International Union of Crystallography
Commission on Crystallographic Computing

WORLD LIST
OF
CRYSTALLOGRAPHIC COMPUTER PROGRAMS

SECOND EDITION

edited by

DAVID P. SHOEMAKER
(Massachusetts Institute of Technology, Cambridge, Mass., U.S.A.)

1966

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I U CR WORLD LIST OF CRYSTALLOGRAPHIC COMPUTER PROGRAMS

SECOND EDITION
JULY 1, 1966

INTERNATIONAL UNION OF CRYSTALLOGRAPHY
COMMISSION ON CRYSTALLOGRAPHIC COMPUTING

GENERAL DESCRIPTION

1. THE FORMAT OF THIS LIST IS THAT OF THE FIRST EDITION, AND OF PREVIOUS LISTS OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION. IT IS BASED ON THE USE OF STANDARD 80-COLUMN IBM CARDS.

2. NORMALLY, EACH PROGRAM LISTED SHOULD BE A DISCRETE ENTITY CAPABLE OF BEING RUN BY ITSELF (ALTHOUGH IT MAY OR MAY NOT NORMALLY BE USED IN CONJUNCTION WITH ONE OR MORE OTHER PROGRAMS). HOWEVER, A PACKAGE OF MINOR PROGRAMS OR ROUTINES EACH OF WHICH HAS LITTLE IMPORTANCE OUTSIDE THE PACKAGE SHOULD PREFERABLY BE LISTED AS A SINGLE ENTRY.

3. A PROGRAM SHOULD NOT BE LISTED UNLESS IT HAS RUN SUCCESSFULLY, ALTHOUGH IT NEED NOT BE DEBUGGED IN ALL RESPECTS. PREFERENCE FOR LISTING IS FOR PROGRAMS WHICH HAVE SOME PROMISE OF BEING USEFUL TO OTHERS AND FOR WHICH SUITABLE WRITE-UPS ARE, OR WILL PROBABLY BECOME, AVAILABLE.

4. EACH PROGRAM IS TO BE REPRESENTED BY AN ENTRY CONSISTING OF --

A. A TITLE COMPRISING A SINGLE IBM CARD (80 COLUMNS) CONTAINING THE ESSENTIAL INFORMATION PERTAINING TO THE PROGRAM IN A VERY COMPRESSED FORM, AND

B. AN (OPTIONAL) ABSTRACT OF NOT MORE THAN ABOUT 50 WORDS, WRITTEN BY THE AUTHOR(S) OF THE PROGRAM, ON ADDITIONAL IBM CARDS. THIS SHOULD GIVE WHATEVER CAN BE BRIEFLY STATED REGARDING TYPE OF APPLICATION, GENERALITY, VERSATILITY, SPEED, STORAGE REQUIREMENTS, AND ACCURACY. REFERENCES TO OTHER PROGRAMS THAT CAN BE USED IN CONJUNCTION WITH IT ARE VALUABLE.

5. THE I U CR WORLD LIST OF COMPUTER PROGRAMS WILL CONSIST PRIMARILY OF THE TITLE AND ABSTRACT CARDS ARRANGED ACCORDING TO MACHINE TYPE AND FUNCTION.

6. TO ASSIST IN THE USE OF THE PROGRAM LIST, A LISTING OF ABBREVIATIONS AND AN AUTHOR INDEX WILL BE MADE AVAILABLE FROM PUNCHED CARD LISTINGS. THE EXTREME DEGREE OF COMPRESSION REQUIRED ON THE TITLE CARD MAY REQUIRE THAT EVEN AUTHORS NAMES BE ABBREVIATED. IN SUCH CASES THE AUTHOR INDEX WILL CROSS-REFERENCE THE ABBREVIATED NAME TO THE CORRECTLY SPELLED NAME. ASIDE FROM SUCH CROSS REFERENCES, EACH ENTRY IN THE AUTHOR INDEX WILL CONSIST OF SURNAME, INITIALS, AND MAILING ADDRESS, ON A SINGLE IBM CARD.

7. THE TITLE, ABSTRACT, AND AUTHOR-INDEX CARDS SHOULD BE PREPARED BY THE PROGRAMMERS THEMSELVES WHENEVER POSSIBLE, IN ACCORDANCE WITH THE FORMAT GIVEN BELOW. IF THIS IS NOT POSSIBLE, THE INFORMATION SHOULD BE SUBMITTED ON PROGRAM LIST FORMS, AVAILABLE ON APPLICATION.

8. THE INFORMATION SHOULD BE KEPT AS CURRENT AND COMPLETE AS POSSIBLE BY FRESH INFORMATION FROM PROGRAMMERS, FOR FUTURE EDITIONS. ESPECIALLY, THE STATUS AND AVAILABILITY INFORMATION IN COLS. 78 - 80 SHOULD BE COMPLETE AND UP-TO-DATE. OBSOLETE PROGRAMS, AND PROGRAMS THAT HAVE NO APPRECIABLE PROSPECT OF BECOMING AVAILABLE OR OF BEING USEFUL TO OTHERS, SHOULD BE WITHDRAWN.

9. A SUBSTANTIAL REVISION OR MODIFICATION OF A PROGRAM SHOULD BE TREATED

AS A NEW PROGRAM WITH A NEW ENTRY IN THE PROGRAM LIST AND A NEW ACCESSION NUMBER. THE OLDER PROGRAM SHOULD BE WITHDRAWN IF MADE OBSOLETE BY THE REVISION.

10. THE LANGUAGE OF THE TITLE CARD SHOULD BE ENGLISH. FOR ABSTRACT CARDS ENGLISH IS PREFERABLE THOUGH NOT NECESSARY. HOWEVER, ONLY THE ROMAN ALPHABET WITH LETTERS AND CHARACTERS AVAILABLE ON ENGLISH-LANGUAGE IBM MACHINES MAY BE USED.

1234567890 ABCDEFGHIJKLMNOPQRSTUVWXYZ .,=+-/()*

11. PROGRAMS SHOULD BE LISTED UNDER PROGRAMMING LANGUAGES (PSEUDO-MACHINES) SUCH AS ALGOL, FORTRAN, ETC., RATHER THAN UNDER THE ACTUAL MACHINES, WHEN THEY ARE MACHINE-INDEPENDENT OR LARGELY SO, BUT THE MACHINE ON WHICH COMPILED AND TESTED SHOULD BE CITED.

12. CERTAIN CRYSTALLOGRAPHIC PROGRAM SYSTEMS, AND INDIVIDUAL PROGRAMS BELONGING TO THEM, ARE LISTED IN A SEPARATE CATEGORY (THE FIRST CATEGORY IN THE LIST).

13. THIS EDITION CONTAINS LISTINGS FOR 697 PROGRAMS, OF WHICH 311 ARE FROM THE FIRST EDITION AND 386 ARE NEW. A FEW OF THE LISTINGS IN THE FIRST EDITION HAVE BEEN REVISED FOR THE NEW EDITION, AND A FEW HAVE BEEN TRANSFERRED FROM ONE MACHINE TO ANOTHER OR TO FORTRAN. LISTINGS IN THE FIRST EDITION BUT NOT IN THE SECOND ARE

A. THOSE SUGGESTED FOR WITHDRAWAL BY THEIR AUTHORS,

B. THOSE (WITH FEW EXCEPTIONS) WITH NO STATUS AND AVAILABILITY INFORMATION IN COLS. 78 - 80 OF THE TITLE CARD, OR STATED IN COL. 80 AS NOT AVAILABLE, AND

C. THOSE FOR CERTAIN OLD MACHINES JUDGED TO BE OBSOLETE, MOST PROGRAMS FOR WHICH HAVE BEEN WITHDRAWN BY THEIR AUTHORS AND NO NEW PROGRAMS FOR WHICH HAVE BEEN SUBMITTED.

DAVID P. SHOEMAKER, EDITOR
MASS. INST. OF TECH.
CAMBRIDGE, MASS. 02139, U.S.A.

I U CR COMMISSION ON CRYSTALLOGRAPHIC COMPUTING
D. W. J. CRUICKSHANK, CHAIRMAN
W. R. BUSING
TH. HAHN
A. LINEK
M. A. PORAY-KOSHITS
D. P. SHOEMAKER
Y. TAKEUCHI

THE REGIONAL AND MACHINE CORRESPONDENTS WHO AIDED IN THE COLLECTION OF THE PROGRAM LISTINGS ARE NAMED BELOW. ACCOMPANYING THEIR NAMES ARE THEIR ASSIGNED RANGES OF ACCESSION NUMBERS.

1 - 2999 W. R. BUSING (CANADA, U. S. A.)
OAK RIDGE NAT. LAB., P. O. BOX X, OAK RIDGE, TENNESSEE, USA
FOR FIRST EDITION --
D. SAYRE
IBM WATSON RESEARCH CTR., P.O. BOX 218, YORKTOWN HEIGHTS, NEW YORK 10598, USA

3001 - 3499 D. ROGERS (ZEBRA, ATLAS, BRITISH COMMONWEALTH)
IMPERIAL COLLEGE, UNIV. OF LONDON, LONDON S.W. 7, ENGLAND

3501 - 3999 D. W. J. CRUICKSHANK (KDF9)
CHEM. DEPT., THE UNIVERSITY, GLASGOW W. 2, SCOTLAND

4001 - 4499 J. ROLLETT (DEUCE, MERCURY)
COMPUTING LAB., U. OF OXFORD, SOUTH PARKS RD., OXFORD, ENGLAND

5001 - 5999 T. HAHN (AUSTRIA, GERMANY, SWITZERLAND)
INST. FUR KRISTALLOGRAPHIE, HOCHSCHULE AACHEN,
51 AACHEN, TEMPLERGRABEN 55, WEST GERMANY

6001 - 6499 S. ASBRINK (SCANDINAVIA)
INST. OF INORG. AND PHYS. CHEM., U. OF STOCKHOLM,

KUNGSTENGATAN 45, STOCKHOLM, SWEDEN

6501 - 6999 A. LINEK (BULGARIA, CZECHOSLOVAKIA, GERMAN DEMOCRATIC REPUBLIC, HUNGARY, POLAND, ROUMANIA)
INST. OF TECHN. PHYS., ACAD. OF SCI., CUKROVARNICKA 10, PRAGUE, CZECHOSLOVAKIA

7001 - 7499 M. TOURNARIE (FRANCE, PORTUGAL, SPAIN)
40, RUE BANGEON, MASSY, 78, FRANCE
FOR FIRST EDITION --
P. MERIEL, C. E. N. SACLAY, B. P. 2, GIF-SUR-YVETTE, SEINE-ET-OISE, FRANCE

7501 - 7999 C. PANATTONI (ITALY, YUGOSLAVIA)
IST. DI CHIMICA ORGANICA, U. OF PADOVA, PADOVA, ITALY

8001 - 8499 MRS. E. W. M. RUTTEN-KEULEMANS (BELGIUM, NETHERLANDS)
CENTRAAL REKENINST., UNIV. OF LEIDEN, LEIDEN, THE NETHERLANDS
FOR FIRST EDITION --
D. W. SMITS, REKENCENTRUM DER UNIVERSITEIT, APPELSTRAAT 11, GRONINGEN, NETHERLANDS

8501 - 8999 Y. TAKEUCHI (JAPAN)
DEPT. OF MINERALOGY, U. OF TOKYO, MOTOFUJIMACHI, BUNKYOKU, TOKYO, JAPAN

THE PUNCHED CARD WORK FOR THIS EDITION WAS DONE MAINLY AT THE M. I. T. COMPUTATION CENTER, MASS. INST. OF TECH., CAMBRIDGE, MASS. 02139, U. S. A.

FORMAT

TITLE CARD

COLS. 1 - 4 PROGRAM ACCESSION NUMBER, TO BE ASSIGNED BY THE EDITOR. PROGRAMS ARE NUMBERED SERIALLY IN CHRONOLOGICAL ORDER OF RECEIPT BY THE EDITOR. TO AVOID CONFUSION, ACCESSION NUMBERS OF OBSOLETED PROGRAMS WILL NOT BE RE-USED. THE UNITS PLACE OF THE NUMBER SHOULD BE IN COL. 4.

COLS. 6 - 13 MACHINE TYPE, BY CODE NAME OR NUMBER. MAY BE FOLLOWED BY ABBREVIATIONS INDICATING SIZE OF STORAGE, MODIFICATIONS, ETC., AND/OR LANGUAGE IN WHICH PROGRAM WAS WRITTEN.

ALTERNATIVELY, FOR A PROGRAM WRITTEN IN A MACHINE-INDEPENDENT MANNER IN A LANGUAGE SUCH AS FORTRAN OR ALGOL, THE LANGUAGE NAME MAY TAKE THE PLACE OF THE MACHINE NAME. IN SUCH A CASE IT IS ASSUMED THAT THE USER MUST ORDINARILY COMPILE THE PROGRAM FOR HIS OWN MACHINE. THE ABSTRACT SHOULD STATE THE TYPE OF MACHINE ON WHICH TESTED, AND INDICATE THE AMOUNT OF STORAGE REQUIRED.

COLS. 15 - 22 FUNCTION OF PROGRAM, BY CODE ABBREVIATIONS. SEE LIST OF ABBREVIATIONS.

COLS. 24 - 38 AUTHORS, PROGRAMMERS, ETC. BECAUSE OF SPACE LIMITATIONS MORE THAN ONE OR TWO NAMES SHOULD BE AVOIDED IF THIS CAN BE DONE WITHOUT INJUSTICE. ONLY SURNAMES SHOULD BE GIVEN EXCEPT WHEN USE OF AN INITIAL IS NECESSARY TO AVOID CONFUSION.

IT MAY BE NECESSARY TO ABBREVIATE SURNAMES. IN THIS CASE CROSS REFERENCES SHOULD BE ENTERED INTO THE AUTHOR INDEX.

TWO OR MORE SURNAMES SHOULD BE SEPARATED BY PUNCTUATION (COMMA, SLASH, OR ASTERISK) BUT NO SPACES. WHERE INITIALS ARE NEEDED THEY SHOULD FOLLOW THE SURNAME, SEPARATED BY SPACES BUT NO PUNCTUATION.

WHERE A SLASH (/) APPEARS BETWEEN TWO NAMES, THE NAMES AFTER THE SLASH ARE THE NAMES NOT OF AUTHORS OR PROGRAMMERS BUT

THOSE OF PERSONS PRESENTLY IN CONTROL OF THE PROGRAM, TO WHOM INQUIRIES REGARDING THE PROGRAM SHOULD BE ADDRESSED.

WHERE AN ASTERISK (*) APPEARS AFTER THE NAME OF AN AUTHOR OR PROGRAMMER, IT INDICATES THAT THAT PERSON, RATHER THAN THE FIRST-NAMED AUTHOR OR PROGRAMMER, IS THE PERSON TO WHOM INQUIRIES SHOULD BE SENT.

THE NAMES OF AUTHORS MAY BE PERMITTED TO EXTEND BEYOND COL. 38 AND ENCROACH ON THE NEXT FIELD IF ABSOLUTELY NECESSARY. IN THIS CASE THE LAST NAME GIVEN SHOULD BE FOLLOWED BY A SLASH TO SEPARATE IT FROM WHAT FOLLOWS.

COLS. 40(41) - 76 IDENTIFICATION AND COMMENTS. IF AN IDENTIFICATION CODE NAME OR NUMBER EXISTS, IT SHOULD BE GIVEN STARTING IN COLUMN 40 AND FOLLOWED BY A SLASH (/). FURTHER COMMENTS BEGIN IMMEDIATELY AFTER THE SLASH, WITHOUT A SPACE BEFORE.

IF THERE IS NO IDENTIFICATION CODE NAME OR NUMBER, COLUMN 40 SHOULD BE LEFT BLANK AND THE COMMENTS SHOULD BEGIN IN COLUMN 41.

COMMENTS SHOULD BE ABBREVIATED AS MUCH AS POSSIBLE AND MUST NOT EXTEND BEYOND COLUMN 76.

COL. 78 STATUS OF PROGRAM OPERABILITY AND AVAILABILITY OF PROGRAM CODE (I.E., ACTUAL LISTING OF PROGRAM IN AUTOMATIC AND/OR SYMBOLIC AND/OR MACHINE LANGUAGE, ADEQUATE FOR TROUBLE-SHOOTING AND MAKING MODIFICATIONS)

- L WELL CHECKED OUT, PROGRAM CODE AVAILABLE
- M WELL CHECKED OUT, PROGRAM CODE NOT AVAILABLE
- N OPERABLE BUT NOT WELL CHECKED OUT

COL. 79 STATUS OF PROGRAM WRITE-UP

- W COMPLETE WRITE-UP IN FINAL FORM AVAILABLE
- P ABBREVIATED OR PROVISIONAL WRITE-UP AVAILABLE
- N NO WRITE-UP AVAILABLE

COL. 80 STATUS OF AVAILABILITY OF PROGRAM IN WORKING FORM (PUNCHED CARDS OR TAPE, PLUS WRITE-UP AND/OR PROGRAM CODE IF SO INDICATED IN 78 AND/OR 79)

- S AVAILABLE THROUGH MACHINE-USER ORGANIZATION (E. G., SHARE)
- M AVAILABLE THROUGH MANUFACTURER OF MACHINE
- A AVAILABLE DIRECTLY FROM AUTHOR OR AUTHORS INSTITUTION
- X PROGRAM IS OF A SPECIAL OR LOCAL NATURE, CONDITIONALLY AVAILABLE
- N NOT AVAILABLE AT PRESENT, PROBABLY AVAILABLE AT LATER DATE

ABSTRACT CARDS

COLS. 1 - 4 PROGRAM ACCESSION NUMBER, THE SAME AS ON THE TITLE CARD.

