN, POS 20 BORGEN LCA
BORGEN,MESTVEDT,TIDEMANN
ORIENTATION OF PLANAR MOLECULAR SUBUNITS.

52 UNC1108 FOR V XNTH CNHM, CHP 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 TAPSI1, 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 CARSI1, 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.

60 UNC1108 FOR V XPROGF STABL1, DRF RRA 2 BORGEN LCS
BORGEN,MESTVEDT
REFERENCE REFLECTION ANALYSIS FOR X-RAY DIFFRACTOMETER DATA.

61 UNC1108 FOR V XPROGF SCALE1, PRO SCL 1 BORGEN LCS
BORGEN,MESTVEDT
SCALING OF ONE OR MORE DATA SETS CONTAINING REFERENCE REFLECTIONS.

62 UNC1108 FOR V XPROGF LISTF1, FED PRT 1 BORGEN LCS
BORGEN,MESTVEDT
DOCUMENTATION ROUTINES FOR X-RAY DATA FILE.

63 UNC1108 FOR V XPROGF FFILE1, FED 5 BORGEN LCS
BORGEN,MESTVEDT
GENERATION OF WORKING FILE FOR STRUCTURE ANALYSIS FROM OBSERVED RAW DATA.COLLECTION OF EQUIVALENT REFLECTIONS ETC.

64 UNC1108 FOR V XRAY*TU COPRO1, MSC CCS 8 BORGEN NNN
BORGEN
INITIATION AND DATA COLLECTION PHASE OF AUTOMATIC,'SELF-ADMINISTRATING' STRUCTURE ANALYSIS FILE-ORIENTED PROGRAM SYSTEM.

65 CDC 6500 FORTRAN4 DIF, OMC OMR 18 LIEDL LIA
ELLIS,LIEDL*
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.

66 IBM36091 FORTRAN4 SPSRM286 40 TOURNAR MIA
BORNE HARDY TOURNARIE*
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)
ORTHOGONAL OR STEREOGRAPHIC PROJECTION
OPTIONAL CONVERSATIONAL SYSTEM FOR ORGANIC STRUCTURES

67 IBM36091 FORTRAN4 SPSRM302 POW, LCP 54 TOURNAR MIA
TOURNARIE
CALCULATION OF CORRECTED COUNTS
RACHINGER CORRECTION OF DOUBLET, SMOOTHING OF DATA
SEPARATION OF THE COMPONENTS OF A MULTIPLET (7 COMPONENTS)
EVALUATION OF THE INTENSITIES, POSITIONS AND WIDTHS
PLOTTING OF CURVES (LISTING, TRACING, PHOTOGRAPHY)

68 IBM36091 FORTRAN4 SPSRM304 MSC, EDN REN 40 TOURNAR MIA
TOURNARIE
INTENSITIES, MODULI, PHASES OF DIFFRACTED ELECTRON BEAMS
DYNAMICAL EFFECTS (EXTINCTION, ABSORPTION)
AS FUNCTION OF WAVELENGTH, THICKNESS, TILTING AND STRUCTURE

69 IBM36091 FORTRAN4 SPSRM307 FOU, FPS FR2 SHF 23 TOURNAR MIA
TOURNARIE
CALCULATION AND PLOT OF FOURIER OR PATTERSON PROJECTION CONTOURS FOR ALL PLANAR GROUPS
FOURIER PEAKS SEARCH
ATTENUATION OF THE TERMINATION EFFECT

OUTPUT CARDS FOR INPUT OF SPSRM386

70 IBM36091 FORTRAN4 SPSRM308 MSC, EOA 10 TOURNAR MIA
TOURNARIE
CONSTRUCTION OF AN APODAL KERNEL
WITHOUT DISTORTION OF THE MOMENTS OF FOURIER PEAKS
OUTPUT CARDS FOR INPUT OF SPSRM307

71 IBM36091 FORTRAN4 SPSRM321 COR, ABA SEX EOA 40 TOURNAR MIA
TOURNARIE
EVALUATION OF EXTINCTION BY COMPARING DIFFERENT CRYSTALS
ACCORDING THE OPTIMAL ALGORITHM
REJECTION OF ERRATIC INTENSITIES
OUTPUT CARDS FOR INPUT OF SPSRM330

72 IBM36091 FORTRAN4 SPSRM330 COR, ABI SEX 16 TOURNAR MIA
BERTINOTTI TOURNARIE* HAMILTON
EXTINCTION AND ABSORPTION CORRECTION
ADAPTATION BY A. BERTINOTTI OF THE HAMILTON CODE
OUTPUT CARDS FOR INPUT OF SPSRM307, SPSRM321, SPSRM386

73 IBM36091 FORTRAN4 SPSRM344 GEO, 40 TOURNAR MIA
TOURNARIE
INERTIAL PLAN THRCUGH A SET OF ATOMS
OPTIMAL PLAN THRCUGH A SET OF ATOMS

74 IBM36075 FORTRAN4 SPSRM360 MSC, EOA 20 TOURNAR MIA
BIBIAN BORNE TOURNARIE*
PERFORMS OPTIMAL ESTIMATES OF IMPLICIT PARAMETERS OF ANY FUNCTION
DEFINED BY USER'S SUBROUTINE. NO DERIVATIVE FORMULA DEMANDED.
NO INTERNAL LIMITATION OF THE NUMBER OF PARAMETERS OR OBSERVATIONS.
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
QUALITY FACTORS, ERROR SCALE ESTIMATED. WEIGHTING AD LIBITUM.
PLOTTING OF CURVES AND OBSERVATIONS (LISTING)

75 IBM36091 FORTRAN4 SPSRM360 MSC, EOA 33 TOURNAR MIA
BIBIAN BORNE TOURNARIE*
PERFORMS OPTIMAL ESTIMATES OF IMPLICIT PARAMETERS OF ANY FUNCTION
DEFINED BY USER'S SUBROUTINE. NO DERIVATIVE FORMULA DEMANDED.
NO INTERNAL LIMITATION ON THE NUMBER OF PARAMETERS OR OBSERVATIONS.
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
QUALITY FACTORS, ERRORS SCALE ESTIMATED. WEIGHTING AD LIBITUM.
PLOTTING OF CURVES AND OBSERVATIONS (LISTING,TRACING,PHOTO.)

76 IBM36075 FORTRAN4 SPSRM379 POW, BRG DHK EOA LCD 25 TOURNAR MIA
TOURNARIE
ALL CRYSTALLOGRAPHIC SYSTEMS, ERRATIC LINES OPTIONALY REJECTED .
EXCENTRICITY CORRECTION (POWDER CAMERA OR GONIOMETER)
ASSUMED INDICES CAN BE TESTED WITHOUT PERTURBATION
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING)
CELL VOLUME AND C/A RATIO OUTPUT.

77 IBM36091 FORTRAN4 SPSRM379 POW, BRG DHK EOA LCD 37 TOURNAR MIA
TOURNARIE
ALL CRYSTALLOGRAPHIC SYSTEMS, ERRATIC LINES OPTIONALY REJECTED .
EXCENTRICITY CORRECTION (POWDER CAMERA OR GONIOMETER)
ASSUMED INDICES CAN BE TESTED WITHOUT PERTURBATION
ADJUSTED PARAMETERS, STANDARD ERRORS AND CORRELATION MATRIX OUTPUT.
PROBABILITY DENSITY MAP AROUND THE SOLUTION (LISTING,TRACING,PHOTO.)

CELL VOLUME AND C/A RATIC OUTPUT.

78 IBM36075 FORTRAN4 SPSRM386 REF, BIS EOA ESD LAY XYZ 40 TOURNAR MIA
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 53 TOURNAR MIA
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 37 TOURNAR MIA
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 64 ELLISON LIA
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 85 ELLISON LIA
LEVY, ELLISON
CONVERTS HKL TO SYMMETRY-UNIQUE SET, ANY POINTGROUP, FRIEDEL LAW OPTIONAL. 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. GENERATES INPUT FOR ORXFLS3 OR ORESTES.

83 IBM36075 FORTRAN4 ORTEP-2 PLT, DRW TEL STE SBL SAN 50 JOHNSON LCA
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,ELLISN,THIESSEN,LEVY ORFLS,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 FORTRAN4 OR FFE3 GEO, ESD SID SAN DIH TOR TEL CBA128 BUSING LIA
BUSING,JOHNSON,THIESSEN,LEVY ORFFE,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 KOYAMA 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, MONOCLINIC 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 FORT+ASM FILMDATA MSC,CCS PRO, DRF,PRC WEI LPC FOB 32 PEARSON LCA
PEARSON,R.H. SUSSMAN,J. HYBL,A.
FILM DATA REDUCTION SYSTEM OF PROGRAMS. INPUT=MAG. TAPE OF OUTPUT FROM SCANNING DENSITOMETER. OUTPUT=LP CORRECTED STRUCTURE FACTORS+WEIGHTS. CARD+PRINTER+1 TAPE DRIVE. IBM360/44PS+DOS,IBM360/91OS,UNC1108/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 FORT+ASM FILMDATA 1COMPAK FED, COMP FORMT 12 PEARSON LCA
PEARSON,R.H.
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) + ACROSS RECORDS). COMP NOT EQUIVALENT TO ENLARGING DENSITOMETER SCAN APERTURE SINCE D=-LOG(T). REQ. 2 TAPES

89 IBM+UNC FORT+ASM FILMDATA 2MAPP FED, PRT SAMP 32 PEARSON LCA
PEARSON.R.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 COMPAK ROUTINE).SPOT ADDRESSES EASILY FOUND BY NOTEING WORD AND RECORD NUMBERS FROM BOX AXES SURROUNDING PRINTOUT.

90 IBM+UNC FORT+ASM FILMDATA 3FILM DRF,PRC WEI LPC WTA FOB SC 32 PEARSON LCA
PEARSON,R.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 ON INPUT PARAMETERS.
IMPROVED VERSION OF PROGRAM DESCRIBED AT A.C.A. 1970 SPRING MEETING

91 IBM+UNC FORT+ASM FILMDATA 4SCALE PRO, LAY AVG CMP DUA SRT 32 PEARSON LCA
PEARSON,R.H. HAMILTON-ROLETT-SPARKS
TENTATIVE R OF DATA SET. AVERAGES EQUIVALENT REFLECTIONS. (PRO, CMP) AND MATCHES AGAINST WEIGHT FROM FILM PROGRAM TO CHECK FOR ERRORS. 2 OUTPUTS,(DRF, FOB+WTA) AND THE RATIO(PRO, CMP)/(DRF, WTA)

RATIO OUTPUT CAN BE USED FOR SUBSEQUENT STASTICAL ANALYSIS.

92 IBM36065 PL/1 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 ALFFT,ALFFDP AND ALFFPROJ. WRITEUP IS2625 AVAILABLE.

93 IBM36065 PL/1 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/1 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 FROM 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/1 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/1 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, SUPERPOSITON 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 ACCES 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 SCOPECUFIT, FLS DLS 32 THOENI LIA
THOENI
FLS PROGRAM TO ADJUSTE 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 MOD. OF BCSU
FULL SPHERE ORIENTER SETTINGS, CALC. STEREOGRAPHIC PROJ. AND PLOTS IT (PLOT LOCAL CODE).

103 CDC6600 FORTRAN4 CELFIX, 17 WOLTEN LIA
WOLTEN
TRANSFMS MONOCLINIC CELLS TO I.U.CR. 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 THETA VALUES IN 5 MINUTES.

113 IBM1130 FORTRAN X-ARC-02 PICK3, DIF HKL OMC OMR LCR GSC 16 TRUTER LIA
BRIGHT MODEl W.C.HAMILTON
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 NRC-3 F.R.AHMED AND P.SINGH
ABSORPTION CORRECTION IS PUNCHED ON OUTPUT CARDS FROM PICKER 4 CIRCLE DIFFRACTOMETER, FOR SUBSEQUENT APPLICATION BY DATA REDUCTION PROGRAM. REQUIRES ORIENTATION MATRIX FROM PICKER SETTING PROGRAM BY R.H.B.MAIS AND D.C.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 NRC-2 F.R.AHMED
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 FORDAP A.ZALKIN
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 SAP1-4B, DIR EHS STF S2I SAP SCP 16 TRUTER NCA
VICKERY NRC-4 S.R.HALL AND F.R.AHMED
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 OCC 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 ISOTROPIC 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 BIJ SCH OCC XYZ 16 TRUTER LIA
VICKERY,MALLINSON*
BLOCK DIAGONAL LEAST-SQUARES REFINEMENT 5X5 OR 10X10 FOR ISOTROPIC 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 CO-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 DIH 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

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

130 IBM1130 FORTRAN X-ARC-29 ELIPS, THV TEL TRUTER NN
MALLINSON
CALCULATION OF U(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 IBM1130 FORTRAN X-ARC-21 RANGE, REF 13 TRUTER LIA
VICKERY
ANALYSIS OF WEIGHTING SCHEME FOR LEAST-SQUARES STRUCTURE REFINEMENT. VALUES OF AVERAGE W*(DELTA 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 ON F(OBS) TO CONSTRUCT EQUALLY POPULATED RANGES.

132 IBM1130 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 IBM36050 FORTRAN4 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 ONE 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 IBM36050 FORTRAN4 NRC-2A PRO, 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 IBM36050 FORTRAN4 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 IBM36050 FORTRAN4 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 IBM36050 FORTRAN4 NRC-4 DIR, SAP CSP TMO STF EHS ORG S2I 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, TMO STF EHS PTN S2I 25 AHMED LCA
HUBER, BRISSE 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 DISPERTION, 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 OST 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 5TO8 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 18TO17 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 OR TIMES AS A FUNCTION OF ANGLE USING A PLOTTER

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

154 ICL4120 ALGOL RFL 334 FIRESPARK 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 POSITION OF MAXIMUM IN A SEQUENCE OF COUNTS BY FOURIER METHOD

158 ICL4120 ALGOL RFL 7083 FIRESTAR LCD T POW UCP 9 F UKAEA LNA
ASTLE G FERGUSON 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
ASTLE G FERGUSON 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
ASTLE G FERGUSON 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
ASTLE G FERGUSON 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
ASTLE G FERGUSON I F *
DETERMINES Y=MX+C CALIBRATION FOR 2CIRCLE DIFFRACTOMETER WITH STANDARD

163 ICL4120 ALGOL RFL 331 FIREDAWG EDITW POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREWOLF

164 ICL4120 FORTRAN4 RFL 332 FIREDOG EDITW POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
AS FIREPUP BUT TAPE IS FOR USE WITH FIREWOLF

165 ICL4120 FORTRAN4 RFL 359 FIREADD EDITF POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
ADDS THE CORRESPONDING ANGLES TO A SEQUENTIAL LIST OF COUNTS

166 ICL4120 FORTRAN4 RFL 360 FIRECOP EDITG POW 1 F UKAEA LNA
FERGUSON I F HUGHES T E
ALTERS THE ANGLES ON A SEQUENTIAL LIST OF ANGLES AND COUNTS

167 ICL4120 ALGOL RFL 267 FIREWOLF INTC POW LB 4? F UKAEA LNA
FERGUSON I F HUGHES T E
INTEGRATES THE INTESITY OF A BRAGG REFLEXION AND FINDS ITS BREADTH

168 ICL4120 ALGOL RFL 231 FIREDRAKE POW BRG DHK DST 8 F UKAEA LNN
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 8 F UKAEA LNN
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 1 F UKAEA LNA
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 1 F UKAEA LNA
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 1 F UKAEA LNA
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 1 F UKAEA LNA
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 7? F UKAEA LNA
FERGUSON I F TSEUNG G C Y
USED IN CONJUNCTION WITH FIRECHOP

175 ICL 4120 FORTRAN4 RFL 340 FIRERICE POW LB 7? F UKAEA LNA
FERGUSON I F TSEUNG G C Y
WITH FIRECHOP REMOVES ALPHA2 COMPONENT OF DOUBLET BY RACHINGERS METHOD