COL. 5 SUCESSIVE CARDS OF AN ABSTRACT ARE LETTERED SERIALLY A, B, C, D, . . .

COLS. 8 - 80 (73 CHARACTERS AND SPACES PER CARD) FOR THE CONTENT OF THE ABSTRACT, WHICH SHOULD BE LIMITED TO NO MORE THAN ABOUT 50 WORDS.

AUTHOR INDEX CARDS -- BEGIN IN COL. 1, AND GIVE SURNAME, INITIALS, AND MAILING ADDRESS, E.G. --

COULTER, C. L., M. R. C. UNIT, CAVENDISH LABORATORY, CAMBRIDGE, ENGLAND

ALL NAME ABBREVIATIONS SHOULD BE EXPLAINED ON ADDITIONAL CARDS, E. G.,

CLTR, SEE COULTER, C. L.

ABBREVIATIONS

FUNCTION ABBREVIATIONS

A	ACENTRIC (NON-CENTROSYMMETRIC) ONLY
ABS	ABSORPTION CORRECTIONS
A-C TEST	ACENTRIC/CENTRIC STAT. TEST
AT	ANISOTROPIC TEMPERATURE FACTORS CAN BE TREATED
BL	BEEVERS-LIPSON TYPE OF (FR) CALCULATION
BLK	SMALL BLOCK OF POINTS, AS IN NEIGHBORHOOD OF FOURIER PEAK
C	CENTRIC (CENTROSYMMETRIC) ONLY
CONTOUR	PRODUCES CONTOURED FOURIER MAPS OR SECTIONS
D	INTERPLANAR SPACINGS
DF	DIFFERENTIAL FOURIER
DEBYE	DEBYE TEMPERATURE
DIR	DIRECT METHODS OF SIGN OR PHASE DETERMINATION
DISPERSN	ANOMALOUS DISPERSION (CORRECTIONS, ETC.)
DM	DIAGONAL (OR MAINLY DIAGONAL) MATRIX
DP	DATA PROCESSING
E	ERROR, STANDARD DEVIATIONS, ETC.
EL	ELECTRON (DIFFRACTION)
EQ	EQUI-INCLINATION GEOMETRY
EXT	EXTINCTION (OR EXT. CORRECTION)
FM	FULL MATRIX
FPK	FOURIER PEAK SHAPE ANALYSIS
FR	FOURIER SYNTHESIS (2 OR 3 DIM)
FT	FOURIER TRANSFORM
GEOM	MOLECULAR GEOMETRY
H	INDEX (HKL) GENERATION
ICA	INDIVIDUAL ATOMIC CONTRIBUTIONS (TO SF) AVAILABLE
ID	INTERATOMIC DISTANCES (AND USUALLY BOND ANGLES)
IT	INPUT
LC	LATTICE CONSTANTS
LF	LITTLE F - FORM FACTORS
LP	LORENTZ-POLARIZATION CORRECTION
LS	LEAST SQUARES REFINEMENT (3D UNLESS OTHERWISE STATED). SEE ALSO SFLS.
N	NEUTRON (DIFFRACTION)
OT	OUTPUT
P	POWDER CALCULATIONS
PARAM	PARAMETER(S)
PATSUP	PATTERSON SUPERPOSITION, MINIMUM FUNCTION, ETC.
PI	POWDER INDEXING
PK	PEAK
PLANE	LEAST-SQUARES PLANE THROUGH GROUP OF ATOMS
PREC	PRECESSION
PRJCTN	PROJECTION
PROF	PROFILE
R	R FACTOR, AGREEMENT FACTOR
ROTF	ROTATION FUNCTION
ROTN(FN)	ROTATION FUNCTION
RB	RIGID BODY
S	SPECIAL
SCL	SCALE FACTOR
SD	STANDARD DEVIATIONS
SF	STRUCTURE FACTORS
SFLS	STRUCTURE FACTORS AND LEAST SQUARES REFINEMENT
SIGN	MANIPULATION OF STRUCTURE FACTOR SIGNS (NOT SAME AS DIR)
SPC	SPECTROMETER SETTINGS
SPEC	SPECIAL
STAT	STATISTICS, PERTAINING PARTICULARLY TO SF
STEREO	CALC OF STEREO STRUCTURE PICTURES
SYSTEM	CRYSTALLOGRAPHIC PROGRAM SYSTEM

TF	TEMPERATURE FACTOR
THETA	BRAGG ANGLE
WEIS	WEISSENBERG
2	TWO-DIMENSIONAL
3	THREE-DIMENSIONAL
2C,3C,4C	2-, 3-, 4-CIRCLE (DIFFRACTOMETER)

MACHINE ABBREVIATIONS

ATLAS	FERRANTI ATLAS
BULL GET	BULL TYPE GAMMA ET (FRANCE)
BULLGAET	BULL TYPE GAMMA AET (FRANCE)
B5000	(NO DEFINITION RECEIVED)
CAB 500	SEA TYPE CAB 500 (FRANCE)
CEP	CALCOLATRICE ELETTRONICA PISANA (PISA UNIVERSITY, PISA, ITALY)
DASK	(DENMARK)
ER 56	STANDARD-ELECTRIC-LORENZ ER 56 (GERMANY)
FACIT	FACIT EDB (SWEDEN)
KDF9	ENGLISH ELECTRIC KDF9
LGP30	ROYAL-MCBEE
MERCURY	FERRANTI MERCURY (BRITAIN)
M1B	MUSASHINO 1B, SOMEWHAT SIMILAR TO PC1 (TOKYO, JAPAN)
NE803	NATIONAL ELLIOTT NE 803
PC1	PARAMETRON COMPUTER, DEPT. OF PHYSICS, UNIV. OF TOKYO, TOKYO, JAPAN
PDP6	DIGITAL EQUIPMENT CORP. PDP6
SILLIAC	SILLIAC (AUSTRALIA)
URAL 1	(USSR)
WGMATIC	WEGEMATIC 1000 (SWEDEN)
X 1	N. V. ELECTROLOGICA, THE HAGUE, NETHERLANDS
ZEBRA	STANTEC ZEBRA, STANDARD TELEPHONES AND CABLES LTD, ENFIELD, ENGLAND
Z22R	ZUSE 22R (GERMANY)
Z23A	ZUSE 23A
1103	REMINGTON RAND UNIVAC 1103
1107	REMINGTON RAND UNIVAC 1107
1410	IBM 1410
1604	CONTROL DATA 1604
1620	IBM 1620
2002	SIEMENS 2002 (GERMANY)
205	BURROUGHS 205
220	BURROUGHS 220
360	IBM SYSTEM 360
5090H	OKIDAC-5090H (JAPAN)
6001	OLIVETTI ELEA 6001. K INDICATES 10000 DIGITS HIGH SPEED STORAGE.
650	IBM 650
704	IBM 704
7040	IBM 7040
7044	IBM 7044
7070	IBM 7070
7074	IBM 7074
709	IBM 709
7090	IBM 7090
7094	IBM 7094
7094DC	IBM 7094 DIRECT COUPLED

NOTE -- IBM 709, 7090, 7094 (IN ORDER OF INCREASING SPEED) ARE LARGELY INTERCHANGEABLE, AND MACHINE-LANGUAGE PROGRAMS ARE READILY INTERCONVERTABLE. THESE MACHINES ARE GROUPED TOGETHER IN THE PROGRAM LISTINGS.

PROGRAMMING LANGUAGES (PSEUDO-MACHINES), USUALLY COMPILABLE ON SEVERAL MACHINE TYPES), WHICH MAY BE CITED IN LIEU OF MACHINE IF SOURCE PROGRAM IS LARGELY MACHINE INDEPENDENT (HOWEVER, ABSTRACT CARDS SHOULD CONTAIN REFERENCE TO MACHINE ON WHICH COMPILED, PREFERABLY WITH INDICATION OF STORAGE REQUIREMENTS) --

ALGOL	ALGORITHMIC LANGUAGE

ALGOL60 DITTO (1960 VERSION)
ATLAS F WRITTEN IN A FORM OF FORTRAN (HARTRAN) FOR THE ATLAS COMPUTER
(HOWEVER, PROGRAMS IN ATLAS F ARE LISTED UNDER ATLAS MACHINE)
AUTOCODE
EMA EXTENDED MERCURY AUTOCODE
EXCHLF (SEE ATSYS)
FORTRAN FORMULA TRANSLATION (IBM)
FORTRAN2 FORTRAN II
FORTRAN4 FORTRAN IV
HARTRAN SEE ATLAS F
MAD MICHIGAN ALGORITHMIC DECODER (RELATED TO ALGOL)
NP/I PROGRAMMING LANGUAGE TO BE IMPLEMENTED UNDER IBM SYSTEM 360

MODIFIERS

AGL WRITTEN IN ALGOL (60), COMPILED ON MACHINE INDICATED BY PRIOR ABBREV.
AUC WRITTEN IN AUTOCODER (7070), COMPILED ON MACHINE INDIC. BY PRIOR ABBREV
AUT WRITTEN IN AUTOCODE, COMPILED ON MACHINE INDICATED BY PRIOR ABBREV.
FTN WRITTEN IN FORTRAN, COMPILED ON MACHINE INDICATED BY PRIOR ABBREV.
FT2 WRITTEN IN FORTRAN II, COMPILED ON MACHINE INDICATED BY PRIOR ABBREV.
8K INDICATED MACHINE MUST HAVE AT LEAST 8192 WORDS HIGH-SPEED STORAGE
4K, 32K MUST HAVE AT LEAST 4096, OR 32,768 WORDS, ETC.

CRYSTALLOGRAPHIC PROGRAM SYSTEMS

ATSYS ATLAS CRYSTALLOGRAPHIC SYSTEM, COMPILED AT IMPERIAL COLLEGE, LONDON.
DEVELOPED MAINLY BY M. G. B. DREW.
X-RAY 63 SYSTEM OF CRYSTALLOGRAPHIC PROGRAMS DEVELOPED BY J. STEWART, NOW AT
UNIV. OF MARYLAND. CONTAINS INDIVIDUAL PROGRAMS WRITTEN BY MANY
OTHERS. INDIVIDUAL PROGRAMS ARE LISTED UNDER 7090/7094 AS
WELL AS UNDER THE X-RAY 63 SYSTEM.

AUTHOR/PROGRAMMER INDEX

BENVENUTI P, CSCE, SERVIZIO CALCOLI, LUNGARNO, PACINOTTI 16, PISA, ITALY
BERGERHOFF,G., CHEM. INST. UNIV.,BONN, GERMANY
BERG., SEE BERGERHOFF
BERNARD, W. H., PHYSICS DEPT., LOUISIANA POLYTECHNIC INST., RUSTON, LA., U.S.A.
BERNSTEIN, J.L. BELL TELEPHONE LABORATORIES, MURRAY HILL,NEW JERSEY
BERTOLUZ, SEE BERTOLUZZA C
BERTOLUZZA, C, CSCE, SERVIZIO CALCOLI, LUNGARNO, PACINOTTI 16, PISA, ITALY
BEURSKENS, P.T., LAB. KRISTALCHEMIE, RIJKSUNIVERSITEIT, UTRECHT, NETHERLANDS
BEU, K. E., GOODYEAR ATOMIC, BOX 628, PORTSMOUTH, OHIO
BIBIAN,F,C.E.N.SACLAY,S.P.S.R.M.,BP2,GIF-SUR-YVETTE,78,FRANCE
BIEDL,A.W., LEHRSTUHL FUR KRIST., RUHR-UNIVERSITAET, 463 BOCHUM,GERMANY
BLAND, J. A., I.C.I. LTD., BILLINGHAM DIV., BILLINGHAM CO., DURHAM, ENGLAND
BLOCK, S., NATIONAL BUREAU OF STANDARDS, WASHINGTON DC
BLOMK, SEE BLOMQVIST, G.
BLOMQVIST, G., A.B. ATOMENERGI, STUDSVIK, TYSTBERGA, SWEDEN
BLOUNT, J., DEPT OF CHEM, UNIVERSITY OF WISCONSIN, MADISON, WISCONSIN
BOMBIERI GABRIELLA, CENTRO DI STRUTTUR. CHIM., VIA F.MARZOLO, 1-PADOVA, ITALY
BOMB, SEE BOMBIERI GABRIELLA
BONNER, R. U., SHELL DEVELOPMENT CO., EMERYVILLE, CALIF.
BOOM,G., INSTITUUT VOOR KRISTALFYSICA, RIJKSUNIVERSITEIT, GRONINGEN, NETHERLANDS
BOONSTRA, E. G., N.PHYS.R.L., C.S.I.R., BOX 395, PRETORIA, SOUTH AFRICA
BOOTH, D. P., BELL TELEPHONE LABORATORIES, MURRAY HILL, N J
BORN, L., MIN.-PETRO INST., KIEL, GERMANY
BOWLER,MISS M.,AERE HARWELL, DIDCOT, BERKS, ENGLAND
BOYKO, E. R., WESTINGHOUSE ELECTRIC CO., BETTIS PLANT, PITTSBURGH, PA.
BRADACZEK,H.,FRITZ-HABER INST., ABT. PROF. HOSEMANN, BERLIN 33, GERMANY
BRACHER, B. H., BLDG. 775, AERE, HARWELL, DIDCOT, BERKS., U.K.
BRANDEN, C. I., AGRICULTURAL COLLEGE OF SWEDEN, UPPSALA 7, SWEDEN
BRAUN,R. UNIVERSITY OF WASHINGTON SEATTLE, WASHINGTON USA
BROWN, B. W., DEPT. CHEM., PORTLAND STATE COLLEGE, PORTLAND, ORE. 97207
BROWN, G. M., CHEM. DIV., OAK RIDGE NAT. LAB., OAK RIDGE TENNESSEE, U. S. A.
BROWN,B.W. PORTLAND STATE COLLEGE PORTLAND ORE. USA
BRUHN, RECHENINSTITUT PROF HAACK, TU BERLIN
BRWN, SEE BROWN, B. W.
BRYDEN, J. H., CHEM. DEPT., CALIF. STATE COLLEGE, FULLERTON, CALIF., U. S. A.
BUJOSA, A., I.B.M., S.A.E., SERRANO 5, MADRID 1, SPAIN
BUJ, SEE BUJOSA, A.
BURKE, MARY E., DEPT CHEM, UNIV OF CALIF, LOS ANGELES 24, CALIF
BURNHAM, C. W., GEOPHYSICAL LAB., 2801 UPTON ST., N.W., WASHINGTON 8, D.C.
BUSING,W. R., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
CANUT, M. L., SCHOOL OF TECH., SOUTHERN ILLINOIS UNIV., CARBONDALE, ILL. 62903
CARPENTER, C.L., STATE UNIVERSITY OF IOWA, IOWA CITY, IOWA
CARPENTER, G. B., BROWN UNIVERSITY, PROVIDENCE, RI
CARTER, F. L., WESTINGHOUSE RESEARCH LABORATORIES, PITTSBURGH 35, PA.
CARTER, J. M., GOODYEAR ATOMIC, BOX 628, PORTSMOUTH, OHIO
CETLIN,B.B.,BELL TELEPHONE LABORATORIES,MURRAY HILL,N.J.,USA
CHAND, SEE CHANDROSS, R.
CHANDROSS, R., DEPT. OF CHEM., MIT, CAMBRIDGE, MASS.
CHAST SEE CHASTAIN,R.V.
CHASTAIN,R.V. UNIVERSITY OF WASHINGTON SEATTLE WASH. USA
CHU, S. C. (MRS), CRYSTALLOGRAPHY LAB., UNIVERSITY OF PITTSBURGH,PITTSBURGH,PA.
CLOSS, S. W.,
CLTR, SEE COULTER, C.L.
COHEN,J B , DEPT.MATERIALS SC.,TECH INST., NORTHWESTERN UNIV.,EVANSTON,ILL.
COJAZZI GIANNA, CENTRO DI STRUTTUR. CHIM., VIA F.MARZOLO, 1-PADOVA, ITALY
COJAZ, SEE COJAZZI GIANNA
COLASANTI,A.,ISTITUTO CHIMICO,VIA MEZZOCANNONE 4,NAPOLI,ITALIA
COL,SEE COLASANTI,A.
COONEY, W. A., SEE HAENDLER, H. M.
CORFIELD, P., CRYSTALLOGRAPHIC LABORATORY, U. OF PITTSBURGH, PITTSBURGH 13, PA.
COULTER, DR. C.L. M.R.C. UNIT, CAVENDISH LABORATORY, CAMBRIDGE, ENGLAND
CRUICK, SEE CRUICKSHANK, D.W.J.
CRUICKSHANK, D. W. J., CHEM. DEPT., THE UNIVERSITY, GLASGOW, W.2, SCOTLAND
CURTIS,A.R.,AERE HARWELL, DIDCOT, BERKS, ENGLAND
DAHL, L.F., DEPT OF CHEM, UNIVERSITY OF WISCONSIN, MADISON, WISCONSIN
DALLINGA, G., KONINKLIJKE/SHELL LABORATORIUM, AMSTERDAM, NETHERLANDS