176 ICL 4120 ALGOL RFL 254 FAIRFAX POW 1 F UKAEA LCA
HUGHES T E
INTERCONVERSION OF THETA D SIN2THETA AND TWOTHETA

177 ICL 4-70 FORTRAN4 HMJSR003 FIREFLY POW BRG CPP DHK DST ASG 136 F UKAEA LCA
FERGUSON I F KIRWAN J E
GIVEN HKL,DETAILS OF THE UNIT CELL AND THE EQUIPMENT THIS PROGRAM

WILL CALCULATE THE INTENSITIES OF UP TO 100 BRAGG REFLEXIONS AND, AS OPTIONS,INTERATOMIC 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 FORTRAN4 HMJSR002 FENRIS POW LB DST F UKAEA LIA
FERGUSON I F KIRWAN J E
GIVEN THE AREAS AND PEAK HEIGHTS OF BRAGG REFLEXIONS THIS PROGRAM DERIVES THE INTEGRAL BREADTHS OF BRAGG REFLEXIONS 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 16 SHIONO LCA
SHIONO
EQUI-INCLINATION, NORMAL BEAM WEISSENBERG, EXTENDED SPOT CORRECTION HIGHER LEVEL PRECESSION

180 IBM1130 FORTRAN PRO, AVG CMP SCL SRT 16 SHIONO LCA
SHIONO
INDEX TRANSFORMATION, SORTING, SCALING, DETERMINATION OF SCALES BETWEEN SETS(UP TO 8), AVERAGING

181 IBM1130 FORTRAN DIR, SCL WSN EHS 16 SHIONO LCA
SHIONO
SCALE AND TEMP. FACTORS BY WILSON PLOT, NORMALIZED SF,SORTED IN DECREASING ORDER OF MAGNITUDE (UP TO 7000 REF.). MAY BE RENORMALIZED IN TERMS OF DIFFERENT CATEGORIES

182 IBM1130 FORTRAN SFC, ASG SAN SFO 16 SHIONO LCA
SHIONO
UP TO 100 ATOMS IN ONE RUN, NO LIMIT IN MULTIPLE RUNS

183 IBM1130 FORTRAN REF, ASG SCL XYZ BLS ESD BIJ 16 SHIONO LCA
SHIONO
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 16 SHIONO LCA
SHIONO
1/1000 TH OF CELL OR ITS MULTIPLE.

185 IBM1130 FORTRAN SCF, ISC 16 SHIONO LCA
SHIONO
N-POINT INTERPOLATION BY AITKEN (N:2-9)

186 IBM1130 FORTRAN LAT, LCR ASG 16 SHIONO LCA
SHIONO
LEAST-SQUARES REFINEMENT OF THE APPROXIMATE VALUES WITH THE OBSERVED SINE THETA VALUES.

187 IBM1130 FORTRAN MSC, ASG HKL BRG DHK DST 16 SHIONO LCA
SHIONO
GENERATES INDEPENDENT OR ALL POSSIBLE REFLEXIONS WITH A GIVEN SPACE GROUP. SORTED OUTPUT.

188 IBM1130 FORTRAN DIF, CIR HKL GSC 16 SHIONO LCA
SHIONO
FOR CARD CONTROLLED PICKER, SETTING ARE SORTED TO OPTIMIZE DIFFRACTO

METER MOVEMENT

189 IBM1130 FORTRAN DRF, LPC CIR SCL 16 SHIONO LCA
SHIONO
FOR FACS-I, CAD-3 ETC. SCALES THE INTENSITIES WITH STANDARDS BY N-POINT INTERPOLATION

190 IBM1130 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 IBM1130 FORTRAN GEO, TOR 16 SHIONO LCA
GARTLAND, SHIONO*
ALL TORSION ANGLES WITH DISTANCES LESS THAN A LIMIT.

192 PDP10 FORTRAN SFT, CSF 32 SHIONO LCA
SHIONO, SAX
PACKS UP TO 2800 REFLEXIONS PER PAGE.PRINTS ONLY RUNNING INDEX EVERY TIME.THE LENGTH OF EACH COLUMN IS AUTOMATICALLY ADJUSTED.

193 CDC 3600 FORTRAN4 CELPAR, LCR XDN WEI ASG 20 WADHWAN LIA
WADHAWAN
LEAST-SQUARES REFINEMENT ON BRAGG THETA OBTAINED FROM ZERO-LAYER WEISSENBERG PHOTOGRAPHS.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 CRYSTL1A PRO,AVG OUA SRT DRF,LPC PRC WEI 15 CROSS LCA
CROSS
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. EQUIVALENT 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 CRYSTL-1 DRF, CIR LPC WTA 32 POWELL LCA
GRIFFITHS,POWELL
A DATA REDUCTION PROGRAM FOR FOUR CIRCLE DIFFRACTOMETER DATA. CORRECTIONS APPLIED ARE 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 CRYSTL-2 PRO/DRF, AVG CMP OUA SCH SRT 32 POWELL LCA
POWELL
A UNIQUE SET OF REDUCED DATA ARE EXTRACTED FROM OUTPUT OF CRYSTL-1. 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 CRYSTL-3 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 TMO 32 POWELL LCA
GRIFFITHS,POWELL
PROGRAM DEALS WITH SPACEGROUPS 1 TO 74 EXCLUDING FDD2 AND FDDD.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, BLS 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 MANIOC, 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 WTA

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 & CCORDINENCE 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 DY 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 POOR 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+NXNXO.002)K.
SPEED (10+ 0.00004XNXNXN) SECS.CHARGE NEGOTIATED FOR COMMERCIAL USE.

209 ICLKDF9 ALGOL JYQ4445 PLT, HKL STE LAU DY 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 CYLINDRICALCAMERAS.
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 LMN DY 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 ALGOL JYQ021 POW, HKL DHK DST 16 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+ 0.002NXN) SECONDS.
CHARGE NEGOTIATED FOR COMMERCIAL USE.

212 IBM36044 FORTRAN LAT, RUC 15 LAWTON LCA
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 32 ALCOCK LCA
ALCOCK
VERY GENERAL IN ATLAS VERSION,INCLUDING MANY RECORDING GEOMETRIES

AND CALCULATION OF EXTINCTION COEFFICIENT. 4130 VERSION IS STAND-ALONE

214 ICL1905 FORTRAN PLT,POL 16 ROTHWL LCA
ROTHWELL
CONSTRUCTION OF POLE FIGURES DRAWN ON A DIGITAL PLOTTER. REFERENCES
LEWIS,D ET AL. STUDY OF TWINNING 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 CII510 ASLOGA S24K AFI,BIS ESD FLS LAD LAY LSP XYZ 12 BASSI LCA
BASSI G C
REFINEMENT ON SINGLE REFLECTIONS.MULTIPLICITY IS ALLOWED.SPACE GROUP IS DESCRIBED AS PRINTED IN THE INTERNATIONAL TABLES.

216 CII510 ASLOGA S24K AFM,BIS ESD FLS LAD LAY LSP XYZ 12 BASSI LCA
BASSI G C
SAME AS AFI PLUS:REFINEMENT ON MULTIPLE REFLECTIONS AS IN POWDER TECNIQUE AND POSSIBILITY OF USING ONE GROUP OF X-RAYS INTENSITIES AND ONE GROUP OF NEUTRONS INTENSITIES

217 CII510 ASLOGA S24K INS,ASG SAD SIS 12 BASSI LCA
BASSI G C
GENERAL PROGRAM GIVING INTENSITY WITH MULTIPLICITY,STRUCTURE FACTOR WITH SIGN OR PHASE.

218 CII510 ASLOGA S24K IND,HKL DST 12 BASSI LCA
BASSI G C
IND TAKES ACCOUNT OF GENERAL CONDITIONS ON (HKL)

219 CII510 ASLOGA S24K DII,ASG BOL 12 BASSI LCA
BASSI G C,GEYNET M
PRINTS ALL DISTANCES LESS THAN ONE LIMIT PER PAIR OF SITES

220 CII510 ASLOGA S24K FOU,FR3 FPD 12 BASSI LCA
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 CII510 ASLOGA S24K GOU,FR3 FPD 12 BASSI LCA
BASSI G C,GEYNET M
SAME AS FOU BUT PERMITS A LOCAL DISTORTION TO INCREASE THE RESOLUTION POWER OF THE MAP

222 CII510 ALGOL S24K AFFIMAILLE,LCR 12 BASSI LCA
BASSI G C,ROUDAUT M
CELL REFINEMENT FROM POWDER DIFFRACTION PATTERNS.SIX SEPARATE PROGRAMS,ONE PER SYSTEM

223 CII510 ALGOL S24K TRACE,PLT DRW 12 BASSI LCA
ROUDAUT M
GENERAL STUCTURE DRAWING WITH POSSIBILITY OF ORIENTED BOUNDS AND DIFFERENT ATOMIC RADII

224 CII510 ALGOL S24K SEPARRAIES,PRS 12 BASSI LCA
BASSI G C,ROUDAUT M
PERFORMS THE DERIVATION OF A MULTIPLE POWDER PEAK INTO GAUSSIAN COMPONENTS WITH SAME OR DIFFERENT HALF-WIDTH AT WILL.

225 CII510 ALGOL S24K ABSORPLAQUES,ABS 12 BASSI LCA
BASSI G C,ROUDAUT M
ABSORPTION CORRECTION FOR FLAT SPECIMEN

226 CII510 ALGOL S24K DIAGNEUTRONS,FOB LPC 12 BASSI LCA
BASSI G C,ROUDAUT M,SIEGFRIED R
SET OF PROGRAMS STARTING FROM SCANNED POWDER INTENSITIES ON A ONE-OR TWO-DETECTORS NEUTRON DIFFRACTOMETER AND GIVING BACK-GROUD AND LORENTZ CORRECTED INTEGRATED INTENSITIES

227 CII510 ALGOL S24K ANGLES,DIF GSC 12 BASSI LCA
BASSI G C,GUITEL J C
COMPUTATION OF SETTING ANGLES IN 4-CIRCLE DIFFRACTOMETER.ORIENTATION MATRIX IS FOUND GEOMETRICALLY

228 CII510 ALGOL S24K GENERATEUR,DIF HKL 12 BASSI LCA
BASSI G C
COMPUTES ALL INDICES BETWEEN TWO ANGULAR LIMITS IN VIEW OF INPUT FOR INTENSITIES MEASUREMENTS ON A FOUR-CIRCLE GONIOSTAT

229 CII510 ALGOL S24K SIMPLEXE,SPW ASD 12 BASSI NNN
BASSI G C
DIRECT STRUCTURE DETERMINATION FROM INTENSITIES WITHOUT PHASE EVALUATION

230 CII510 ASLOGA S24K LAMI,DIF CCD CIR GSC OMC OMR RTS 12 BASSI MCA
BASSI G C,GEYNET M,GUITEL J C
GENERAL REAL TIME SYSTEM USING AN ORIENTED LANGUAGE CALLED LAMI, GIVING ACCESS TO ALL GEOMETRICAL POSSIBILITIES OF A DIFFRACTOMETER INCLUDES PEAK POSITION OPTIMISATION,INTENSITIES MEASUREMENTS UNDER VARIOUS CONDITIONS,ROTATION AROUND THE DIFFUSION VECTOR,LEAST SQUARES AUTOMATIC ORIENTATION MATRIX DETERMINATION

231 CDC6600 FORTRAN4 SEKO, DIF GSC HKL 30 FLETCHR NIS
FLETCHER, STEPHENS
A COMPUTER PROGRAM TO CALCULATE SETTING ANGLES AND GENERATE PAPER STEERING TAPES FOR THE FIVE-POINT MEASURENENT MODE OF DATA COLLECTION ON A SIEMENS OFF-LINE X-RAY DIFFRACTOMETER.

232 CDC6600 FORTRAN4 SODI, PRO OUA NET SCL LPC 30 FLETCHR NIS
STEPHENS
A COMPUTER PROGRAM TO PROCESS THE OUTPUT OF A SIEMENS OFF-LINE X-RAY DIFFRACTOMETER AND PRODUCE A LIST OF OBSERVED INTENSITIES CORRECTED FOR LORENTZ AND POLARISATION FACTORS

233 NEAC2200 FORTRAN UNICS DIR, STF S2I TMO 40 ASHIDA LIA
ASHIDA
'SIGMA' PERFORMS WILSON STATISTICS AND SIGMA 2 INTERACTIONS SEARCH

234 NEAC2200 FORTRAN UNICS DIR, PTN TMO 40 ASHIDA LIA
ASHIDA

235 NEAC2200 FORTRAN UNICS REF, BLS XYZ BIJ SCL ESD 40 ASHIDA LIA
ASHIDA
'HBLS-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 (TMO)

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 CISOSF AND CANILS,IN THE HURAY SYSTEM.
PROGRAM WORKS WITH ICL GEORGE 3 OPERATING SYSTEM ONLY.

238 ICL1905E FORTRAN HURAY-10 CANILS,TMO BIJ BLS 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 CISOSF,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 CFOURR,TMO FPD FRS 29 CMORGAN LIA
HALL,MORGAN*
DOES NOT ACCEPT FOD2 OR FODD.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 CFOURR IN ANY OF 6 POSSIBLE ORIENTATIONS ON LINE PRINTER
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 UNC1108 FORTRAN FFOCUS1, SAXS DESM 16 VONK LCA
VONK
SAXS DESMEARING PROCEDURE. SEE J.APPL.CRYST.(1971) 4,340

244 IBM36065 ALGOL60 LSP, POW UCP(HKL IND DHK DST) 24 VISSER LIA
VISSER 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 LCA
VISSER 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 LCA
VISSER 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 THIESSN LIA
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.