DAMIANI,A.,ISTITUTO CHIMICO,VIA MEZZOCANNONE 4,NAPOLI,ITALIA
DANIELSEN, J., DEP. OF INORG. CHEM., AARHUS UNIVERSITY, AARHUS, DENMARK
DANIELS, SEE DANIELSEN, J.
DARLOW, S.F., PHYS. DEPT., COLLEGE OF SCI. AND TECH., MANCHESTER 1, ENGLAND
DARLOW, MRS J. V., SEE DARLOW, S. F.
DAYHOFF, M. O.,NAT'L BIOMEDICAL RESEARCH FDN. 8600 16 ST. SILVER SPRING, MD.
DAYH, SEE DAYHOFF, M. O.
DEANGELIS, R. J., DEPT. OF METALL. ENG., U. OF KENTUCKY, LEXINGTON, KY.
DEGRIF, SEE DE GRIFFI ELENA
DE GRIFFI ELENA, OLIVETTI, VIA CLERICI, MILANO, ITALY
DELF, B. W., PHYS. DEPT., UNIVERSITY COLLEGE, CARDIFF, WALES
DENNER,K H ,DAW,INSTITUT FUER STRUKTURFORSCHUNG,BERLIN-ADLERSHOF,GDR
DE VRIES, A., LAB. KRISTALCHEMIE, RIJKSUNIVERSITEIT, UTRECHT, NETHERLANDS
DIA, SEE DIAMAND, R. D.
DIAMAND, R. D., ROYAL INSTITUTION, LONDON W.1, ENGLAMD
DICKINSON,C.W. NAVAL ORDNANCE LAB. WHITE OAK, SILVER SPRING, MD. USA
DICSN SEE DICKINSON,C.W.
DIDRIKSEN, F., IBM, OSLO, NORWAY
DIETRICH,H., FRITZ'HABER'INSTITUT,BERLIN'DAHLEM,FARADAYWEG 4'6, GERMANY
DODGE, R. UNION CARBIDE RES. INST., BOX 324, TUXEDO, N.Y.
DOL, SEE DOLLIMORE, J.
DOLLIMORE,J., UNIV.LOND.INST.COMPUTER SCI., 44 GORDON SQ., LONDON WC1, ENGLAND
DOMENICANO, A., CENTRO STRUTTURISTICA CNR, CITTA UNIVERSITARIA, ROMA, ITALY
DOMENICI,M., SORIN, SALUGGIA, ITALY
DOME, SEE DOMENICANO, A.
DOMIANO,P., CENTRO DI CALC.ELETTR., UNIV.OF PARMA,VIA M.D,AZEGLIO 85 PARMA ITALY
DONNAY, J.D.H., CRYSTAL. LAB., JOHNS HOPKINS UNIV., BALTIMORE, MD.21218
DREW, M. G. B., CHEM. DEPT., IMPERIAL COLLEGE, LONDON S.W.7, ENGLAMD
DUCHAMP,D.J.,THE UPJOHN COMPANY,KALAMAZOO,MICHIGAN
DUISENBERG, A.J.M., LAB.KRISTALCHEMIE, RIJKSUNIVERSITEIT, UTRECHT, NETHERLANDS
EDSTRAND, M., FORSKN. AVD., A.B. BOFORS NOBELKRUT, BOFORS, SWEDEN
EHRLICH, H. W. W., ICI LTD, HEAVY ORG. CHEMICALS DIV., BILLINGHAM, CO DURHAM, UK
EICHHORN, E. L., 7802 ALLAN STRUGES TERR., FALLS CHURCH, VA. 22041, USA
ELLISON, R.D., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE.
ESPOSITO,U.,ISTITUTO CHIMICO,VIA MEZZOCANNONE 4,NAPOLI,ITALIA
ESP,SEE ESPOSITO,U.
ESQUIVEL,A.L.,MAT LS RES LAB,MP-105,MARTIN CO.,ORLANDO,FLA 32805
FARRAR, R. A., FACULTY OF ENG., KWAME NKRUMA UNIV., KUMASI, GHANA
FENN, R.H., PHYS.DEPT., PORTSMOUTH COLL.OF TECH., PARK RD.,PORTSMOUTH,HANTS, UK
FITZW, SEE FITZWATER, D.
FITZWATER, D., IOWA STATE UNIVERSITY, AMES, IOWA
FRASS, SEE FRASSON EDOARDO
FRASSON EDOARDO, CENTRO DI STRUTTURISTICA CHIMICA, VIA F.MARZOLO,1, PADOVA,ITALY
FREEMAN, H. C., SCH. OF CHEM., UNIVERSITY OF SYDNEY, SYDNEY, AUSTRALIA
FREER,S. UNIVERSITY OF CALIFORNIA AT SAN DIEGO LA JOLLA CALIF. USA
GABE, E.J., INST. FOR CANCER RESEARCH, 7701 BURHOLME AVE., PHILADELPHIA 11, PA.
GALLAHER,L.J. E.E.S. GEORGIA INST. OF TECHNOLOGY,ATLANTA,GA. U.S.A.
GANTZEL, PETER K. , DEPT CHEM, UNIV OF CALIF, LOS ANGELES 24, CALIF
GEISE, H. J., LAB. ORGANIC CHEMISTRY, UNIV. LEIDEN, LEIDEN, THE NETHERLANDS
GERGELY, G., COMPUTING CENTER OF THE HUNG. ACAD. OF SCIENCES, BUDAPEST, HUNGARY
GIGLIO,E.,ISTITUTO CHIMICO,VIA MEZZOCANNONE 4,NAPOLI,ITALIA
GIG,SEE GIGLIO,E.
GILMARTIN,MRS J.,AERE HARWELL, DIDCOT, BERKS, ENGLAND
GOEBEL,J.B., APPLIED MATH., BATTELLE-NORTHWEST, RICHLAND, WASHINGTON
GRAF, D. L., ILLINOIS GEOLOGICAL SURVEY, URBANA, ILL.
GRANT, D. F., PHYS. DEPT., UNIVERSITY COLLEGE, CARDIFF, WALES
GREEN, D.W., ROYAL INSTITUTION, LONDON W.1, ENGLAND
GROENBAEK, RITA, DEPT. OF INORG. CHEM., AARHUS UNIVERSITY, AARHUS, DENMARK
GRUBISS, SEE GRUBISSICH CLAUDIO
GRUBISSICH CLAUDIO, C.E.C.S., VIA PAOLOTTI 9, PADOVA, ITALY
GTZL, SEE GANTZEL, PETER K.
GUERRI L., CSCE, SERVICIO CALCOLI, LUNGARNO, PACINOTTI 16, PISA, ITALY
HAENDLER, H. M., DEPT CHEM, UNIV OF NH, DURHAM, NH
HAHN,TH.,INST.FUR KRIST.,TECHN.HOCHSCHULE,51 AACHEN,TEMPLERGRABEN 55, GERMANY
HALL,S.R.,PHYSICS DEPT.,UNIV. OF W.A.,NEDLANDS,WESTERN AUSTRALIA
HAMILTON, W. C., BROOKHAVEN NATIONAL LABORATORY, BROOKHAVEN, NY

HAMOR, T. A., CHEM. DEPT., UNIV. OF BIRMINGHAM, BIRMINGHAM 15, ENGLAND
HARD, SEE HARDING, M. M.
HARDING, MRS. M. M., CHEM. CRYST. LAB., SOUTH PARKS ROAD, OXFORD, ENGLAND
HARDING,M.M., EDINBURGH UNIV. CHEM. DEPT., WEST MAINS ROAD, EDINBURGH 9,SCOTLAND
HARRIS,D.R. DEPT. OF COMP. SCIENCE, UTAH STATE UNIV., LOGAN, UTAH
HEATON, L. ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS
HECKEL, R.W., DEPT. OF MET. ENG., DREXEL INST. OF TECH., PHILADELPHIA 4, PA.
HELLNER, E., MIN.-PETRO. INST., KIEL, GERMANY
HENDE, SEE VAN DEN HENDE, J. H.
HESPER, B., LAB. BIOCHEMISTRY, UNIV. LEIDEN, LEIDEN, THE NETHERLANDS
HIGH,D.F. UNIVERSITY OF CALIFORNIA AT SAN DIEGO LA JOLLA CALIF. USA
HILDEB, SEE HILDEBRAND
HILDEBRAND, R., MIN. INST. UNIV., FRANKFURT , SENCKENBERG ANLAGE 30,GERMANY
HINE. R., PHYSICS DEPT., UNIVERSITY COLLEGE, CARDIFF, WALES
HIRSHFELD, F., DEPT. OF CHEM, UNIV. OF MINN., MINNEAPOLIS, MINN.
HOLDEN,J.R. NAVAL ORDNANCE LAB. WHITE OAK, SILVER SPRING, MD. USA
HOP., SEE HOPPE
HOPPE,W., MPI. EIWEISSFORSCHUNG, MUENCHEN, LUISENSTR. 39, GERMANY
HOUSTON, B. J.,
HUBER,R., MPI. EIWEISSFORSCHUNG, MUENCHEN, LUISENSTR. 39, GERMANY
HUNT, , CHEM. DEPT., IMPERIAL COLLEGE, LONDON S.W. 7, ENGLAND
IANDOLO,A.,ISTITUTO CHIMICO,VIA MEZZOCANNONE 4,NAPOLI,ITALIA
IAN,SEE IANDOLO,A.
IBERS, J. A., DEPT. CHEM., NORTHWESTERN UNIV., EVANSTON, ILL., USA
IITAKA, Y., FAC. OF PHARMACEUTICAL SCI., UNIV. OF TOKYO, BUNKYO-KU, TOKYO, JAPAN
JACOBSON, R. A., DEPT. OF CHEM., UNIV. OF MINN., MINNEAPOLIS, MINN.
JAMARD,C., 91 RUE VILLIERS DE L,ISLE ADAM, PARIS 20E, FRANCE
JAMES, , BLDG. 775, AERE, HARWELL, DIDCOT, BERKS., U.K.
JEFFREY, G. A., CRYSTALLOGRAPHIC LAB., UNIVERSITY OF PITTSBURGH, PITTSBURGH, PA.
JENSEN, L. H., DEPT. BIOL. STRUCT., UNIV. OF WASHINGTON, SEATTLE, WASH. 98105
JMS, SEE JAMES
JOHANSSON, G., DEPT. OF INORG. CHEM., INST. OF TECHNOLOGY, STOCKHOLM 70, SWEDEN
JOHNSON, C. K., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE, U.S.A.
JOHNSON, Q., UNIV. OF CALIFORNIA, BERKELEY, CALIF.
JONES, UNIV. OF CALIFORNIA, BERKELEY, CALIF.
JSTEW SEE STEWART,J.M.
KAPLOW, R., METALLURGY DEPT., MIT, CAMBRIDGE, MASS.
KASPER, H., CHEM. INST. UNIV. 53 BONN, MECKENHEIMER ALLEE 168, GERMANY
KATZ, L., DEPT. OF BIOLOGY, M.I.T., CAMBRIDGE MASS. 02139, U.S.A.
KAY,M.I. E.E.S. GEORGIA INST. OF TECHNOLOGY, ATLANTA, GA. U.S.A.
KEEFE,W. MEDICAL COLLEGE OF VIRGINIA RICHMOND, VA. USA
KEILHAU, H., NORWEGIAN DEFENCE RESEARCH ESTABLISHMENT, KJELLER, NORWAY
KEMPTER,C.P.,LOS ALAMOS SCIENTIFIC LABORATORY,LOS ALAMOS,NM
KEULEMANS, E. W. M., LAB. VOOR KRISTALLOGRAFIE, UNIV. OF AMSTERDAM, NETHERLANDS
KEUL, SEE KEULEMANS, E. W. M.
KEUNING, W., CENTR. PROEFSTATION, STAATSMIJNEN, HOENSBROEK, NETHERLANDS
KEYES, P. A., IOWA STATE UNIVERSITY, AMES, IOWA
KING, G. S. D., E. R. A., 95 RUE GATTI DE GAMOND, BRUSSELS 18, BELGIUM
KOENE, A. A., STATISTICAL DEPT., T.N.O., THE HAGUE, NETHERLANDS
KOENIG, D. F., BIOLOGY DEPT., BROOKHAVEN NAT. LAB., UPTON, LONG ISLAND, N.Y.,USA
KRAUSE,CH ,DAW,INSTITUT FUER STRUKTURFORSCHUNG,BERLIN-ADLERSHOF,GDR
KRAUT, J., DEPT.CHEM., U. OF CAL.SAN DIEGO., LA JOLLA, CALIF. 92038, USA
KRETSCHMER,R G ,DAW,INSTITUT FUER STRUKTURFORSCHUNG,BERLIN-ADLERSHOF,GDR
KRUECKEBERG,F., MATH. INST. UNIV. BONN,GERMANY
KRUECKEBG, SEE KRUECKEBERG
LAGERWALL, X., ADP INST., CHALMERS UNIV. OF TECHN., GIBR.G.5, GOTHENBURG, SWEDEN
LAI, T. F., CHEM. DEPT., UNIVERSITY OF HONG KONG
LANGHAMMER, D., PHYSICS DEPT., BRADLEY UNIV., PEORIA, ILLINOIS, U. S. A.
LANGHMR, SEE LANGHAMMER, D.
LARSEN, F., DANISH INST. FOR COMPUTING MACHINERY, GL CARLSBERGV 2, VALBY,DENMARK
LARSON, A.C. LOS ALAMOS NATL. LAB., LOS ALAMOS, N.M.
LEDLEY, R. S., NAT'L BIOMEDICAL RESEARCH FDN. 8600 16 ST. SILVER SPRING, MD.
LEFKER, R., USASRDL-XE, FORT MONMOUTH, NJ
LEMM,K., FRITZ-HABER-INST. M.P.G., ABT. PROF. HOSEMANN, BERLIN-33, GERMANY
LENHERT, P.GALEN., PHYS. DEPT., VANDERBILT UNIV., NASHVILLE, TENN.
LESJAK, J., COMPUTING CENTRE, LEPI POT 11, LJUBLJANA, JUGOSLAVIA

LEVY,H. A., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
LIMINGA, R., DEPT. OF CHEMISTRY, UNIV. OF UPPSALA, UPPSALA, SWEDEN
LIND, M.D., UNION OIL RESEARCH CTR., BREA, CALIF.92621, USA
LINEK, A., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
LING SEE LINGAFELTER,E.C.
LINGAFELTER, E. C., DEPT. CHEM., UNIV. OF WASHINGTON, SEATTLE, WASH. 98105
LINGFTR, SEE LINGAFELTER, E. C.
LIPSCOMB, W. N., JR., DEPT. OF CHEM., HARVARD UNIVERSITY, CAMBRIDGE, MASS.
LIPSC, SEE LIPSCOMB, W. N., JR.
LOMBARD, SEE LOMBARDI SILVANA
LOMBARDI SILVANA, OLIVETTI, VIA CLERICI, MILANO, ITALY
LOVELL, F.M. SCHOOL OF CHEM., UNIV. OF SYDNEY, N.S.W., AUSTRALIA
LOVE, W. E., BIOPHYSICS DEPT., JOHNS HOPKINS UNIV., BALTIMORE, MD.
LOV, SEE LOVELL, F.M.
LUNDBERG, B.K.S. , UNIVERSITY OF UMEA, UMEA, SWEDEN
LUNDBRG, SEE LUNDBERG, B.
MAC SEE MACINTYRE, W.M.
MACGILL, SEE MACGILLAVRY, C. H.
MACGILLAVRY, C. H., LAB. VOOR KRISTALLOGRAFIE, UNIV. OF AMSTERDAM, NETHERLANDS
MACINTYRE, W. M., DEPT. OF CHEM., UNIVERSITY OF COLORADO, BOULDER, COLO.
MAIN, P., PHYSICS DEPT., COLLEGE OF SCI. AND TECHNOLOGY, MANCHESTER 1, ENGLAND
MAIR, G.A., ROYAL INSTITUTION, 21 ALBERMARLE ST., LONDON W.1, ENGLAND
MALLETT, G. R., DOW CHEMICAL CO., BOX 2131, DENVER, COLO.
MARIANI C., INSTITUTO DO CHIMICA FISICA, UNIVERSITA DI MILANO, MILANO, ITALY
MARSH, R. E., CALIF. INST. OF TECH., PASADENA, CALIF
MARTIN,K. O., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
MAR, SEE MARTIN,K. O.
MASAKI, N., FAC. OF PHARMACEUTICAL SCI., KYOTO UNIV., SAKYO-KU, KYOTO, JAPAN
MASLEN,E.N.,PHYSICS DEPT.,UNIV. OF W.A.,NEDLANDS,WESTERN AUSTRALIA
MATHER, K., P. O. DR. 2131 JACKSON, MISS.
MATHEWS,
MATTES,R., LABORATORIUM FUER ANORG. CHEMIE DER T.H. STUTTGART, GERMANY
MCGANDY, E. L., CHEM. DEPT., BOSTON UNIVERSITY, BOSTON, MASS.
MCGREGOR,D.R., CHEM. DEPT., THE UNIVERSITY, GLASGOW W.2, SCOTLAND
MCMULLAN, R. K., DEPT. OF CHEM., UNIV. OF PITTSBURGH, PITTSBURGH, PENNSYLVANIA
MEDRUD, R. C., IOWA UNIVERSITY, IOWA CITY, IOWA
MEYER, E.F.H., DEPT. CHEMISTRY, TEXAS UNIVERSITY, AUSTIN, TEXAS
MIGLIORISI, G., SORIN, SALUGGIA, ITALY
MIGLIO, SEE MIGLIORISI, G.
MILLER, D. P., TEXAS INSTITUTE, DALLAS, TEXAS
MINKIN,J.A., INST. FOR CANCER RESEARCH, 7701 BURHOLME AVE.,PHILADELPHIA PA.19111
MOHN, G. J., WESTINGHOUSE ELECTRIC CO., BETTIS PLANT, PITTSBURGH, PA.
MONDRUP, P.,DANISH INST. FOR COMPUTING MACHINERY, GL CARLSBERGV 2,VALBY,DENMARK
MOORE, F. H., BLDG. 775, AERE, HARWELL, DIDCOT, BERKS., U.K.
MORE, SEE MOORE, F. H.
MORGAN, C. H., CHEM. DEPT., QUEENS COLLEGE, DUNDEE, SCOTLAND
MORINO, Y., DEPT. OF CHEM., UNIV. OF TOKYO, BUNKYO-KU, TOKYO, JAPAN
MOROSIN,B. SANDIA CORPORATION ALBUQUERQUE, NEW MEXICO USA
MORROW, J. C., UNIV. OF NORTH CAROLINA, CHAPEL HILL, NC
MOSELEY,JERRY, CHEMISTRY DEPT., UNIVERSITY OF COLORADO,BOULDER,COLO.
MOZZI, R., RESEARCH DIV., RAYTHEON CO., WALTHAM 54, MASS.
MUELLER, M.H. ARGONNE NATIONAL LABORATORY ARGONNE, ILLINOIS
MUIR,K.W., CHEM. DEPT., THE UNIVERSITY, GLASGOW W.2, SCOTLAND
MUSATTI,A., CENTRO DI CALC.ELETTR., UNIV.OF PARMA,VIA M.D,AZEGLIO 85 PARMA ITALY
MUSIL, F. J., GOODYEAR ATOMIC, BOX 628, PORTSMOUTH, OHIO
NADRCHAL, J., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
NADR, SEE NADRCHAL, J.
NEETHLING, J. D., N. P. R. L., PRETORIA, SOUTH AFRICA
NEWELL, J., RESEARCH DIV., RAYTHEON CO., WALTHAM 54, MASS.
NIIZEKI, N., ELEC. COMM. LAB. JAPAN TEL-TEL PUB. CORP., TOKYO, JAPAN
NKB, SEE NOVAK, B.
NORMENT, H., CALLERY CHEMICALS,
NORRESTAM,R., INST. INORG. AND PHYS. CHEM., UNIV. OF STHLM., STOCKHOLM VA,SWEDEN
NORTH, A.C.T., ROYAL INSTITUTION, 21 ALBEMARLE ST., LONDON W. 1, ENGLAND
NOVAK, B., NUM. CENTR. OF MAT., CHARLES UNIV., PRAGUE, CZECHOSLOVAKIA
NOVAK, C., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA

NVK, SEE NOVAK, C.
NYBORG, J., DEP.OF INORG. CHEM., AARHUS UNIVERSITY, AARHUS, DENMARK.
OCENASKOVA,D., INST . OF SOLID STATE PHYS., C.S.A.V., PRAGUE, CZECHOSLOVAKIA
OCKEN, H. HAMMOND LABORATORY, YALE UNIVERSITY, NEW HAVEN, CONN.
OCONNOR,B.H.,PHYSICS DEPT.,UNIV.OF W.A.,NEDLANDS,WESTERN AUSTRALIA
OGAWA, Y., INSTITUTE FOR PROTEIN RESEARCH, OSAKA UNIV., KITAKU OSAKA JAPAN
OLOVSON, SEE OLOVSSON, I.
OLOVSSON, I., DEPT. OF CHEMISTRY, UNIV. OF UPPSALA, UPPSALA, SWEDEN
ONKEN, H., LEHRST. F. KRISTALLOGR., UNIV. SAARBRUECKEN, WEST GERMANY
OSAKI, K., FAC. OF PHARMACEUTICAL SCI., KYOTO UNIV., SAKYO-KU, KYOTO, JAPAN
OTTE,H.M., MAT LS RES LAB,MP-105,MARTIN CO,ORLANDO,FLA. 32805
PALENIK,G.J.,CODE 5058, USNOTS ,CHINA LAKE,CALIFORNIA
PALMER,R.A.,BIRKBECK COLLEGE RES.LAB., 21 TORRINGTON SQ., LONDON W.C.1, ENGLAND
PALM, J. H., LAB. TECHN. PHYSICA, TECHNISCHE HOGESCHOOL, DELFT, NETHERLANDS
PANATT, SEE PANATTONI CARLO
PANATTONI CARLO, CENTRO DI STRUTTURISTICA CHIMICA, VIA F.MARZOLO,1,PADOVA,ITALY
PATT SEE PATTERSON, A.L.
PATTERSON, A.L., INST FOR CANCER RESEARCH, 7701 BURHOLME AVE, PHILADELPHIA 11,PA
PAULING, PETER, CHEM. DEPT., UNIVERSITY COLLEGE, GOWER ST., LONDON W.C.1,ENGLAND
PEACOR, D.R., DEPT OF GEOL AND GEOPHYS, MIT, CAMBRIDGE 39, MASS
PENFOLD, B., DEPT. OF CHEM., HARVARD UNIVERSITY, CAMBRIDGE, MASS.
PEPINSKY, R., DEPT. OF PHYSICS, PENN. STATE UNIV., UNIVERSITY PARK, PA.
PETERS, MRS. G., MATH. DIV., NATIONAL PHYSICAL LAB., TEDDINGTON, MIDDX., ENGLAND
PETERSON, D. P., DOW CHEMICAL COMPANY, MIDLAND, MICH.
PETERSE,W.J.A.M.,LAB.TECHN.PHYSICA,TECHNISCHE HOGESCHOOL,DELFT,NETHERLANDS
PIPPY, M.E., NATIONAL RESEARCH COUNCIL, OTTAWA 2, ONTARIO, CANADA
PISTORIUS, C. W. F. T., N.PHYS.R.L., C.S.I.R., BOX 395, PRETORIA, SOUTH AFRICA
PISTORIUS, M.C., N.R.I.MATH.SC., C.S.I.R., BOX 395, PRETORIA, SOUTH AFRICA
PLEHWE, A. VON, INST. ANG. MATH. UNIV. 78 FREIBURG/BRSG., HEBELSTR. 40, GERMANY
PREWITT, C. T., DEPT. OF GEOLOGY, MASS. INST. OF TECH., CAMBRIDGE, MASS.
PROUT, C. K., CHEM. CRYST. LAB., SOUTH PARKS RD., OXFORD, ENGLAND
PTRSON, SEE PETERSON, D. P.
RAE,A.I.M.,PHYSICS DEPARTMENT,UNIVERSITY OF W.A.,NEDLANDS,WESTERN AUSTRALIA.
RAE,A.I.M.,PHYSICS DEPT.,UNIV.OF W.A.,NEDLANDS,WESTERN AUSTRALIA
RICHARDS, J. P. G., PHYS. DEPT., UNIVERSITY COLLEGE, CARDIFF, WALES
ROGERS, D., CHEMISTRY DEPT., IMPERIAL COLLEGE, LONDON, S.W.7, ENGLAND
ROLLETT, J. S., OXFORD UNIV. COMPUTING LAB., SOUTH PARKS ROAD, OXFORD, ENGLAND
ROMMING, CHR., CHEMISTRY DEPARTMENT, UNIVERSITY OF OSLO, BLINDERN, NORWAY
ROSSMANN,M.G.,M.R.C.LAB OF MOLECULAR BIOLOGY,HILLS RD.,CAMBRIDGE,ENGLAND
ROWE,J.M., I.C.I.LTD.,HEAVY ORG. CHEMICALS DIV., THE FRYTHE,WELWYN,HERTS,ENGLAND
RUDEE, M.L., DEPT. OF MATERIALS SCI., STANFORD, CALIFORNIA
RUDOLPH, G. J., N.R.I.MATH.SC., C.S.I.R., BOX 395, PRETORIA, SOUTH AFRICA
RUTTEN-KEULEMANS, E. W. M., CENTRAAL REKENINST., UNIV. LEIDEN, THE NETHERLANDS
RUTTEN-KEULEMAN, SEE RUTTEN-KEULEMANS, E. W. M.
SAMET P., CO H.P. STADLER, KINGS COLLEGE, NEWCASTLE UPON TYNE, ENGLAND
SANBORN, M. A., I.B.M. MFG. RES. LAB., ENDICOTT, N. Y.
SANDS, D. E., LAWRENCE LABORATORY, LIVERMORE, CALIF.
SANTA, L., COMPUTING CENTER OF THE HUNG. ACAD. OF SCIENCES, BUDAPEST, HUNGARY
SASADA, Y., INSTITUTE FOR PROTEIN RESEARCH, OSAKA UNIV., KITA-KU, OSAKA, JAPAN
SASS, R., RICE INSTITUTE, HOUSTON, TEXAS
SASVARI, K., CRYST. LAB. U. OF PITT., PITTSBURGH 13, PA, ON LEAVE FROM HUNGARY
SAYRE, D., IBM CO., 590 MADISON AVE., NYC
SCHAPIRO, P. J., DEPT. OF CHEM., U. OF OKLAHOMA, NORMAN, OKLAHOMA, USA
SCHMDMT, SEE SCHMITZ-DU MONT, O
SCHMITZ-DU MONT, O., CHEM. INST. UNIV. 53 BONN, MECKENHEIMER ALLEE 168, GERMANY
SCHMID,E., RECHENINSTITUT DER TECHN. HOCHSCHULE, STUTTGART, HERDWEG 51 GERMANY
SCHOONE, J. C., LAB. VOOR KRISTALCHEMIE, UNIVERSITY OF UTRECHT, NETHERLANDS
SCHULZ, H., MINERAL. INST. D. UNIVERS., HAMBURG 13, GRINDELALLEE 48, GERMANY
SCHULTZERHONHOF, SEE SCHULTZE-RHONHOF,E.
SCHULTZE-RHONHOF, E., CHEM. INST. UNIV. 53 BONN, MECKENHEIMER ALLEE 168, GERMANY
SCHWARTZ,L.H.,MAT. SCI. DEPT., NORTHWESTERN U. EVANSTON,ILL.
SEGMUELLER, A., IBM RESEARCH LABORATORY, 8803-RUESCHLIKON, SWITZERLAND
SENKO, M. E., IBM COMPANY, POUGHKEEPSIE, N Y
SHEFTER, , BLDG. 775, AERE, HARWELL, DIDCOT, BERKS., U.K.
SHFTER, SEE SHEFTER
SHIONO, R., CRYSTALLOGRAPHIC LAB., UNIVERSITY OF PITTSBURGH, PITTSBURGH. PA.

SHOEMAKER, C. B., DEPT. OF CHEM., MIT, CAMBRIDGE, MASS.
SHOEMAKER, D. P., DEPT. OF CHEM., MIT., CAMBRIDGE, MASS.
SHO, SEE SHOEMAKER, D. P.
SILVERTON, J. V., CORNELL UNIV., DEPT. OF CHEMISTRY, ITHACA, NY.
SIME,J.G., CHEM. DEPT., THE UNIVERSITY, GLASGOW W.2, SCOTLAND
SIMPSON, P. G., DEPT. OF CHEM., STANFORD UNIV., STANFORD, CALIF. 94305, USA
SIMPSON, S.M., DEPT. OF GEOL., M. I. T., CAMBRIDGE, MASS. 02139, USA
SLITER, J. A., 2162 14TH ST., TROY, N Y
SMITH, D. K., LAWRENCE RADIATION LABORATORY, LIVERMORE, CALIF.
SMITH, J. G., CHEM. DEPT., THE UNIVERSITY, GLASGOW W2, SCOTLAND
SMITH, A. E., SHELL DEVELOPMENT CO., EMERYVILLE, CALIF.
SMITH, J., SEE SMITH, J.G.F.
SMITH, J. G. F., CHEM. DEPT., THE UNIVERSITY, GLASGOW, W.2, SCOTLAND
SMITS, D. W., REKENCENTRUM DER RIJKSUNIVERSITEIT, GRONINGEN, THE NETHERLANDS
SPARKS, R. A., IBM CORP., TIME-LIFE BLDG., NYC
SPEAKMAN, J. C., CHEM. DEPT., THE UNIVERSITY, GLASGOW, W.2, SCOTLAND
SPKS, SEE SPARKS, ROBERT A.
SRIVASTAVA, R. C., DEPT. OF CHEM., U. OF WASHINGTON, SEATTLE, WASHINGTON
STADLER, H. P., THE UNIVERSITY, NEWCASTLE-UPON-TYNE, ENGLAND
STALEC, F., COMPUTING CENTRE, LEPI POT 11, LJUBLJANA, JUGOSLAVIA
STEMMLER, R. S., ILLINOIS GEOLOGICAL SURVEY, URBANA, ILL.
STEWART, J. M., DEPT. CHEM., UNIV. OF MARYLAND, COLLEGE PARK, MARYLAND
STOUT, G. H., DEPT CHEM, UNIV. OF WASHINGTON, SEATTLE 5, WASH.
STWRT, SEE STEWART, J. M.
SUMNER, G. G., MELLON INST., PITTSBURGH, PA.
SVETICH, G., 7126 S 130TH ST., SEATTLE, WASH., USA
TAKEDA, HIROSHI, CRYSTAL. LAB., JOHNS HOPKINS UNIV., BALTIMORE, MD.21218
TAKEUCHI, Y., DEPT. OF MINERALOGY, UNIV. OF TOKYO, HONGO, TOKYO, JAPAN
TAYLOR, F. C., EES, GEORGIA INSTITUTE OF TECHNOLOGY, ATLANTA, GEORGIA
TEMPLETON, D. H., UNIV, OF CALIFORNIA, BERKELEY, CALIF.
TEMP, SEE TEMPLETON, D. H.
THURN,H.,LEHRST.ANORG.ANALYT.CHEMIE T.H.STUTTGART,SCHELLINGSTR.26,GERMANY
TICHY, K., INST. OF SOLID STATE PHYS., C.S.A.V., PRAGUE, CZECHOSLOVAKIA
TOEPFER, RECHENINSTITUT PROF HAACK, TU BERLIN
TOMAN, K., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
TOURNARIE,M.,40,RUE-MANGEON,MASSY,78,FRANCE
TRAUB, W., COLUMBIA UNIVERSITY (COLLEGE OF PHYSICIANS AND SURGEONS), NYC
TRBD, SEE TRUEBLOOD, K. N.
TREUTING, R. G., BROOKHAVEN NATIONAL LABORATORY, BROOKHAVEN, NY
TREUTNG, SEE TREUTING, R. G.
TROTTER, J., DEPT. OF CHEM., UNIV. OF BRIT. COLUMBIA, VANCOUVER, CANADA
TRUEBLOOD, K.N. , DEPT CHEM, UNIV OF CALIF, LOS ANGELES 24, CALIF
TRUTER, M.R., SCHOOL OF CHEM., UNIVERSITY, LEEDS 2, ENGLAND
TULINSKY, A., DEPT. OF CHEMISTRY., YALE UNIVERSITY, NEW HAVEN, CONN.
TUVLIND, S.O., ADP INST., CHALMERS UNIV. OF TECHN., GIBR.G.5, GOTHENBURG, SWEDEN
UEDA,I., GENERAL EDUCATION DEPT., KYUSHU UNIV., OTSUBO-MACHI, FUKUOKA, JAPAN
URBAN, J., FRITZ-HABER-INST., ABT. PROF. HOSEMANN, BERLIN 33, GERMANY
VACIAGO, A., CENTRO STRUTTURISTICA CNR, CITTA UNIVERSITARIA, ROMA, ITALY
VAC, SEE VACIAGO, A.
VAND, V., GROTH INST., PENN. STATE UNIV., UNIVERSITY PARK, PA.
VAN DEN HENDE, J. H., LEDERLE LABAROTORIES, AMER. CYANAMIDE, PEARL RIVER, N. Y.
VAN DER HELM, D. CHEM.DEPT.,UNIV. OF OKLAHOMA, NORMAN, OKLA., USA.
VAN DER SLUIS, , 51 CATHARIJNESINGEL, UTRECHT, NETHERLANDS
VAN EIJCK, B.P., LAB. KRISTALCHEMIE, RIJKSUNIVERSITEIT, UTRECHT, NETHERLANDS
VDHELM SEE VAN DER HELM, D.
VISSER,J.W.,TECHN,PHYS.DEPT.,P.O.BOX 155, DELFT,NETHERLANDS
VOGEL,R.E., KAMAN CORP COLO SPRINGS,COLO
VON STEINWEHR,H.E., INST.MIN.PETR., UNIVERSITAT, PPOSTFACH 606, 65 MAINZ,GERMANY
VONK, C. G., CENTRAAL LAB. STAATSMIJNEN, GELEEN, NETHERLANDS
VOS,A,LAB. VOOR STRUCTUURCHEMIE BLOEMSINGEL 10, GRONINGEN,NETHERLANDS
WAX,S. NASA GODDARD SPACE FLIGHT CENTER GREENBELT MD USA
WEHE,D. J., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
WEH, SEE WEHE,D. J.
WEISS, H. G., DAW-STRUKTURFORSCHUNG, BERLIN, GDR
WEISS,H G ,DAW,INSTITUT FUER STRUKTURFORSCHUNG,BERLIN-ADLERSHOF,GDR
WENGELIN,R.F.,INORG.CHEM.,UNIV.OF GOTHENBURG,GOTEBORG S,SWEDEN