Reference table

100	CDC	FTN IV		SCOPECUFIT, FLS DLS	32	THOENI	LIA
99	CDC	FTN IV	ETHOS	DLS, FLS	33	MEIER	LCA
193	CDC3600	FORTRAN4		CELPAR, LCR XDN WEI ASG	20	WADHWAN	LIA
65	CDC6500	FORTRAN4		DIF, OMC OMR	18	LIEDL	LIA
86	CDC6600	FORTRAN		SEARCHER, AHA SIS FPS BLS DRW	96	KOYAMA	LCA
106	CDC6600	FORTRAN4		ANGLES,	17	WOLTEN	LIA
110	CDC6600	FORTRAN4		ASTM7,SCH		WOLTEN	NIA
101	CDC6600	FORTRAN4		BCSU,ASG BRG DHK DST HKL GSC	28	WOLTEN	LIA
108	CDC6600	FORTRAN4		BRAGG		WOLTEN	LIA
103	CDC6600	FORTRAN4		CELFIX,	17	WOLTEN	LIA
104	CDC6600	FORTRAN4		LIM,		WOLTEN	LIA
107	CDC6600	FORTRAN4		PRECES,PRC		WOLTEN	LIA
231	CDC6600	FORTRAN4		SEKO, DIF GSC HKL	30	FLETCHR	NIS
232	CDC6600	FORTRAN4		SODI, PRO OJA NET SCL LPC	30	FLETCHR	NIS
102	CDC6600	FORTRAN4		SPHERE,ASG GSC HKL GRT DST STE	28	WOLTEN	LIA
109	CDC6600	FORTRAN4		STACK	20	WOLTEN	LIA
105	CDC6600	FORTRAN4		TWIN,TMO		WOLTEN	LIA
225	CII510	ALGOL	S24K	ABSORPLAQUES,ABS	12	BASSI	LCA
222	CII510	ALGOL	S24K	AFFIMAILLE,LCR	12	BASSI	LCA
227	CII510	ALGOL	S24K	ANGLES,DIF GSC	12	BASSI	LCA
226	CII510	ALGOL	S24K	DIAGNEJTRONS,FOB LPC	12	BASSI	LCA
228	CII510	ALGOL	S24K	GENERATEJR,DIF HKL	12	BASSI	LCA
224	CII510	ALGOL	S24K	SEPARRAIES,PRS	12	BASSI	LCA
229	CII510	ALGOL	S24K	SIMPLEXE,SPW ASD	12	BASSI	NNN
223	CII510	ALGOL	S24K	TRACE,PLT DRW	12	BASSI	LCA
215	CII510	ASLOGA	S24K	AFI,BIS ESD FLS LAD LAY LSP XYZ	12	BASSI	LCA
216	CII510	ASLOGA	S24K	AFM,BIS ESD FLS LAD LAY LSP XYZ	12	BASSI	LCA
219	CII510	ASLOGA	S24K	DII,ASG BOL	12	BASSI	LCA
220	CII510	ASLOGA	S24K	FOU,FR3 FPD	12	BASSI	LCA
221	CII510	ASLOGA	S24K	GOU,FR3 FPD	12	BASSI	LCA
218	CII510	ASLOGA	S24K	IND,HKL DST	12	BASSI	LCA
217	CII510	ASLOGA	S24K	INS,ASG SAD SIS	12	BASSI	LCA
230	CII510	ASLOGA	S24K	LAMI,DIF CCD CIR GSC OMC OMR RTS	12	BASSI	MCA
211	HONTS	ALGOL	JYQ021	POW, HKL DHK DST	16	CLARKE	LIC
87	IBM+UNC	FORT+ASM	FILMDATA	MSC,CCS PRO, DRF,PRC WEI LPC FOB	32	PEARSON	LCA
88	IBM+UNC	FORT+ASM	FILMDATA	1COMPAK FED, COMP FORMT	12	PEARSON	LCA
89	IBM+UNC	FORT+ASM	FILMDATA	2MAPP FED, PRT SAMP	32	PEARSON	LCA
90	IBM+UNC	FORT+ASM	FILMDATA	3FILM DRF,PRC WEI LPC WTA FOB SC	32	PEARSON	LCA
91	IBM+UNC	FORT+ASM	FILMDATA	4SCALE PRO, LAY AVG CMP OUA SRT	32	PEARSON	LCA
188	IBM1130	FORTRAN		DIF, CIR HKL GSC	16	SHIONO	LCA
181	IBM1130	FORTRAN		DIR, SCL WSN EHS	16	SHIONO	LCA
189	IBM1130	FORTRAN		DRF, LPC CIR SCL	16	SHIONO	LCA
179	IBM1130	FORTRAN		DRF, LPC PRC WEI	16	SHIONO	LCA
184	IBM1130	FORTRAN		FOU, TMO FBL FPD FR3	16	SHIONO	LCA
190	IBM1130	FORTRAN		GEO, ASG SBL SID SAN	16	SHIONO	LCA
191	IBM1130	FORTRAN		GEO, TOR	16	SHIONO	LCA
186	IBM1130	FORTRAN		LAT, LCR ASG	16	SHIONO	LCA
187	IBM1130	FORTRAN		MSC, ASG HKL BRG DHK DST	16	SHIONO	LCA
180	IBM1130	FORTRAN		PRO, AVG CMP SCL SRT	16	SHIONO	LCA
183	IBM1130	FORTRAN		REF, ASG SCL XYZ BLS ESD BIJ	16	SHIONO	LCA
185	IBM1130	FORTRAN		SCF, ISC	16	SHIONO	LCA

182	IBM1130	FORTRAN		SFC, ASG SAN SFO	16	SHIONO	LCA
111	IBM1130	FORTRAN	X-ARC-00	X-RAYARC, MSC CCS XDN		TRUTER	LCA
113	IBM1130	FORTRAN	X-ARC-02	PICK3, DIF HKL OMC OMR LCR GSC	16	TRUTER	LIA
115	IBM1130	FORTRAN	X-ARC-03	PRED,PRO DRF NET OUA LPC FOB WTA	8	TRUTER	LIA
117	IBM1130	FORTRAN	X-ARC-04	DATAR, SCF ISC	7	TRUTER	LCA
118	IBM1130	FORTRAN	X-ARC-05	FODAP, FOU FBL FPD FR3 FPS ASG	16	TRUTER	LIA
120	IBM1130	FORTRAN	X-ARC-06	MAMIE,REF BIS XYZ OCC LAY FLS	15	TRUTER	LCA
119	IBM1130	FORTRAN	X-ARC-07	SAP1-48, DIR EHS STF S2I SAP SCP	16	TRUTER	NCA
132	IBM1130	FORTRAN	X-ARC-08	BANGL, GEO SBL SID SAN	9	TRUTER	LIA
124	IBM1130	FORTRAN	X-ARC-10	MPLN, GEO MPL DIH	11	TRUTER	LCA
122	IBM1130	FORTRAN	X-ARC-11	HGEN, GEO	9	TRUTER	LIA
126	IBM1130	FORTRAN	X-ARC-12	INIAX, PLT DRW	16	TRUTER	LIA
114	IBM1130	FORTRAN	X-ARC-13	ABSEP, COR ABI	16	TRUTER	NIS
125	IBM1130	FORTRAN	X-ARC-14	TORSN, GEO TOR	7	TRUTER	LCA
112	IBM1130	FORTRAN	X-ARC-19	DEES, POW HKL DHK BRG DST	16	TRUTER	LCA
121	IBM1130	FORTRAN	X-ARC-20	BLOK,REF BLS LAD BIJ SCH OCC XYZ	16	TRUTER	LIA
131	IBM1130	FORTRAN	X-ARC-21	RANGE, REF	13	TRUTER	LIA
127	IBM1130	FORTRAN	X-ARC-22	FTAB, SFT CSF	16	TRUTER	LIA
128	IBM1130	FORTRAN	X-ARC-23	RCELL, POW UCP	9	TRUTER	NNN
116	IBM1130	FORTRAN	X-ARC-24	FSORT, FED FST	5	TRUTER	LIA
129	IBM1130	FORTRAN	X-ARC-26	ECALC, DIR EHS	16	TRUTER	LCA
123	IBM1130	FORTRAN	X-ARC-27	BOND, SBL SAN	10	TRUTER	LCA
130	IBM1130	FORTRAN	X-ARC-29	ELIPS, THV TEL		TRUTER	NN
4	IBM1800	FORTRAN		ABSG, ABS CIR ABI LPC SEX	13	PEW	LIA
3	IBM1800	FORTRAN		ABSW, ABS WEI ABI LPC SEX	9	PEW	LIA
13	IBM1800	FORTRAN		DIF, CCD WEI HKL ASG VAR OUA	8	NSTAM	LIS
1	IBM1800	FORTRAN		PIRUM, POW UCP HKL IND DHK	13	PEW	LIA
29	IBM1800	FORTRAN		POW, CPP BRG DHK	5	NORD	LCA
2	IBM1800	FORTRAN		PURUM, POW UCP DHK	13	PEW	LIA
17	IBM1800	FORTRAN		REF, BLS BIS LAY XYZ WAN ASG	8	BRANDT	LCA
7	IBM1800	FORTRAN2		CHOW, GEO MPL SAN SID SBL TOR	10	KOENIG	LIA
5	IBM1800	FORTRAN2		PHASE2, DIR ASG S2I SAP PTN MLT	10	KOENIG	LIA
8	IBM1800	FORTRAN4		DIR, CSP MLT ORG SAP S1I S2I	10	NSTAM	LIA
10	IBM1800	FORTRAN4		DIR, TMO MLT WSM S2I	10	NSTAM	LIA
9	IBM1800	FORTRAN4		DIR, TMO OES S1I S2I	10	NSTAM	LIA
14	IBM1800	FORTRAN4		GEO, MPL DIH VAR	8	NSTAM	LIA
15	IBM1800	FORTRAN4		GEO, TOR PRH	8	NSTAM	LIA
12	IBM1800	FORTRAN4		PRO, NET OUA CMP VAR WTA	5	NSTAM	LIA
16	IBM1800	FORTRAN4		SFT, CSF AGR	8	NSTAM	LIA
212	IBM36044	FORTRAN		LAT, RUC	15	LAWTON	LCA
133	IBM36050	FORTRAN4	NRC-1	DIF, GSC CIR HKL ASG LPC	4	AHMED	LCA
141	IBM36050	FORTRAN4	NRC-10	REF, BLS XYZ BIJ BIS OCC SCL ESD	22	AHMED	LCA
142	IBM36050	FORTRAN4	NRC-12	GEO, SBL SAN SID ESD POL	23	AHMED	LCA
143	IBM36050	FORTRAN4	NRC-14	AGA	4	AHMED	LCA
135	IBM36050	FORTRAN4	NRC-2	DRF, FOB ISC CIR WEI LPC SHF WTA	8	AHMED	LCA
134	IBM36050	FORTRAN4	NRC-2A	PRO, AVG CMP OUA NET SCH SCL SRT	22	AHMED	LCA
144	IBM36050	FORTRAN4	NRC-21	POW, DHK DST HKL ASG	10	AHMED	LCA
145	IBM36050	FORTRAN4	NRC-22	GEO, MPL DIH	6	AHMED	LCA
146	IBM36050	FORTRAN4	NRC-23	SFT, CSF	13	AHMED	LCA
147	IBM36050	FORTRAN4	NRC-24	PRJ, ORT	4	AHMED	LCA
136	IBM36050	FORTRAN4	NRC-3	COR, ABS ABI CIR	9	AHMED	LCA
137	IBM36050	FORTRAN4	NRC-4	DIR, SAP CSP TMO STF EHS ORG S2I	22	AHMED	LCA
138	IBM36050	FORTRAN4	NRC-5	DIR, TMO STF EHS PTN S2I	25	AHMED	LCA
139	IBM36050	FORTRAN4	NRC-8	FOU, FPD FR3 FUM SHF ASG	23	AHMED	LCA
140	IBM36050	FORTRAN4	NRC-9	REF, DFS XYZ ESD	27	AHMED	LCA
245	IBM36065	ALGOL60		ITO-ALG, POW LCD	32	VISSER	LCA
244	IBM36065	ALGOL60		LSP, POW UCP(HKL IND DHK DST)	24	VISSER	LIA
97	IBM36065	FORTRAN		VMS, VMF TMO	32	JACOBSN	LCA
98	IBM36065	FORTRAN		VMS, VVR	32	JACOBSN	LCA
201	IBM36065	FORTRAN4		FOU, FBL ASG FR3 FUM SHF SAN SAD		ARAKI	MCA

96	IBM36065	PL/1		FED, ASG GRT	32	JACOBSN	LCA
92	IBM36065	PL/1		FOU, FCT ASG FPD FR3	32	JACOBSN	LCA
95	IBM36065	PL/1		FOU, FCT FPD FRI FR2	32	JACOBSN	LCA
93	IBM36065	PL/1		FOU, FCT FTM FR3	32	JACOBSN	LCA
246	IBM36065	PL/1		ITO-PL/1, POW LCD	32	VISSER	LCA
94	IBM36065	PL/1		MSC, 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 WEI LPC PEX SEX	26	BRANDT	LCA
33	IBM36075	FORTRAN		DRF, HKL NET LPC OUA FOB	26	BRANDT	LCA
22	IBM36075	FORTRAN		DRF, PEX SEX	13	BRANDT	LCS
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	50	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, BLS 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	FORTRAN4		DIF, CIR HKL ASG	15	NSTAM	LIA
6	IBM36075	FORTRAN4		FALFA, REF FLS FAZ EXT LAD OCC	20	KOENIG	LIA
83	IBM36075	FORTRAN4	ORTEP-2	PLT, DRW TEL STE SBL SAN	50	JOHNSON	LCA
74	IBM36075	FORTRAN4	SPSRM360	MSC, EOA	20	TOURNAR	MIA
76	IBM36075	FORTRAN4	SPSRM379	POW, BRG DHK EOA LCD	25	TOURNAR	MIA
78	IBM36075	FORTRAN4	SPSRM386	REF, BIS EOA ESD LAY XYZ	40	TOURNAR	MIA
207	IBM36091	FORTRAN4	DR012	FIGATOM, DRW PLT STE ASG SPL	400	LANGLET	LIS
85	IBM36091	FORTRAN4	OR FFE3	GEO, ESD SID SAN DIH TOR TEL CBA	128	BUSING	LIA
84	IBM36091	FORTRAN4	OR XFLS3	REF, FLS ASG BIJ LAD LAX OCC LAY	128	BUSING	LIA
81	IBM36091	FORTRAN4	ORDATLIB	DRF, ABI FOB LPC CIR ADL SCL	64	ELLISON	LIA
82	IBM36091	FORTRAN4	ORDATSRT	DRF, SRT AVG CMP SCL SCH ASG	85	ELLISON	LIA
247	IBM36091	FORTRAN4	ORESTES	DIR, EHS STF BIJ ASG ACT WSN WTA	25	THIESSN	LIA
66	IBM36091	FORTRAN4	SPSRM286		40	TOURNAR	MIA
67	IBM36091	FORTRAN4	SPSRM302	POW, LCP	54	TOURNAR	MIA
68	IBM36091	FORTRAN4	SPSRM304	MSC, EON REN	40	TOURNAR	MIA
69	IBM36091	FORTRAN4	SPSRM307	FOU, FPS FR2 SHF	23	TOURNAR	MIA
70	IBM36091	FORTRAN4	SPSRM308	MSC, EOA	10	TOURNAR	MIA
71	IBM36091	FORTRAN4	SPSRM321	COR, ABA SEX EOA	40	TOURNAR	MIA
72	IBM36091	FORTRAN4	SPSRM330	COR, ABI SEX	16	TOURNAR	MIA
73	IBM36091	FORTRAN4	SPSRM344	GEO,	40	TOURNAR	MIA
75	IBM36091	FORTRAN4	SPSRM360	MSC, EOA	33	TOURNAR	MIA
77	IBM36091	FORTRAN4	SPSRM379	POW, BRG DHK EOA LCD	37	TOURNAR	MIA
79	IBM36091	FORTRAN4	SPSRM386	REF, BIS EOA ESD LAY XYZ	53	TOURNAR	MIA
80	IBM36091	FORTRAN4	SPSRM388		37	TOURNAR	MIA
203	IBM7094	FORTRAN2		MANIOC, EST ASG	32	BAUR	LIA
209	ICLKDF9	ALGOL	JYQ4445	PLT, HKL STE LAU	DY	CLARKE	LIC
208	ICLKDF9	ALGOL	JYQ6160	MSC, POW DEC	DY	CLARKE	LIC
210	ICLKDF9	ALGOL	JYQ8484	MSC, XDN KOS DHK LMN	DY	CLARKE	LIC
214	ICL1905	FORTRAN	PLT,POL		16	ROTHWL	LCA
237	ICL1905E	FORTRAN	HURAY-05	CINTER,ISC	05	CMORGAN	LIA
238	ICL1905E	FORTRAN	HURAY-10	CANILS,TMO BIJ BLS ESD FDG LSP	20	CMORGAN	LIA
239	ICL1905E	FORTRAN	HURAY-11	CISOSF,SIS TMO	16	CMORGAN	LIA
240	ICL1905E	FORTRAN	HURAY-20	CFOURR,TMO FPD FRS	29	CMORGAN	LIA
241	ICL1905E	FORTRAN	HURAY-21	CFOUT	21	CMORGAN	LIA
242	ICL1905E	FORTRAN	HURAY-40	CMOLGY,MPL	17	CMORGAN	LIA
178	ICL4-70	FORTRAN4	HMJSR002	FENRIS POW LB DST		F UKAEA	LIA
177	ICL4-70	FORTRAN4	HMJSR003	FIREFLY POW BRG CPP DHK DST ASG	136	F UKAEA	LCA
169	ICL4120	ALGOL	RFL SS	FIREBALL POW INT	8	F UKAEA	LNN
176	ICL4120	ALGOL	RFL 254	FAIRFAX POW	1	F UKAEA	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 INTC POW LB	4?	F	UKAEA	LNA
163	ICL4120	ALGOL	RFL 331	FIREDAWG EDITW POW	1	F	UKAEA	LNA
161	ICL4120	ALGOL	RFL 7037	FIRESTAR LCD C POW	7	F	UKAEA	LCA
162	ICL4120	ALGOL	RFL 7062	FIRECRACKER CAL POW	1	F	UKAEA	LCA
159	ICL4120	ALGOL	RFL 7069	FIRESTAR LCD MO POW UCP	10	F	UKAEA	LCA
160	ICL4120	ALGOL	RFL 7072	FIRESTAR LCD TEHR POW UCP	9	F	UKAEA	LCA
158	ICL4120	ALGOL	RFL 7083	FIRESTAR LCD T POW UCP	9	F	UKAEA	LNA
151	ICL4120	FORTRAN4	RFL 292	FIRETWIST INVERT POW	1	F	UKAEA	LNA
153	ICL4120	FORTRAN4	RFL 330	FIREPUP EDIT POW	1	F	UKAEA	LNA
155	ICL4120	FORTRAN4	RFL 333	FIREGLOW EDITS POW	1	F	UKAEA	LNA
149	ICL4120	FORTRAN4	RFL 336	FIRESCALP 18TO17 POW	1	F	UKAEA	LNA
150	ICL4120	FORTRAN4	RFL 337	FIREPAIR TOTAL POW	1	F	UKAEA	LNA
175	ICL4120	FORTRAN4	RFL 340	FIRERICE POW LB	7?	F	UKAEA	LNA
170	ICL4120	FORTRAN4	RFL 347	FIRECUB POW SKH LB	1	F	UKAEA	LNA
172	ICL4120	FORTRAN4	RFL 348	FIREHEX POW SKH LB	1	F	UKAEA	LNA
173	ICL4120	FORTRAN4	RFL 349	FIRETANGLE POW SKH LB	1	F	UKAEA	LNA
171	ICL4120	FORTRAN4	RFL 350	FIREPRISM POW SKH LB	1	F	UKAEA	LNA
174	ICL4120	FORTRAN4	RFL 352	FIRERICE POW LB	7?	F	UKAEA	LNA
164	ICL4120	FORTRAN4	RFL 332	FIREDOG EDITW POW	1	F	UKAEA	LNA
165	ICL4120	FORTRAN4	RFL 359	FIREADD EDITF POW	1	F	UKAEA	LNA
166	ICL4120	FORTRAN4	RFL 360	FIRECOP EDITG POW	1	F	UKAEA	LNA
148	ICL4120	NEAT	RFL 226	ALGCON 5TO8 POW	2?	F	UKAEA	LNA
38	ICL4130	ALGOL	DPS	DY1DQF, VMS VPS REC	5		TOLLIN	LIA
36	ICL4130	ALGOL	DPS	DY2DQF, VMS VPS REC	5		TOLLIN	LIA
34	ICL4130	ALGOL	DPS	IMITHP, VMS VOS REC	3		TOLLIN	LIA
35	ICL4130	ALGOL	DPS	IMRFNIA, VMS VOS REC	5		TOLLIN	LIA
37	ICL4130	ALGOL	DPS	RFLTEA, VMS VOS REC RAB	5		TOLLIN	LIA
195	ICL4130	FORTRAN	CRYSTL-1	DRF, CIR LPC WTA	32		POWELL	LCA
196	ICL4130	FORTRAN	CRYSTL-2	PRO/DRF, AVG CMP OUA SCH SRT	32		POWELL	LCA
197	ICL4130	FORTRAN	CRYSTL-3	PRO/DRF, LAY SCL ISC WSN FOB	32		POWELL	LCA
198	ICL4130	FORTRAN	CRYSTL-4	FOU, FR3 FBL FPD SHF TMO	32		POWELL	LCA
199	ICL4130	FORTRAN	CRYSTL-5	REF, BLS XYZ BIJ FDG LAY LSP SCH	32		POWELL	LCA
200	ICL4130	FORTRAN	CRYSTL-6	GEO, SAN SBL SID ESD MPL DIH TEL	32		POWELL	LCA
194	ICL4130	FORTRAN	CRYSTL1A	PRO,AVG OUA SRT DRF,LPC PRC WEI	15		CROSS	LCA
39	ICL4130	FORTRAN	DPS	EFITF , VMS VOS REC	3		TOLLIN	LIA
41	ICL4130	FORTRAN	DPS	EFPATS, FPD VOS	3		TOLLIN	LIA
42	ICL4130	FORTRAN	DPS	EF1DQF, VMS VPS REC	5		TOLLIN	LIA
40	ICL4130	FORTRAN	DPS	EF2DQF, VMS VPS REC	5		TOLLIN	LIA
213	ICL4130	FORTRAN	XRAY63	ABS,ABA	32		ALCOCK	LCA
234	NEAC2200	FORTRAN	UNICS	DIR, PTN TMO	40		ASHIDA	LIA
233	NEAC2200	FORTRAN	UNICS	DIR, STF S2I TMO	40		ASHIDA	LIA
236	NEAC2200	FORTRAN	UNICS	GEO, DIH MPL ROT SAN SID SBL ASG	16		ASHIDA	LIA
235	NEAC2200	FORTRAN	UNICS	REF, BLS XYZ BIJ SCL ESD	40		ASHIDA	LIA
192	PDP10	FORTRAN		SFT, CSF	32		SHIONO	LCA
47	UNC1108	FOR IV	XNTH	DISTAN, GEO SID SBL	10		BORGEN	NNS
43	UNC1108	FOR IV	XNTH	FOUFU1, FOU FBL FPD FR2 FR3	20		BORGEN	LCA
44	UNC1108	FOR IV	XNTH	FOUFU1, FOU FBL FPD FR2 FR3	20		BORGEN	LCA
45	UNC1108	FOR IV	XNTH	FOUPLA, FOU FPL FUM SHF	50		BORGEN	LCA
48	UNC1108	FOR IV	XPROGF	PAFIV2, GEO SAN SID SBL	30		BORGEN	LIA
56	UNC1108	FOR V		GRUGEN, MSC REP	20		BORGEN	LCS
55	UNC1108	FOR V		SYMVEC, THV CSC	65		RA	LCS
61	UNC1108	FOR V	XPROGF	SCALE1, PRO SCL	1		BORGEN	LCS
54	UNC1108	FOR V	XNTH	BESPLA, GEO MPL	4		BORGEN	LCA
52	UNC1108	FOR V	XNTH	CNHM, CHP	2		BORGEN	MNS
50	UNC1108	FOR V	XNTH	PLOSTR, PLT DRW TEL	30		BORGEN	LIA