WERKEMA,MARILYN, CHEMISTRY DEPT., UNIVERSITY OF COLORADO, BOULDER,COLO.
WERNER, P.E., INST. INORG. AND PHYS. CHM., UNIV. OF STHLM., STOCKHOLM VA, SWEDEN
WESTM, SEE WESTMAN, S.
WESTMAN, S., INST. INORG. CHEM., UNIV. OF STOCKHOLM, STOCKHOLM 50, SWEDEN
WHITTIER, V. E., DOW CHEMICAL COMPANY, MIDLAND, MICH.
WILLIAMS, D. E., IOWA STATE UNIVERSITY, AMES, IOWA
WILL,G., MPI. EIWEISSFORSCHUNG,MUENCHEN,LUISENSTR. 39, GERMANY
WILSON, A.S., CHEM. RESEARCH, BATTELLE-NORTHWEST, RICHLAND, WASHINGTON
WOLFEL, E. R., ABT. FUR. STRUKTURFORSCHUNG, DARMSTADT, GERMANY
WOLTEN, G.M. AEROSPACE CORP., BOX 95085, LOS ANGELES 45, CALIF.
WOOLFSON,M.M., MANCHESTER COLLEGE OF SCIENCE AND TECHNOLOGY, MANCHESTER, ENGLAND
WRIGHT, D.A., DEFENSE STANDARDS LABS, BOX 50, ASCOT VALE, W2, VICTORIA, AUSTRAL.
WUENSCH, B. J., DEPT. OF METALLURGY, M. I. T., CAMBRIDGE, MASS., 02139, USA
WUNDERLICH, J., CENTRAL SCI. INDUSTR. RES. ORG., MELBOURNE, AUSTRALIA
YAKEL,H.L.,OAK RIDGE NATIONAL LAB.,OAK RIDGE,TENN.
ZAKRAJSEK, E., COMPUTING CENTRE, LEPI POT 11, LJUBLJANA, JUGOSLAVIA
ZAKRAJS, SEE ZAKRAJSEK, E.
ZALKIN, A., LAWRENCE RADIATION LAB., P O BOX 808, LIVERMORE, CALIF.
ZANOVELLO RENATO, C.E.C.S., V. PAOLOTTI 9, PADOVA, ITALY
ZANO, SEE ZANOVELLO RENATO
ZELENKO,B., INST.R.BOSCOVICH BIJENICKA 54 , ZAGREB, JUGOSLAVIA
ZILAHI-SEBESS, L., M.T.A.KOZP.KEM.KUT.INT., BUDAPEST, HUNGARY
ZUCCA, T., SORIN, SALUGGIA, ITALY

CNRS BELLEVUE = LABORATOIRE DE CRISTALLOGRAPHIE APPLIQUEE DU CNRS, 1 PLACE ARISTIDE BRIAND, BELLEVUE, S ET O, FRANCE
DAW-STRUKTURFORSCHUNG, BERLIN, GDR = INSTITUT FUR STRUKTURFORSCHUNG DER DAW, BERLIN-ADLERSHOF, GERMAN DEMOCRATIC REPUBLIC
INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA = USTAV FYSIKY PEVNYCH LATEK CSAV, PRAHA-STRESOVICE, CUKROVARNICKA 10, CZECHOSLOVAKIA
LAB.CALC.CNRS = LABORATOIRE DE CALCUL DU CNRS, IMPASSE D*AUBERVILLIERS, PARIS 19, FRANCE
M.T.A.KOZP.KEM.KUT.INT., BUDAPEST, HUNGARY = CENTRAL RESEARCH INSTITUTE OF CHEMISTRY OF THE HUNGARIAN ACADEMY OF SCIENCES, BUDAPEST, HUNGARY
NUM.CENTR.OF MAT., CHARLES UNIV., PRAGUE, CZECHOSLOVAKIA = CENTRUM NUMERICKE MATEMATIKY KARLOVY UNIVERSITY, PRAHA-MALA STRANA, CZECHOSLOVAKIA

LIST OF PROGRAMS

LISTED ACCORDING TO MACHINE TYPE AND FUNCTION.

TO FIND A PROGRAM WHEN ONLY THE ACCESSION NUMBER IS KNOWN, CONSULT THE ACCESSION NUMBER INDEX WHICH GIVES THE MACHINE AND FUNCTION UNDER WHICH THE PROGRAM IS LISTED.

IN THE INTEREST OF LEGIBILITY, THE ACCESSION NUMBERS AND SERIAL LETTERS (A, B, ETC.) ON THE ABSTRACT CARDS (COLS. 1 - 5) HAVE BEEN SUPPRESSED.

CRYSTALLOGRAPHIC PROGRAM SYSTEMS AND PROGRAMS BELONGING THERETO --

3068 ATSYS SYSTEM DREW ATSYS/ ATLAS CRYSTALLOGRAPHIC SYSTEM
IMPERIAL COLLEGE SYSTEM OF CRYSTALLOGRAPHIC PROGRAWORKING IN CONJUNCTION WITH A SINGLE MAGNETIC TAPE WHICH CONTAINS ALSO THE DATA AND WORKING SPACE FOR 20 - 30 JOBS. ALL PROGRAMS WRITTEN IN EXCHLF. THEY ARE
FIFI DATA REDUCTION, WEISSENBERG (DIAMAND, DREW.
PLIP DATA RECUTION, PRECESSION (DOLLIMORE, DREW)
LSCD LS FIT POWD. OR S.C. DATA FOR CELL DIM. (DIAMAND)
POLO SCALES DATA ON TWO OR MORE AXES (DREW)
PEPE FOURIER (HARDING, DREW)

KIKI PAPER TAPE TO MAG TAPE DATA STORAGE (DREW)
BABA BLOCK DIAG. SF LS, SIMILAR TO ROLLETT,S MERCURY PGM(DIAMAND,DREW)
ELSI BOND DISTANCES AND ANGLES (DIAMOND, DREW)
DIDO WEIGHTED LS PLANE THRU GROUP OF ATOMS (SPARKS, HUNT)
DIAN DIHEDRAL ANGLES, ETC., FOR MODEL BLDG. (DIAMAND)
FOR DETAILS CONCERNING THE SYSTEM, WRITE TO MR. M. G. B. DREW, IMPERIAL COLLEGE, UNIVERSITY OF LONDON, LONDON S.W. 7, ENGLAND

413 X-RAY-63 GENERAL JSTEW*HIGH,HOLDEN,CHAST,DICSN,BROWN,DAYH,MOROSIN,LING LWA ,JENSEN,TAKEDA,WAX,KEEFE,AMMON,BRAUN,ALDEN/EACH PROGRAM OF THIS SYSTEM IS ALSO LISTED BY ITS FUNCTION. MAJOR CODING IS IN FORTRAN II WITH NEEDED FAP SUBROUTINES. SYSTEM IS EXECUTABLE ALONE OR UNDER ANY OTHER MONITOR. WRITE-UP AVAIL AS 1401 PROGRAM, SYMBOLIC DECKS ALSO FROM 1401. ALL ON MAG. TAPE OF SPECIFIED DENS. 2 REELS OF TAPE 8K IBM 1401 REQ. FORTRAN IV-NPL VERSION IN PREPARATION.

419 X-RAY-63 CONTOUR DAYHOFF,STEWART*/CONTUR/ CONTOUR MAP LINK LWA
CONTOUR PLOTS OF A THREE DIMENSIONAL FOURIER MAP ARE PRODUCED. UP TO 17,000 POINTS PER LAYER CAN BE HANDLED. THE LOGIC IS DESCRIBED IN COMM. ACM 6, (1963), 620-622

423 X-RAY-63 DIR DICKINSON/JSTEW ESORT/PROGRAM TO SORT E VALUES LWA
(QUASI-NORMALIZED STRUCTURE FACTS.) PRELIMINARY TO KARLE SYMBOLIC ADDITION PROCEDURE.

440 X-RAY-63 DP CHASTAIN/JSTEW DATCO1/SPECTROMETER DATA SCALING AND LWA
INTENSITY CORRECTION(INCLUDING BURNHAM GEN.ABS.CORR.)

439 X-RAY-63 DP CHASTAIN/JSTEW DATCOR/INTER-FILM DATA SCALE AND AVE LWA

443 X-RAY-63 DP CHASTAIN/JSTEW IFORMS/GEN REF NEEDED + FORMS FOR LWA
RECORDING INTENSITIES FROM FILM DATA AS WELL AS INPUT TO DATCOR LINK.

441 X-RAY-63 DP HOLDEN/JSTEW DATCO2/INTER-FILM DATA SCALING LWA

421 X-RAY-63 DPDIR HOLDEN,STEWART* DATFIX/CONVERSION OF F-RELATIVE LWA
INTO QUASI-NORMALIZED STRUCTURE FACTORS(E-FACTORS)(KARLE-HAUPTMAN) THESE MAY THEN BE USED FOR THE SYMBOLIC ADDITION PROCEDURE OR FOR COEFFICIENTS IN SHARPENED ORIGIN REMOVED PATTERSON (VECTOR-MAP) OR E-MAPS BY THE FOURR LINK. ESTIMATE OF OV T.F. AND SCALE GIVEN.

438 X-RAY-63 DP JSTEW*CHAST,MOROSIN/DATRDN/THIS LINK OF THE X-RAY SYS LWA
SERVES TO BUILD THE COMPOUND REFLECTION TAPE WITH ALL SYMMETRY AND CELL INFORMATION STORED ON IT. ITS FUNCTIONS ARE PRELIMINARY TO ALL OTHER MAJOR LINKS OF THE SYSTEM. IT CALCULATES 1/LP FOR POW,WEIS,PREC,SPECTROM, IT DOES BOND ABS CORR.,INTERPOLATES FORM FACTOR FROM LITT BY 4-POINT, SETS LEAST SQUARES WEIGHTS,AND GENERALLY SCANS PRELIMINARY DATA. MOST IMPORTANT FUNCTION IS BUILDING OF FOURIER AND LEAST SQUARES GEN SYM CODE

442 X-RAY-63 DP TAKEDA,JSTEW* INCOR/WEIS INTEN.CORR.1/LP,BURNHAM LWA
GENERAL ABSORPTION CORR.

418 X-RAY-63 FR HIGH,JENSEN,HOLDEN,JSTEW*FOURR/3D FOURIER,ALL SPC GRP LWA
ALL SETTINGS,ANY INTERVAL TO 2000THS IN 1ST SUM,400THS IN 2ND SUM 200THS IN 3RD SUM DIRECTION,14 POSS COEF.(FO,DELTAF,E,FC,ETC.)WILL GIVE UNDISTOR SECTIONS,BINARY OUTPUT TO PLOTTER AND PEAK SEARCH LINKS OF SYSTEM. WILL TAKE VERY LARGE CELLS WITHOUT MODIFICATION.

431 X-RAY-63 FRBLK HOLDEN/STEWART FOUREF/BLOCK FOURIER ATOMIC COORD REF LWA
MOVES ATOMS TO MAXIMUM IN ED.CALCS,FC AND BLOCK,CYCLES,SHIFTS OVERALL TF. ANY SPACE GROUP

433 X-RAY-63 ID CHAST,HIGH,JSTEW*BONDLA/GENERAL LENGTH ANG.GEN H COOR LWA

434 X-RAY-63 ID BUSING,MARTIN,LEVY/STEWART/ORFFE/X-RAY-SYSTEM COPY LWA

427 X-RAY-63 LC ALDEN,AMMON,CHAST,HIGH/JSTEW*/PARAM/ REFINE CELL CONSTANTS FROM THETA VALUES BY LEAST SQUARES

416 X-RAY-63 LSBLK STEWART*DICSN BLOKLS/BLOCK DIAGONAL LEAST SQUARES LWA
MIXED T.F. 200 ATOMS,850 PARAM,UNLIM REF,ALL SPACE GROUPS SOME PATCH REQ

415 X-RAY-63 LSDM STEWART*LING DIAGLS/DIAGONAL LEAST SQUARES MIXED T LWA
F.,250 ATOMS,1400 PARAM, UNLIM REF,ALL SPACE GROUPS,SOME SPEC POS PATCH

417 X-RAY-63 LSFM STEWART*/EXTENSIVE MOD OF BUSING,MARTIN,LEVY F.M.LEAS LWA
SQUARES,45 ATOMS,190 PARAM,UNLIM REF,ALL SPACE GROUPS,FIXED AT.SOME SPEC POS.PATCH REQ.MIXED T.F.REQ X-RAY SYSTEM REFLECTION TAPE.

436 X-RAY-63 LSPL CHASTAIN/STEWARTLSQPL/METHOD OF SHOMAKER ET.AL. FITS LWA
AN ARRAY OF POINTS TO A LINE OR PLANE,GIVES INTER PL ANGS, DISTS FROM PL.

432 X-RAY-63 PATSHL HOLDEN/STEWART SHLPAT/GIVES SHELLS AS MERCATOR PROJ LWA

437 X-RAY-63 SPEC CHASTAIN/STEWARTDELSIG/LEAST SQUARES WEIGHT ESTAB- LWA
LISHMENT. EST EXTINCTION IN DATA PLOT FO/FC AS FN OF FO OR SNTH/LAMBDA

420 X-RAY-63 PK DAYHOFF,STEWART*/PEKPIK/ PEAK PICKING LINK LWA

THE PRECISE COORDINATES AND DENSITIES OF THE PEAKS IN A 3 DIMENSIONAL FOURIER MAP ARE CALCULATED. UP TO 20,000 POINTS PER LAYER CAN BE SEARCHED. SYMMETRICALLY UNIQUE PICKS ARE LISTED. THREE ORTHOGONAL PROJECTION PLOTS OF ALL PEAKS IN ONE UNIT CELL ARE MADE ON THE 1401.

414 X-RAY-63 SF STEWART*HIGH FC/GENERAL STRUCTURE FACTORS ALL SPAC LWA
GROUPS ALL SPECIAL POSITIONS,MIXED T.F.,DISPERSION,POPULATION OF SITE,ETC 2400 ATOMS/CELL OV.TF.2000 AT/CELL IND.ISO.TF.1000 AT/CELL IND.ANIFO.TF.

445 X-RAY-63 SPEC CHASTAIN/JSTEW WUUD/4K1401 SYS WRITE UP PRINTING LWA

422 X-RAY-63 SPEC STEWART MODIFY/SEARCH AND MODIFY REFLECTION LWA
TAPE. GENERATE PSEUDO-DATA OF KNOWN ERROR FOR TEST PURPOSES.

430 X-RAY-63 SPEC STEWART STUJOB/GENERATE 2D STUDENT PROBLEMS LWA

425 X-RAY-63 SPEC TAKEDA,DONNAY/JSTEW/TRXLS/TRANSFORMATIONS OF CRYST LWA
SETTINGS AND SPACE GROUP SYMBOLS

444 X-RAY-63 SPEC WAX,STEWART* UDATE/8K1401 SYS MAINTENANCE LWA

424 X-RAY-63 STAT HIGH,STEWART* FCLIST/LIST STRUCTURE FACTORS LWA

426 X-RAY-63 STAT KEEFE,STEWART* RLIST/LIST R VALUES FOR ZONES ETC LWA

435 X-RAY-63 STERO BRAUN,HIGH/JSTEWPROJCT/ORTH OR PERSP PROJ OF MOL ON LWA
ARBITRARY PLANE

428 X-RAY-63 THETASET FREER,AMMON,CHAST,HIGH/JSTEW*/GESET/ GENERATION OF LWA
SPECTROMETER SETTINGS FROM CELL DATA AND ORIENTATION INFORMATION

429 X-RAY-63 WEISDP HOLDEN/JSTEW FLMSET/MM COOR OF REF ON WEIS FLMS LWA

PROGRAMS LISTED UNDER PROGRAMMING LANGUAGES (PSEUDO-MACHINES) --

8039 ALGOL60 ABS DUISENBERG UTR.D1/ABSORPTION COEFFICIENT LPA
ABS.CORR. FOR CONVEX POLYHEDRON OR ARBITRARILY SHAPED CRYSTAL AND CORR. FOR INHOMOGENEOUS X-RAY BEAM. X1 8K

5051 ALGOL 60 ABS LP SCHULZ ABS, LP FOR EQUI-INCL.-WEIS LWA
PROGR. CONVERTS FILM-DENSITIES TO INTENSITIES. THESE INTENSITIES ARE MULTIPLIED WITH THE LP-FACTOR AND ABSORP. FACTOR FOR SPHERICAL SPECIMENS. TESTED ON TR4. STORAGE ABOUT 1500. INPUT (H, K, L, DENSI). OUTPUT (H, K, L, INTENSI)

5048 ALGOL 60 ABS LPPK SCHULZ ABS, LP, PK-COR. EQUI-INCL.-WEIS LWA
PROGR. CONVERTS FILM DENSITIES TO INTENSITIES. THESE INTENSITIES ARE MULTIPLIED WITH THE LP-FACTOR AND ABSORPT.FACTOR FOR SPHERICAL SPECIMENS. PEAK-INTENSITIES ARE CONVERTED TO INTEGRAL INTENSITIES BY THE METHOD OF PHILLIPS (ACTA CRYS (1954), 7, 746-751). TESTED ON TR4. STORAGE ABOUT 2000. INPUT (H, K, L, DENSI). OUTPUT (H, K, L, INTENSI)

236 ALGOL D EICHHORN RECW/RECIPR.TRANSL.FROM WEISSBG.DATA LPM
PROGRAM COMPUTES RECIPROCAL TRANSLATIONS FROM AXIAL DATA ON WEISSENBERG FILMS, AND OPTIMIZES FOR FILM SHRINKAGE AND SIMILAR ERRORS.

248 ALGOL DF EICHHORN DSBM/DIFF.SYNTHESIS(DS-ONE) LPM
SIMPLE 3-BY-3 PLUS 6-BY-6 MATRIX DIFFERENTIAL SYNTHESIS FOR P-BAR-ONE, FOR UNLIMITED NUMBER OF REFLEXIONS BUT NUMBER OF ATOMS AND SCATTERING TYPES LIMITED BY AVAILABLE MEMORY. GOODNESS-OF-FIT AND ACCURACIES ARE COMPUTED SIMULTANEOUSLY WITH REFINEMENT. PROGRAM IS SELF-CYCLING.

249 ALGOL DF EICHHORN DSSO/DIFF.SYNTHESIS(DS-TWO) LPM
PROGRAM AS DS-ONE, BUT COMPUTES TAYLOR EXPANSION OF POSITIONAL ERROR TO SECOND ORDER APPROXIMATION.

250 ALGOL DF EICHHORN DSEI/DIFF.SYNTHESIS(DS-THREE) LPM
PROGRAM AS DS-TWO, BUT ALSO COMPUTES DEBIJE-WALLER SHIFTS TO SECOND ORDER CORRECTIONS. A RELAXATION METHOD IS APPLIED TO SOLVE EQUATIONS.

251 ALGOL DF EICHHORN DSTT/DIFF.SYNTHESIS(DS-FOUR) LPM
HAS ALL FEATURES OF DS-ONE, BUT IS BASED ON COMPARISON OF OBSERVED AND CALCULATED THIRD DERIVATIVES OF RHO, THUS YIELDING 10-BY-10 MATRIX. THE PROGRAM THUS CATERS TO INDIVIDUAL ATOMIC SCALE FACTORS.

8034 ALGOL60 DIR BEURSKENS UTR.B6/SIGNDETERM. FOR PROJECTIONS LWA
USING NONCENTR. 3DIM DATA FORMULA B3,0 KARLE AND HAUPTMAN 1959 X1

8035 ALGOL60 DIR BEURSKENS UTR.B10/SYMBOLIC ADDITION METHOD MPA
SIGNDETERM. FOR CENTR.STRUCT. KARLE AND KARLE 1963, BEURSKENS 1964 X1

8032 ALGOL60 DP BEURSKENS UTR.B2/CALC. OF E-VALUES X1 LWA

6038 ALGOL60 DP JOHANSSON G LR/X-RAY DATA ON LIQUIDS LPA
COMPILED AND RUN ON FACIT. CORE 2K, DRUM 8K

7557 ALGOL DP PANATT/BOMB/COJAZ/SOME GEOMETRIC PROGRAMS LPA
COMP. ON 6001 1K. 1) BOND ANGLES AND DISTANCES, 2) BEST PLANE WITH LS.,

3) GEOMETRICAL DETERMINATION OF THIRD COORD. FROM TWO KNOWN, 4) DP VALUES FOR TWO CIRCLE NEUTRON DIFFRACTOMETER

8059 ALGOL60 DP WEISS GEISE,HESPER OX1/INTENSITIES TO SF WILSON PLOT LWA
USES LP CORRECTION, PHILLIPS CORR., AND ABSORPTION FOR CYLINDER OPTIONAL PROD INPUT FOR OX3, OX4, OX5, OX8, OX9 . TESTED ON X1 8K.

247 ALGOL E ID EICHHORN ESDV/ESD AND MPE OF POS.BONDS,ANGLES LPM
FROM THE ESD VALUES OF X,Y,Z THE MOST PROBABLE ERRORS OF BONDS AND ANGLES ARE COMPUTED TOGETHER WITH THE BONDS AND ANGLES.

256 ALGOL FR EICHHORN FRSY/TRICLINIC FOURIER SYNTHESIS LPM
FOURIER SYNTHESIS PROGRAM (3-DIMENSIONAL) FOR TABULATOR PRINT-OUT. INDEX LIMITATION IS FACTOR OF AVAILABLE STORAGE.

5012 ALGOL FR 2 HOPPE 2 DIM NO SYMMETRY SIMPLIFICATION LWA

8028 ALGOL60 FR23 BL PETERSE H182/GENL ALL SPACEGROUPS LWA
IT.IND.REFL.AND SPACEGR.DEPENDING PROC.TO GENERATE DEP.REFL,CONTOUR IF WANTED FROM PAPERTAPE OT,UP TO 4000 REFL. AGLTR4 8K

8529 ALG FR 2 3 UEDA,I. UFO-1/FR GRID N/120 TRI MONO ORTH LPA
FOR TRI MONO ORTH. GRID N/120. CHOICE OF SECTION FREE. TWO VALUES OF ABS(HKL) LESS THAN 30. PATT,FOURIER,D-F POSSIBLE. INPUT-M.T. OUTPUT-PRINTS. PROG.TEST REFER SFU-1.

6036 ALGOL60 H WENGELIN GENTRAI/GENERATES TRANSFORMS INDICES LWA
TRANSFORMS TO NEW CELL. GENERATES BY MAX 2 TWIST, 3 REFLEXION-MATRICES. CHECKS AND SURPRESSES IDENTICAL REFLECTIONS WITHIN EACH GENERATION. COMPILED AND RUN ON 16K DATASAAB D21.

240 ALGOL H LC EICHHORN CELL/CELL CONSTANTS,LIMITING SPHERE LPM
PROGRAM COMPUTES COMPLETE SET OF CELL DATA FROM OBSERVED DATA ABOUT TWO AXES, THEN COMPUTES ALL NON-REDUNDANT INDEX COMBINATIONS SUBJECT TO SPACEGROUP CONSTRAINTS WITHIN GIVEN LIMITING SPHERE (WAVE LENGTH).

5049 ALGOL 60 ID SCHULZ DIST.+ANGLES BY GIVEN KOORD. LWA
DISTANCES OR ANGLES ARE CALCULATED BY INPUT OF KOORD. TRIPLES (2 OR 3). TESTED ON TR4. STORAGE ABOUT 300.

6041 ALGOL60 ID NYBORG.DANIELS* ND1/COMPLETE SET OF DISTANCES. LWA
GIER AGL FAST STORE 1024 WORDS. DRUM STORE 12800 WORDS. SPEC INSTRUCTIONS FOR DRUM OPERATIONS. ALL RELEVANT DISTANCES AND ANGLES BETWEEN ATOMS IN 27 UNIT CELLS. STANDARD DEVIATIONS.

409 ALGOL ID E GALLAHER,TAYLOR ALGOL FUNCTION AND ERROR LWA
ALGOL TRANSLATION OF OAK RIDGE FORTRAN FUNCTION AND ERROR BY BUSING, MARTIN, AND LEVY. I/O SUITABLE FOR BURROUGHS B5000 AND B5500

241 ALGOL LC EICHHORN ROTO/AXES FROM LAYERLINES LPM
PROGRAM CALCULATES AXIAL TRANSLATIONS FROM ROTATION-OSCILLATION DATA, AND OPTIMIZES FOR FILM SHRINKAGE ERRORS AND NON-CYLINDRICAL CAMERA SHAPE.

243 ALGOL LF EICHHORN SCCS/SCATTERING CURVES LPM
PROGRAM CONVERTS PUBLISHED SCATTERING DATA INTO UNIFORM SET OF 100 VALUES AND DIFFERENCES, TO GIVE CARD SET OF 25 CARDS FOR INPUT INTO STRUCTURE FACTOR AND REFINEMENT PROGRAMS LISTED BELOW.

238 ALGOL LP EICHHORN WEIS/LORENTZ-POL.WEISSBG.DATA LPM
PROGRAM CALCULATES LP FACTOR ACCORDING TO 3-DIMENSIONAL EXPRESSION AND OBTAINS BOTH PATTERSON AND FOURIER COEFFICIENT FROM RAW INTENSITY.

244 ALGOL LP EICHHORN PREC/LORENTZ-POLAR.PRECESSION DATA LPM
PROGRAM USES THE MODIFIED WASER EXPRESSION TO OBTAIN LP FACTORS FOR PRECESSION INTENSITIES. THESE ARE CONVERTED INTO THE PATTERSON AND FOURIER COEFFICIENTS.

7548 ALGOL LS BASSI 1/X.RAYS/NEUTRONS OBSREV. LPN
LEAST SQUARES REFINEMENT,FM,ISOTROPIC AND ANISOTROPIC TF,ALL SPACE GROUPS LF LINEAR INTERPOLATION,E,R,SCL, CORRELATIONS MATRIX,INTERAT.BOND LENGTHS

7549 ALGOL LS BASSI 2/X RAYS AND NEUTRONS MIXED OBSERV. LPN
LEAST SQUARES REFINEMENT,FM,ISOTROPIC AND ANISOTROPIC TF,ALL SPACE GROUPS LF LINEAR INTERPOLATION,E,R,SCL, CORRELATIONS MATRIX,INTERAT.BOND LENGTHS

252 ALGOL LS EICHHORN LSAN/LEAST SQUARES REF.(LS-ONE) LPM
LEAST SQUARES ANALOG OF DS-ONE.

253 ALGOL LS EICHHORN LSFM/LEAST SQUARES REF.(LS-TWO) LPM
HAS ALL OPTIONS OF DS-ONE AND LS-ONE, BUT COMPUTES 9-BY-9 MATRIX.

6037 ALGOL60 LS JOHANSSON G FLR/REFINEMENT X-RAY DATA ON LIQUIDS LPA
COMPILED AND RUN ON FACIT. CORE 2K, DRUM 8K

6039 ALGOL60 LS,AT GROENBAEK 3X3,6X6 BLOCK DIAGONAL LS LPA
GIER AGL. FAST STORE 1024 WORDS. DRUM STORE 12800 WORDS.SPEC INSTRUCTIONS FOR DRUM OPERATIONS. PROGRAM MODIFICATIONS FOR MOST

SPACE GROUPS AND SPEC POS.

410 ALGOL LS AT FM GALLAHER,KAY ALGOL LEAST SQUARES SF,FM,AT LWA
ALGOL TRANSLATION OF OAK RIDGE FORTRAN LEAST SQUARES BY BUSING, MARTIN, AND LEVY. I/O SUITABLE FOR BURROUGHS B5000 AND B5500

8024 ALGOL60 LS LC P VISSER JW H932/TRICL.MONOCL. ORTHOR. LPA
AGLTR4,IT.RECIPR.LC,OBS.REFL.OT.LC,LIST OF OBS.REFL.AND ALL CALC.REFL.,INCREASING THETA

5052 ALGOL LP PREC BAERNIGHAUSEN LP CORRECTION FOR PREC DATA FOR ANY LWA
LAYER PARALLEL A*,B*. IT RECIPROCAL LC, LAYERINDEX L, PREC-ANGLE, HK AND INTENSITY. OT SF AND SQUARE OF SF.

5072 ALGOL 60 P THTA D VON STEINWEHR ARRAU 170565 LWA

8025 ALGOL60 PDIAGRAM VISSER JW H627/POWDERDIAGRAM FROM LITERAT.DATA LPA
AGLTR4,CALCUL.INTEGR.INTENS.,IT.RECIPR.LC,POS.TF,OT.DIAGRAM FOR ANY INSTR

7551 ALGOL PI BASSI H BETWEEN 0 AND THETA MAX. LPN

8030 ALGOL60 PI PETERSE H81/Q-DIFFERENCES NOT-TRICL.SYSTEMS LWA
AGLTR4 IT.Q-VALUES,OT.FREQUENCY OF DIFFERENCES

8027 ALGOL60 PI 2,3 KUYPERS/PETERSE H142,H127A/ZONEMETHOD GENL
IT.Q-VALUES,2D DETERMINES INDEP.ZONES,3D COMBINES 2 ZONES TO RECPR.LATT. AGLTR4

246 ALGOL PROF EICHHORN LSPL/MARSH-WASER LEAST SQU.PLANE LPM
THE MARSH-WASER RECIPE IS APPLIED TO COMPUTE THE (OPTIMIZED) LEAST SQUARES PLANE THROUGH A SET OF POINTS.

6040 ALGOL60 REFINEM. DANIELSEN D45/R MINIM BY TEST FOR EACH PARAM. LWA
GIER AGL FAST STORE 1024 WORDS. DRUM STORE 12800 WORDS. SPEC INSTRUCTIONS FOR DRUM OPERATIONS. REFINEMENT BY SYSTEMATIC VARIATION OF THE PARAMETERS METHOD BY BHUIYA AND STANLEY, ACTA CRYST 16,981(1963). ISOTROPIC TF.

239 ALGOL S EICHHORN THSC/THRESHOLD SCANNER LPM
PROGRAM DETERMINES THRESHOLD INTENSITY VALUE FOR EACH OBSERVABLE BUT NOT OBSERVED REFLEXION, FROM LP EXPRESSION AND MINIMUM VISIBLE INTENSITY.

245 ALGOL S EICHHORN FILM/ACCURACY OF FILM READINGS LPM
PROGRAM COMPUTES MOST PROBABLE ERROR FOR CELL CONSTANTS FROM ESTIMATED STANDARD DEVIATIONS OF INDIVIDUAL READINGS.

257 ALGOL SCF HOLM SCFA/PNL(N) AND Z-CONTR. LPM
HIGHLY SPECIALIZED INTEGRATION PROGRAM TO CALCULATE SELFCONSISTENT FIELDS FOR HARTREE FIELDS OF LANTHANIDES.

258 ALGOL SCF HOLM SCFB/Y(R) AND Y*(NL,R) LPM
HIGHLY SPECIALIZED INTEGRATION PROGRAM TO CALCULATE SELFCONSISTENT FIELDS FOR HARTREE FIELDS OF LANTHANIDES.

259 ALGOL SCF EICHHORN ATOM/WAVEFIELD INTEGRATION LPM
CURVEFITTING INTEGRATION OF WAVEFIELDS TO OBTAIN ATOMIC SCATTERING FACTORS FOR DIFFRACTION USES.

7552 ALGOL SF BASSI X.RAYS OR NEUTRONS STRUCT.FACT. LPN
POWDER SYSTEMATIC COMPUTATION OF SF FOR BRAGG ANGLES FROM 0 TO A GIVEN MAXIMUM,OR ONLY FOR A LIST OF GIVEN H,K,L ,ISOTROPIC OR ANISOTROPIC

254 ALGOL SF EICHHORN ISOF/IND.ISOTROPIC STRUCTURE F LPM
SIMPLE STRUCTURE FACTOR AND PERCENTAGE DISCREPANCY CALCULATION FOR ISOTROPIC TEMPERATURE FACTORS.

255 ALGOL SF EICHHORN ANIF/IND.ANISOTR.STR.FACTORS LPM
SIMPLE STRUCTURE FACTOR AND PERCENTAGE DISCREPANCY CALCULATION FOR ANISOTROPIC TEMPERATURE FACTORS.