51	UNC1108	FOR V	XATH	TOLLIN, POS	20	BORGEN	LCA
53	UNC1108	FOR V	XATH	TORCOR, THV RIG	10	BORGEN	LIA
59	UNC1108	FOR V	XPROGF	ABSCO1, DRF ABS	6	BORGEN	LCS
58	UNC1108	FOR V	XPROGF	CARSI1, DRF FOB LPC CIR	4	BORGEN	LCS
63	UNC1108	FOR V	XPROGF	FFILE1, FED	5	BORGEN	LCS
62	UNC1108	FOR V	XPROGF	LISTF1, FED PRT	1	BORGEN	LCS
46	UNC1108	FOR V	XPROGF	LSFIV4, REF BMIX ESD FLS LAY XYZ	40	BORGEN	LIA
60	UNC1108	FOR V	XPROGF	STABL1, DRF RRA	2	BORGEN	LCS
57	UNC1108	FOR V	XPROGF	TAPSI1, DRF FOB LPC CIR	4	BORGEN	LCS
64	UNC1108	FOR V	XRAY*TU	COPRO1, MSC CCS	8	BORGEN	NNN
243	UNC1108	FORTRAN		FFOCUS1, SAXS DESM	16	VONK	LCA
49	UNC1108	NU ALGOL	XATH	FOUPL1, PLT FOR	10	BORGEN	NCA
204	360/370	FORTRAN4		CALHPO, GEO ASG	32	BAUR	LIA
205	360/370	FORTRAN4		LPFPRE, COR LPC PRC ASG	32	BAUR	LIA
206	360/370	FORTRAN4		OUTPICK, PRO DRF ASG	64	BAUR	LIS
202	360/370	FORTRAN4		SADIAN69, GEO SAN SBL DRW PRJ	32	BAUR	LI

Dictionary of Abbreviations

Programming languages

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

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 SYNTHESES
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 I.
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 BY BIT UNPACKING THEN REPACKING, I.E. BYTES TO WORDS
FOU	FOURIER TYPE CALCULATION
FPD	FOURIER, PATTERSON & DIFFERENCE SYNTHESES
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