8528 ALG SF UEDA,I. SFU-1/SF 6KINDS 150ATOMS ISO-TF LPA
FOR TRI MONO ORTH 6KINDS 150ATOMS ISO-TF. SCALE OF FOBS,R FACOTRS OF 10 REGIONS ARE CALCULATED. INPUT-CARDS. OUTPUT-PRINTS,M.T.(TO BE USED FOR FOURIER).PROG.IS TESTED BY OKITAC-5090-H(8K) WITH 3M.T.,1DRUM,CARD-READER,PRINTER.

8026 ALGOL60 SF 1,2,3 VISSER J W H628/BHUIYA-STANLEYMETH.ACTA 16,987 LPA
AGLTR4,SINGLE CRYST.,NO LIMIT ON REFL.PARAM.POS.SCL,OVERALL-B 12K IF 3D

5014 ALGOL SF 3 HUBER/ANZENHOF. 3 DIM ANY PLANE WANTED NNN

5050 ALGOL 60 SF 3 SCHULZ 3 DIM INDIV. ISOTR. TEMP. + MULT. LWA
STRUCTURE FACTORS FOR INDIVIDUAL ISOTROPIC TEMPERATURE FACTORS AND INDIVIDUAL MULTIPLIERS ARE CALCULATED AND THE AGREEMENT FACTOR IS ESTIMATED. TESTED ON TR4. STORAGE ABOUT 2500.

8029 ALGOL60 SFLS PETERSE.PALM H562/BLOCK DM AT E GENL R LWA
AGLTR4,SF DATA ON MAGNETIC TAPE,ALL SPACEGROUPS,NO LIMIT ON REFL.ANALYTIC AL LF,VARIABLE WEIGHTINGSCHEME,AUTOMATIC REF.OF COORD.AND AT OF ALL SPEC. POSITIONS,PARAMETERS.SCL,ANISOTR. AND ISOTR.TF,POSITIONS

8023 ALGOL60 SF P VISSER J W H952/BHUIYA-STANLEYFOR POWDER ACTA 16 LPA
ALGTR4,IT.OBS.INTEGRATED INTENS.OF ALLINSTRUM.,PROGR.ALSO HANDLES COIN CIDING LINES,PARAM.POSITIONS,SCL,OVERALL-B
237 ALGOL SF S EICHHORN TRER/TRIAL AND ERROR STR.F LPM
THIS PROGRAM WILL ROTATE AND TRANSLATE A RIGID GROUP SYSTEMATICALLY AND COMPUTE THE STRUCTURE FACTOR SET FOR EACH MODEL. THE TRIAL AND ERROR PROCESS IS SELF-OPTIMIZING AND WILL CONVERGE UPON A SET R-FACTOR.
8040 ALGOL60 SPC DUISENBERG UTR.D2/CRYSTAL POSITION AND SETTING LPA
INPUT OBSERVED CHI AND PHI FOR 3 REFLEXIONS. CALC EXACT POSITION OF THE CRYSTAL AND SETTING ANGLES FOR GENERAL-ELECTRIC AND NONIUS DIFFR. X1
7550 ALGOL SPEC BASSI N POWDER PATTERNS CORRECTIONS LPN
8031 ALGOL60 STAT BEURSKENS UTR.B1/WILSON PLOT, LS FIT X1 LWA
8033 ALGOL60 STAT BEURSKENS UTR.B3/DISTRIBUTION FUNCTION OF E-VAL
DETERM. OF A CENTER OF SYMM. RAMACHANDRAN AND SRINIVASAN 1959 X1
8036 ALGOL60 STAT DE VRIES A UTR.V5/MAKES INPUT FOR UTR.V7 AND V9 LWA
2DIM TABLE OF FO-FC OR FC/FO AGAINST I AND THETA FROM FO AND FC. X1 8K
8037 ALGOL60 STAT DE VRIES A UTR.V7/EXTINCTION CONSTANT LWA
CALC. EXTINCTION, SCF AND TF CORRECTION FROM FC/FO SEE UTR.V5
8038 ALGOL60 STAT DE VRIES A UTR.V9/LS WEIGHTING SCHEME LWA
ANALYSIS OF FO-FC TABLE SEE UTR.V5 IN TERMS OF THE PRODUCT OF A FUNCTION OF I AND A FUNCTION OF THETA SEE ACTA CRYST 18,1077
8060 ALGOL60 STEREO GEISE, RUTTEN OX12/CALC. MOLECULAR GEOMETRY LWA
CALC ANGLES NON INTERSECTING LINES, ANGLES BETWEEN PLANES, AND LINE AND PLANE. CALC LS PLANES AND DIST TO PLANES. TESTED ON X1 8K.
8061 ALGOL60 STEREO GEISE, RUTTEN OX20/CALC.HYDR.POS. (TEST ON X1 8K) LWA
8041 ALGOL60 TF VAN EIJCK UTR.E1/V1BRATIONAL ELLIPSOIDS LWA
CALCULATES VIBRATIONAL ELLIPSOIDS FROM GIVEN U-VALUES
242 ALGOL TF S EICHHORN ZERO/ZERO-APPR.ANISOTR.TEMP.FACTORS LPM
PROGRAM CONSTRUCTS ZERO-APPROXIMATE SET OF ANISOTROPIC DEBIJE-WALLER PARAMETERS FROM CELL CONSTANTS AND OPTIMIZED ISOTROPIC TEMP.FACTORS.
502 BALGOL THETA RUDEE , M.L. CALC PK CENTROID BY PIKE WILSON METH. LWA
CALCULATES CENTROID OF A PEAK BY THE METHOD OF PIKE AND WILSON, BRIT. J. APPL. PHYS., V.10, P.57, (1959).
466 FTN 1410 ABS SCHAPIRO ABS2/POLYHEDRAL XTALS ON XRD-5 LWA
CARD INPUT FROM DP2, CARD OUTPUT FOR RECLP
450 FORTRAN2 ABS 3 BERNARD,LANGHMR EXACT ABS CORR. PARALLELOGRAM CRYST. LPA
FOR EQUI-INCL WEIS. FOR MONOCL, ORTHO, TETR, CUB, NEEDLE CRYSTALS HAVING PARALLELOGRAM CROSS SECTIONS, ROTATING ABOUT NEEDLE AXIS. 32K REQUIRED. TESTED AT 25 SEC/REFLECTION ON 60K 1620. USED FOR MU=378.
362 FORTRAN2 ABS 3 BUSING*LEVY ORABS/ABSORPTION CORR,ARBITRARY SHAPE LWA
USES GAUSS INTEGRATION TO CALCULATE ABSORPTION FACTOR FOR CRYSTAL DEFINED BY PLANE FACES. GENERAL THREE-DIMENSIONAL REFLECTION DESCRIBED BY ANGLES READ BY SUBROUTINE WHICH MAY BE WRITTEN BY USER. SUBROUTINES INCLUDED FOR ONE ZONE AND FOR GE ORIENTER. USES TAPE STORAGE IF NEEDED. WRITTEN IN FORTRAN 2. TESTED ON 704, 7090, AND 1604A.
225 FORTRAN2 ABS EXT HAMILTON ESAF-GONO9/ABS,EXT,POLYHEDRAL XTL LW1
CALCULATES ABSORPTION AND SECONDARY EXTINCTION CORRECTIONS FOR POLYHEDRAL CRYSTALS IN GONIOSTAT GEOMETRY. MAIN PROGRAM CAN BE RECOMPILED FOR OTHER GEOMETRIES. SECONDARY EXTINCTION CORRECTION IS VALID EVEN FOR SEVERE EXTINCTION, SINCE THE COUPLED DIFFERENTIAL EQUATIONS OF THE DARWIN TYPE ARE SOLVED IN A GENERAL WAY. TESTED ON IBM 7094 . RUNNING TIME TYPICALLY TWO SECONDS PER REFLECTION. SEE ACTA CRYST 16,609.
449 FT2 CONTOUR DAYHOFF CONTOUR MAP SUBROUTINES (7094) LWA
USER WRITTEN MAIN PROGRAM STORES MATRIX AND CALLS CONTOUR MAP SUB-ROUTINES ONCE FOR EACH CONTOUR LEVEL. SUBROUTINES PRODUCE PLOT POINTS FOR EACH CONTOUR CURVE. USER WRITTEN PLOT ROUTINE IS CALLED EACH TIME POINTS FOR ONE CURVE ARE READY. SEE COMM. ACM 6 (1963), 620-622
3044 FORTRAN2 DEBYE HALL FOBS-FCAL FIT FOR TEMP FAC,EXT PARAM LWA
FITS FOBS AND FCAL TO GIVE BEST SCALE,TEMP. FACTOR AND EXTINCTION PARAMETER. CORRECTIONS ARE APPLIED TO DATA AND R IS CALCULATED
472 FTN 1410 DEBYE SCHAPIRO THERMAL/PR.AXES ,RMS VIB. AMPL. LWA
7535 FORTRAN4 DP DOME,VACIAGO PRFR/PREPAR. OF FOURIER AMPLITUDES LNA
THE PROGRAM PREPARES FOURIER (OR DIFFERENCE FOURIER) AMPLITUDES FROM THE OUTPUT OF SF PROGRAM (FAST). CAN ALSO BE USED TO PREPARE PATTERSON AMPLITUDES. AVAILABLE AT PRESENT IN A TEMPORARY VERSION FOR SPACEGROUPS 1,2,10,12,14,15,19,29,47,53,61,62, BUT DEVISED FOR ALL TRICLINIC,

MONOCLINIC AND ORTHORHOMBIC SPACEGROUPS. TESTED ON 16K 7040.

465 FTN 1410 DP SCHAPIRO DP1,DP2/CALC.OF IOBS AND STD.DEV.IOBS LWA
CARD INPUT OF XRD-5 DATA,CARD OUTPUT FOR PROGRAMS ABS2 OR RECLP

476 FORTRAN DP TROTTER DATAPR/GONIOSTAT SETTINGS, DATA PREP LWA
PROGRAM GENERATES INDICES HKL AND COMPUTES SETTINGS FOR G.E. GONIOSTAT. APPLIES LP FACTORS FOR EQUI-INCLINATION WEISSENBERG FILMS, INTERPOLATES ON UP TO 8 SCATTERING CURVES. IBM 7040 32K

120 FORTRAN2 DP WRIGHT,CHAND,SHO*/DATAPR/SCL+TF,FCOEF,UNTRY F,PATCOEF LPA
DOES WILSON PLOT (BY LEAST SQUARES) TO GIVE OVERALL ISOTROPIC TF AND PRELIM SCL FACTOR. GIVES PATTERSON COEFS MODIFIED BY ANY DESIRED SHAPE FUNCTION AND WITH ORIGIN PEAK REMOVED. THEN RECALCULATES SCL FACTOR BY CONSIDERATION OF PAT ORIGIN. PUNCHES F (ABS SCL) FOR BUSING (PGM 360) AND PREWETT (PGM 364) LS PGMS. ALSO PUNCHES UNITARY SF CARDS. COMPILED ON 32K 7090, SHOULD RUN ON 8K MACHINE.

7023 FORTRAN EL TOURNARIE 304C/ELECTRON DYNAMICAL DIFFRACTION MPA

478 FORTRAN FR TROTTER FOURIE/3-D FOURIER PROGRAM LWA
ANY SPACE GROUP. 1/120 THS OR MULTIPLES OF CELL EDGES. 16 X 31 X 31 POINTS IN ONE PASS. IBM 7040 32K

344 FORTRAN FR2 KAY IT A,B(CAL),FOBS.OT FR/DIF. NPA
CALCULATES EL. DENSITY OR DIFFERENCE MAP USING SIN. TABLE CHECKED ON 8000 WORD 704

504 FORTRN63 FR 2, 3 HEATON,MUELLER B114/GENL,BL,120 GRID (MIFRI) LWA
FORTRAN MODIFICATION OF MIFRI(PGM118) 64K REQUIRED. GENERALLY SIMILAR BUT MANY INPUT INSTRUCTIONS PERFORMED AUTOMATICALLY BY SUPPLYING INTL TABLES SPACE GROUP NUMBER(1-74). INPUT ALSO IN FORM OF ACTUAL DIFFRACTION COORDINATES. STRAIGHT OR DIFFERENCE FOURIER WITH VARIABLE FORMAT OUTPUT SHEETS FOR CONTOURING. 32K VERSION AVAILABLE AS B149.

7534 FORTRAN4 FR 3 BL DOME,VACIAGO FOUR/GENERAL 3-D FOURIER, GRID N/100 LNA
BEEVERS-LIPSON PRINCIPLE. SIN, COS VALUES BY TABLE LOOK-UP. INPUT TAPE FROM PRFR. THE SORTING ORDER OF DATA ON THE INPUT TAPE DETERMINES ON WHICH AXIS THE SECTIONS ARE CUT. THE OUTPUT SHEETS PERMIT DIRECT CONTOURING. TESTED ON 16K 7040.

7030 FORTRAN FT BUJOSA LPA
THIS PROGRAM COMPUTES THE DIFFERENCE FOURIER TRANSFORM (DFT) OF MOLECULES IT HAS BEEN PROGRAMED FOR TRICLINIC CRYSTALS AND STRUCTURE FACTORS MAY BE EVALUATED AS WELL. THIS PROGRAM HAS BEEN WRITTEN FOR IBM 1620 DP SYSTEM PROGRAM STORAGE' 12296. WORK STORAGE' 2980.

395 FORTRAN FT, DFT ASHWORTH,CANUT FT AND DIFFUSE SCATTERING DFT, TDS1/K LPA
GENERATES FRACTIONAL HKL AND CALCULATES MOLECULAR FT, DIFFERENCE FT AND THE STRUCTURE DEPENDENT PART OF THE THERMAL WAVES DIFFUSE SCATTERING. FORTRAN II ON THE IBM 1620, 40K WITH A 1311 DISK. FORTRAN IV ON THE IBM 7040, 32K WITH 8 TAPES.

7025 FORTRAN FT2 ID TOURNARIE 307C/FOURIER TRANSFORM WHITH PICTURE MWA

411 FORT2FAP GENERAL STEWART*HIGH X-RAY-63/SYSTEM FOR IBM 709-7094-(DC) LWA
SEE ALSO UNDER X-RAY-63 ENTRY IN LIST FOR MORE DETAIL

7543 FORTRAN HYDR GEN COL,ESP,GIG*IAN HYDROGEN COORDINATES GENERATION LNA

506 FORTRAN ID BAUR BOND LENGTHS AND ANGLES LWA
GIVEN THE ATOMIC COORDS AND EQUIVALENT POSITIONS IT SEARCHES FOR ALL THE INTERATOMIC BOND LENGHTS AND ANGLES WITHIN SPECIFIED LIMITS. 7090

7541 FORTRAN ID COL,ESP,GIG*IAN ID AND ANGLES IN TRICLINIC CELL LNA
ALSO INTERMOLECULAR DISTANCES LESS THAN A FIXED DISTANCE,1620 20K

396 FORTRAN4 ID,E HARRIS,D.R. DAESD/7044 LPA
INTERATOMIC DISTANCES AND ANGLES WITH THEIR EST STANDARD DEV. DISTANCES BETWEEN ASYMMETRIC UNIT AND ALL EQUIVALENT POSITIONS IN UNIT CELL AND 26 NEAREST NEIGHBOR CELLS ARE GIVEN. OPTIONAL OUTPUT OF CART COORD (ANG).

3046 FORTRAN2 ID OCONNOR DISTS,ANGLES BETWEEN SPECIFIED POSNS LWA
CALCULATES DISTS AND ANGLES BETWEEN SPECIFIED ATOMS ONLY, GIVEN THE FRACTIONAL COORDINATES

3045 FORTRAN2 ID RAE BOND DISTANCE SEARCH LWA
ALL INTERATOMIC DISTANCES LESS THAN A GIVEN MAXIMUM ARE CALCULATED FROM THE COORDINATES IN THE ASYMM. UNIT AND EXPRESSIONS FOR THE EQUIVT. POSNS.

471 FTN 1410 ID SCHAPIRO BONDS/DIST. AND ANGLES FOR SEL. ATOMS LWA

470 FTN 1410 ID SCHAPIRO VSET/ INTRA,INTER-MOLEC. VECT.AND DST LWA

532 FORTRAN2 ID SHOEMAKER, D. DISTAN/DISTANCES,ANGLES,DIHEDRAL ANG. LPA
CALCULATES INTERATOMIC DISTANCES, BOND ANGLES, AND DIHEDRAL ANGLES.

GIVES ALL PARAMETERS NEEDED FOR CRYSTAL MODEL CONSTRUCTION. ALL SPACE GROUPS AVAILABLE, SPECIFIED BY SYMMETRY CARDS, ONE FOR EACH GENERATOR. ALL NECESSARY INSTRUCTIONS ON COMMENT CARDS (NO SEPARATE WRITE-UP). TESTED ON IBM 7090.