LPC	LORENTZ AND POLARIZATION CORRECTIONS
LSP	LEAST SQUARES WITH ALLOWANCE FOR ATOMS IN SPECIAL POSITIONS
MD.	MARYLAND
MFF	MAGNETIC FORM FACTOR DETERMINATION
MLT	MULTISOLUTION PROCEDURE
MO	MONOCLINIC AND ORTHORHOMBIC ONLY
MPD	CORRECTION FOR MULTIPLE DIFFRACTION
MPL	MEAN PLANE THROUGH A SET OF ATOMS BY LEAST SQUARES
MSC	MISCELLANEOUS
MSD	MAGNETIC STRUCTURE DETERMINATION
NDN	NEUTRON DIFFRACTION
NET	CALCULATION OF NET COUNTS
NSC	NEUTRON SCATTERING FACTOR DETERMINATION
NSG	NON-CENTROSYMMETRIC SPACE GROUPS ONLY
OCC	REFINEMENT OF OCCUPANCY FACTORS
OES	ORIGIN AND ENANTIOMORPH SELECTION
OMC	ORIENTATION MATRIX CALCULATION
OMR	ORIENTATION MATRIX REFINEMENT
ORG	ORIGIN SELECTION
ORT	ORTHOGONAL PROJECTION
OSC	OSCILLATION FILMS IN WEISSENBERG GEOMETRY, ANY MU ANGLE
OUA	OBS/UNOBS ASSIGNMENT
PAS	PHASE ESTIMATION FROM ANOMALOUS SCATTERING
PEX	CORRECTION FOR PRIMARY EXTINCTION
PIA	PHASE ESTIMATION FROM ISOM. REPL. AND ANOM. SCAT.
PIR	PHASE ESTIMATION FROM ISOMORPHOUS REPLACEMENT
PIRUM	PROGRAM FOR INDEXING AND REFINEMENT OF UNIT CELL MATRIX
PLS	PHASE ESTIMATION BY LEAST SQUARES
PLT	PLOTTER PROGRAMS
PLT	AUTOMATIC PLOTTING OF THERMAL ELLIPSOIDS
PLT C	PLOTS COUNTS OR TIMES AS A FUNCTION OF ANGLE
PLT MAX	PLOTS COUNTS AGAINST ANGLE AND LOCATES MAXIMUM BY FOURIER METHOD
POL	CONSTRUCTION OF POLE FIGURES
POL	COORDINATION POLYHEDRA
POS	PLANE ORIENTATION SEARCH
POW	POWDER DIFFRACTION
PRC	PRECESSION GEOMETRY
PRH	PREDICTION OF HYDROGEN POSITIONS FROM GEOMETRICAL CONSIDERATIONS
PRI	PRIMITIVE UNIT CELLS ONLY
PRJ	PROJECTIONS OF THE STRUCTURES
PRO	PROCESSING OF RAW INTENSITY DATA
PRS	POWDER PEAKS SEPARATION
PRT	PROTEIN WORK
PRT	PRINT FILE CONTENTS
PST	PHASE REFINEMENT BY THE SQUARED TANGENT FORMULA
PTN	PHASE REFINEMENT BY THE TANGENT FORMULA
PURUM	PROGRAM FOR REFINEMENT OF UNIT CELL MATRIX
RAB	REFERENCE ROSSMANN AND BLOW 1962 ACTA CRYST, 15, 24
RBL	RIGID BODY LEAST SQUARES
REC	CALCULATION PERFORMED IN RECIPROCAL SPACE
REF	REFINEMENT OF ATOMIC PARAMETERS
REN	RENNINGER EFFECT
REP	GENERATION OF OPERATORS, AND REPRESENTATIONS FOR POINT GROUPS
RID	RIDING MOTION
RIG	RIGID BODY MOTION
ROT	ROTATION ANGLES
RRA	REFERENCE REFLEXION ANALYSIS
RTS	REAL TIME SYSTEM
RUC	REDUCTION OF UNIT CELL
SAD	STRUCTURE FACTORS WITH ANOMALOUS DISPERSION
SAMP	COMPACTION OF VOLUME OF DATA BY USING MAXIMUM VALUE OF GROUP
SAN	STRUCTURE FACTORS WITH ANISOTROPIC THERMAL PARAMETERS
SAN	SCAN OF ANGLES
SAP	SYMBOLIC ADDITION PROCEDURE
SAXS	SMALL ANGLE X-RAY SCATTERING

SBL	SCAN OF BOND LENGTHS
SC	SCREENLESS FILM TECHNIQUE
SCF	SCATTERING FACTOR DETERMINATION
SCH	SCHOMAKER'S CORRECTION OF THERMAL PARAMETER SHIFTS
SCH	SEARCH OF THE ASTM POWDER FILE
SCH	SEARCH FOR UNMEASURED REFLEXIONS
SCL	SCALING OF THE INTENSITIES
SCL	REFINEMENT OF OVERALL SCALE FACTOR
SEX	CORRECTION FOR SECONDARY EXTINCTION
SFC	STRUCTURE FACTOR CALCULATION
SFO	S. F. WITH FRACTIONAL OCCUPANCIES
SFT	S. F. TRIALS BY ADDITION OR SUBTRACTION OF ATOMS
SFT	STRUCTURE FACTOR TABLES FOR PUBLICATION
SGG	SPACE GROUP GENERALITIES
SHF	SHARPENING FUNCTION APPLICATION
SHF	SHARPENING FUNCTION APPLIED
SIC	STRUCTURE INVARIANT CALCULATION
SID	SCAN OF INTERMOLECULAR DISTANCES
SIS	STRUCTURE FACTORS WITH ISOTROPIC THERMAL PARAMETERS
SKH	CALCULATION OF SCHERRER CONSTANTS
SPW	SIMPLEX METHOD
SRG	CONTRIBUTION OF RIGID GROUP
SRT	SORT ON THE INDICES
STE	STEREOSCOPIC PROJECTION
STE	STEREOGRAM
STF	SCALE AND TEMPERATURE FACTOR ESTIMATION
STP	STRUCTURE REFINEMENT FROM POWDER PATTERN BY LEAST SQUARES
SYR	SAYRE'S EQUATION APPLICATION
S1I	SIGMA 1 INTERACTIONS SEARCH
S2I	SIGMA 2 INTERACTIONS SEARCH
T	TRICLINIC ONLY
TDS	THERMAL DIFFUSE SCATTERING
TEHR	TETRAGONAL HEXAGONAL AND RHOMBOHEDRAL ONLY
TEL	THERMAL ELLIPSOIDS
TEL	THERMAL ELLIPSOIDS CALCULATION
THV	THERMAL VIBRATION ANALYSIS
TMO	TRICLINIC, MONOCLINIC, AND ORTHORHOMBIC SYSTEMS ONLY
TOR	TORSIONAL ANGLES
TOTAL	COUNTS THE NUMBER OF ANGLE/COUNT PAIRS ON A TAPE
UCP	UNIT CELL REFINEMENT FROM POWDER PATTERN BY LEAST SQUARES
USF	UNITARY STRUCTURE FACTORS
VAR	VARIANCE
VHA	VECTOR HEAVY ATOM ANALYSIS
VMF	VECTOR MINIMUM FUNCTION
VMS	VECTOR MAP SOLVING AND MANIPULATION
VOS	VECTOR ORIENTATION SEARCH
VPS	VECTOR POSITION SEARCH
VVR	VECTOR VERIFICATION
WAN	WEIGHT ANALYSIS
WEI	WEISSENBERG GEOMETRY
WSM	WEIGHTED SUM FORMULA. WTA USED IS ESTIMATE OF 1/VAR
WSN	WILSON STATISTICS
WTA	WEIGHT ASSIGNMENT
X-ARC	X-RAY ARC
XDN	X-RAY DIFFRACTION
XSC	X-RAY SCATTERING FACTOR DETERMINATION
XYZ	REFINEMENT OF POSITIONAL PARAMETERS
18TO17	CONVERTS ANGLE/COUNT DATA FROM FIELD WIDTH 18 TO 17
360/370	IBM 360 AND IBM 370 SYSTEMS
5TO8	CONVERTS MERCURY 5-HOLE TAPE TO 8-HOLE ISO 7 EVEN PARITY TAPE

Computer abbreviations

CONTROL DATA	CDC 3600	CDC3600
	CDC 6500	CDC6500

	CDC 6600	CDC6600
	CDC 6400/6500	CDC
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	CII510
NEAC	2200	NEAC2200

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