479 FORTRAN ID TROTTER CRRES/LENGTHS, ANGLES, MEAN PLANES ETCLWA
COMPUTES BOND LENGTHS, VALENCY ANGLES, MEAN PLANES, INTERMOLECULAR DISTANCES. IBM 7040 32K

7020 FORTRAN LC BIBIAN,TOURNARIE/341A/OPTIMAL SPACING MPA

386 FORTRAN2 LC P PI HECKEL POWD SOLN-CUBIC-MULTIPHASE PATTERN LPA
MULTIPHASE POWD PATT DATA FITTED TO CUBIC HKL SEQ (BCC,FCC,SC,DC). PGM HANDLES EXTRA LINES, ABSENT LINES, IDENTIFIES LATTICE(S), CALC LC, EXTRAPOLATES LC TO COS SQ THETA EQUALS ZERO. PRINTS D SPACING, LC, LATTICE TYPE(S), EXTR LC

226 FORTRAN LC MUELLER,HEATON B106/CUBIC THROUGH TRICLINIC LWA
PROGRAM PERMITS THE DETERMINATION OF LATTICE CONSTANTS INCLUDING EDGES AND ANGLES FOR ALL CRYSTAL SYSTEMS USING LEAST SQUARES. PROVISION MADE FOR USING AS MANY AS THREE SEPARATE CORRECTION TERMS FOR ECCENTRICITY, ABSORPTION, ETC.-HOWEVER, ONE, TWO, THREE OR NONE AT ALL MAY BE USED. NO REITERATION IS NECESSARY.

463 FTN 1410 LC SCHAPIRO LSLAT/LS FIT OF WTED TWO THETA VALUES LWA
COV.MAT.FOR REC. EL AND STD.DEV. CELL VOL

501 FORTRAN2 LC WILLIAMS,D.E. LCR2/LATTICE CONSTANT REFINEMENT LWA
LEAST SQUARES TREATMENT OF FILM OR COUNTER DATA. ANY CRYSTAL SYMMETRY. ECCENTRICITY, ABSORPTION, AND CALIBRATION ERRORS ARE CONSIDERED.

507 FORTRAN LP BAUR PREC ANY LEVEL LWA
ANY SYMMETRY, ANY ORIENTATION OF CRYSTAL WITH RESPECT TO CAMERA. 7090

7536 FORTRAN LP GIGLIO GENERAL,FIVE KINDS OF ATOMS,PHILLIPS LNA
INDICES TRANSFORMATION,ATOMIC SCATTERING FACTORS,1620 20K,NO S FEATURES

467 FTN 1410 LP SCHAPIRO RECLP/ LP FOR XRD-5 LWA
CARD INPUT FROM DP2 OR ABS2,CARD OUTPUT FOR STAT1-4

3043 FORTRAN2 LPPREC HALL LP CORRECTIONS FOR PRECESSION METHOD LWA
GENERATES HKL AND LP FACTORS OR GIVES F AND FSQUARED FOR INPUT OF HKL AND INTENSITIES

313 FORTRAN2 LS3 P FM HAMILTON POWLS/GENERAL LS,OVERLAPPING P DATA LWA
REFINES ARBITRARY FUNCTIONS OF SF FOR POWDER DATA, E. G., SUM OF INTENSITIES OF TWO OR MORE REFLECTIONS. NON-DIAGONAL WEIGHT MATRIX CAN BE USED. USER MUST SUPPLY SUBROUTINE FOR DEFINITION OF OBSERVATIONS IN TERMS OF PARAMETERS. AVAILABLE DIMENSIONED FOR 50 OBSERVATIONS AND 20 REFINED PARAMETERS. ALSO AVAILABLE FOR 200 OBSERVATIONS AND 72 PARAMETER ALTHOUGH THE LATTER VERSION USES DIAGONAL WEIGHTS ONLY. TESTED ON 7094.

528 FORTRAN LS AT CARPENTER G BXLS/GENL SF AND LS, BLOCK DIAG. LWA
FLEXIBLE BUT SMALL SF AND LS. ADJUSTS COORDS., ISO. OR ANISO. TEMP. PARAMETERS, ATOM SCALE FACTORS, AND OVERALL SCALE FACTOR. 10 X 10 BLOCK DIAG. MATRIX. MAX. 24 INDEP. ATOMS, 36 EQUIV. POSITIONS. COMPILED AND USED ON 5K 7070.

477 FORTRAN LS AT DM TROTTER LS SQR/SFLS PROGRAM LWA
STRUCTURE FACTOR LEAST SQUARES. UP TO ORTHORHOMBIC (EXTENDABLE TO HIGHER SYMMETRIES). UP TO 60 ATOMS, 30 ANISOTROPIC. REFINES POSITIONAL AND THERMAL PARAMETERS, AND SCALE FACTOR. STANDARD DEVIATIONS, NEW BOND LENGTHS COMPUTED. IBM 704032K

390 FORTRAN LS AT FM LEVY,ELLISON* BMFLS/FTN LS,BIG MATRIX.SF,FM,AT,DSPN LPA
MODIFICATION OF XFLS, ACCESSION NO. 389. PROGRAM IS SEGMENTED TO ALLOW FOR LARGER MATRIX. AS COMPILED ON 1604A (32K), MATRIX OF ORDER 243 CAN BE USED. OTHER PROVISIONS SAME AS XFLS.

389 FORTRAN LS AT FM LEVY,ELLISON* XFLS/FTN LS. SF, FM, AT, DISPERSN LPA
MODIFICATION OF ORFLS, ACCESSION NO. 360. PROVISION FOR ANOMALOUS SCATTERING, UNLIMITED NO. OF OBSERVATIONS, INFORMATION TRANSFER TO XFOUR (AC 391), ORFFE(AC 363), ANALYZE(AC 392), EDIT(AC 393). CONDENSED OUTPUT AND SEARCH OF CORRELATION MATRIX AVAILABLE. TESTED ON 1604A. ACCOMODATES ORDER 187 MATRIX WITH 32K MEMORY.

7530 FORTRAN4 LS DM A ALBA,DOME*VAC MNQA/ANY SPACEGROUP, AT LNA
THE SAME AS MNQC FOR ACENTRIC STRUCTURES. TESTED ON 16K 7040. PARAMETERS OF ABOUT 70 ANISOTROPIC, 200 ISOTROPIC ATOMS CAN BE REFINED (WITH 16K).

7529 FORTRAN4 LS DM C ALBA,DOME*VAC MNQC/ANY SPACEGROUP, AT LNA
BLOCK-DIAGONAL LEAST SQUARES FOR CENTRIC STRUCTURES. ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTORS CAN BE TREATED. BLOCKS 4X4 OR 9X9 PLUS

ONE BLOCK 2X2 FOR SCALE AND OVERALL B. EVERYTHING IS STORED IN HIGH-SPEED MEMORY. TESTED ON 16K 7040. PARAMETERS OF ABOUT 85 ANISOTROPIC, 250 ISOTROPIC ATOMS CAN BE REFINED (WITH 16K).

7528 FORTRAN4 LS FM ALBA,DOME*VAC MNQF/ANY SPACEGROUP, AT LNA
FULL MATRIX LEAST SQUARES. ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTORS CAN BE TREATED. EVERYTHING IS STORED IN HIGH-SPEED MEMORY. TESTED ON 16K 7040. REFINES UP TO ABOUT 110 PARAMETERS (WITH 16K).

7542 FORTRAN LS PLANE DAMIANI,GIGLIO* SCHOMAKER ET AL. METHOD,1620 20K LNA

469 FTN 1410 LSSF SCHAPIRO LSSF/AT,ICA,DISPERSN,FM OR BLOCK DM LWA
VARIABLE SIZE DIAG.BLOCKS. CAN INCLUDE OVERAL SCALE IN EA BLOCK,CHANGE SF BETWEEN BLOCKS. SYMMETRY INTERNAL FOR ANY POSN IN ANY SPACE GROUP CALC.PAR.COV.MAT. AND STD.DEV. SUMS WTED ID AND ANGLES. SF SUB-PROGRAM

7022 FORTRAN N TOURNARIE 303B/POWDER DIAGRAM EXPLOITATION MWA

345 FORTRAN N,DP,2 KAY NPD AND SPECTR.IT FOR 100PART TABLE NPA
CHECKED ON 8000 WORD 704

385 FORTRAN2 N SF MAG KAY,CROMER MAGNETIC STRUCTURE FACTOR LWA
CALCULATES MAGNETIC STRUCTURE FACTORS FROM SPIN VECTORS AND ATOMIC POSITIONS FOR EACH ATOM.

5061 FORTRAN2 PATSUP ONKEN QCOMPA/MOD OF SF FOR SHIFT PAT OR SUM LWA
QCOMPA MODIFIES SF. THE OUTPUT CAN BE PROCESSED BY ERFR2.THE COEFFICIENTS ARE USED TO COMPUTE SHIFTED WEIGHTED PAT., SHARPEND PAT., SUM AND RELATED FUNCTIONS USING UP TO 100 VECTORS AND SPACE GROUP SYMMETRY.

452 FORTRAN PATSUP SIMPSON,LIPS* HASUP LWZ
USES ERFR2 BINARY OUTPUT AS INPUT. STORES ENTIRE PATTERSON MAP. COMPUTES MINIMUM FUNCTION FOR UP TO 20 VECTORS.

482 FORTRAN PI GOEBEL,WILSON INDEX CUBIC POWDER PATTERNS LWA
INDEXES POWDER PATTERNS ON CUBIC BASIS, USES MODIFIED LEAST SQUARES TO CALCULATE MILLER INDICES, LATTICE CONSTANTS, STANDARD DEVIATIONS, ERROR TERM AND FORMULA UNITS PER UNIT CELL. TESTED ON 7090. USED 5K STORAGE LOCATIONS.

483 FORTRAN PI GOEBEL,WILSON INDEX HEX AND TETRAG POWD PATTERNS LWA
INDEXES POWDER PATTERNS ON HEXAGONAL AND TETRAGONAL BASIS. USES MODIFIED LEAST SQUARES TO CALCULATE MILLER INDICES, LATTICE CONSTANTS, STANDARD DEVIATIONS, ERROR TERM AND FORMULA UNITS PER UNIT CELL. TESTED ON 7090. USES 5K STORAGE LOCATIONS.

484 FORTRAN PI GOEBEL,WILSON INDEX ORTHORHOMBIC POWDER PATTERNS LWA
INDEXES POWDER PATTERNS ON ORTHORHOMBIC BASIS. USES MODIFIED LEAST SQUARE METHOD TO CALCULATE MILLER INDICES, LATTICE CONSTANTS, STANDARD DEVIATION ERROR TERM AND FORMULA UNITS PER UNIT CELL. TESTED ON 7090. USES 5K STORAGE LOCATIONS.

481 FORTRAN PI GOEBEL,WILSON INDEX ORTHO HEX TETRAG CUBE POWD PAT NNA
INDEXES POWDER PATTERNS ON CUBIC, HEXAGONAL, TETRAGONAL, AND ORTHORHOMBIC BASIS, USES MODIFIED LEAST SQUARES TO CALCULATE MILLER INDICES, LATTICE CONSTANTS, STANDARD DEVIATIONS, ERROR TERM AND FORMULA UNITS PER UNIT CELL. TESTED ON 7090. USES 8K STORAGE LOCATIONS.

7032 FORTRAN4 PI JAMARD CTHO/CUB.TETRAG.HEX.ORTHO. POWD.INDX. LWS
CTHO MEANS CUBIC, TETRAGONAL, HEXAGONAL, AND ORTHORHOMBIC, IN WHICH SYSTEMS THE PROGRAM INDEXES POWDER DIAGRAM, GIVEN EXPERIMENTAL D/D**2 AND MAXIMUM EXPERIMENTAL ERROR IN SAME. PROGRAM CAN REJECT SOME IMPURITY LINES. TESTED ON 1107 UNIVAC

535 FORTRAN2 PI LS LC SHOEMAKER,C.B. LSCELP/INDEXES P,REFINES LC 7094 LPA
FOR ALL CRYSTAL SYSTEMS,INPUT 1/D OR THETA OBS AND
1/D CALC IN ORDER OF INCREASING 1/D

3047 FORTRAN2 PLC LAWN LS FIT FOR CUBIC CELL PARAMETER LWA
CALCULATES CELL DIMENSIONS FROM POWDER LINE POSNS.USING WEIGHTED LEAST SQUARES MODIFIED FOR NELSON-RILEY EXTRAPOLATION

7024 FORTRAN PROF TOURNARIE 306H/SIZE DISTRIBUTION WHITHOUT T.F. MPA

5074 FORTRAN PROJECTN BIEDL,SHOEMAKER DISTAN-PRO
DISTAN-PRJCTN COMPUTES THE ORTHOGRAPHIC PROJECTION ON ANY PLANE (HKL) OF AN ATOMIC STRUCTURE. IN ADDITION INTERATOMIC DISTANCES, BOND ANGLES, AND DIHEDRAL ANGLES ARE COMPUTED. (THE DISTANCE-ANGLE PROGRAM *DISTAN* WAS WRITTEN BY D. P. SHOEMAKER)

5060FORTRAN S GASSMANN 3DIMCONVOLUTION FOR BIG STRUCTURES LWA
CONVOLUTION ACCORDING TO SAYRES EQUATION (AC5,52,P.60). DEVISED MAINLY FOR PHASEDETERMINATION IN PROTEINSTRUCTURES (AC15,62,P.13) WITH MORE THAN 1000 ATOMS AND UP TO 25000 UNIQUE REFLECTIONS (IBM 7090). ALL REFLEC

TIONS ARE IN CORE STORAGE FOR MAXIMUM SPEED. PROGRAM WORKS IN ALL SPACE GROUPS. CALCULATIONS ON MYOGLOBIN HAVE BEEN PERFORMED.

7028 FORTRAN S TOURNARIE 3120/X-RAY DYNAMIC IN BENDED CRYSTAL MPA

7533 FORTRAN4 SCL TF DOME,VACIAGO WILS/WILSON PLOT LNA
THE PROGRAM PREPARES AND PRINTS OUT A WILSON PLOT FOR THE DETERMINATION OF THE SCALE FACTOR AND THE OVERALL B.

7537 FORTRAN SCL TF GIGLIO OBS INTENSITIES ON ABS SCALE,WILSON LNA

7532 FORTRAN4 SF AT ALBA,DOME*VAC FAST/ANY SPACEGROUP, UP TO 200 ATOMS LNA
GENERAL STRUCTURE FACTORS. ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTORS CAN BE TREATED. CONTRIBUTIONS TO SF FROM NEW ATOMS CAN BE ADDED (OR SUBTRACTED) TO THOSE OF THE OTHER ATOMS. TESTED ON 16K 7040. THE PROGRAM ALSO CALCULATES SCALE FACTOR AND R.

398 FORTRAN4 SFLS HARRIS,D.R. BDLSQ/AT,DISPERSN,BDM,ICA,7044 LPA
SUBSTANTIAL REVISION OF SPARKS-TRUEBLOOD-OKAYA BLOCK DIAGONAL LS FOR IBSYS WITH MAP PACKING ROUTINE. MAX 18X18 MATRIX FOR TWO ATOMS, UP TO 6 COORD AND UP TO 12 TF PARAMETERS PER MATRIX. 18X18 MATRIX FOR SCL AND FIRST 17 ISO TF. ALL SPACE GROUPS, 100 ATOMS, 2000 PLANES IN CORE.

7021 FORTRAN 2SPC N BIBIAN,TOURNARIE/323B/3 AXE SPECTROMETER SETTING MWA
SETTING DETERMINATION OF A THREE AXIS SPECTROMETER BY SIMULTANEOUS STEPS SCANNING OF SEVERAL VARIABLES IN NEUTRON INELASTIC DIFFUSION . THE SIX ANGLES ARE PUNCHED ON CARDS TO BE USED DIRECTLY BY THE COMMAND UNIT

314 FORTRAN2 SPC LP SHOEMAKER MIXG2/GEN HKL,SPECTROGON STGS,LP,ETC LPA
EXECUTIVE PROGRAM AND PACKAGE OF SUBROUTINES. SUBROUTINE INDEX GENERATES NEW HKL AND CARTESIAN COORDS OF RL POINT EACH TIME CALLED. GENERATES INDICES ASYMMETRIC UNIT ANY LATTICE ANY LAUE GROUP. INPUT IS CELL CONSTANTS TRICLINIC OR OTHER. PGM CALCULATES SETTINGS PHI CHI PSI FOR GE XRD5 SINGLE CRYSTAL ORIENTER (GONIOSTAT) OR MAY BE ADAPTED TO SETTINGS IN WEISSENBERG OR OTHER GEOMETRY. OPTIONALLY CALCULATES LP OR OTHER NEEDED DATA. COMPILED ON 32K 709, SHOULD RUN ON 8K. GENERALIZATION OF PGM 119.

522 FORTRAN2 SPC KING M V DSA2/GONIO STGS FOR CUBIC XTLS LWA
PROGRAM COMPUTES SETTINGS CHI, PHI, 2 THETA ON DIFFRACTOMETER EQUIPPED WITH GONIOSTAT FOR LAUE-INDEPENDENT REFLECTIONS OF A CUBIC CRYSTAL WITH GIVEN LATTICE PARAMETER AND WAVE LENGTH, HAVING ANY GIVEN R. L. VECTOR IN VERTICAL (CHI = 90) POSITION. AVAILABLE IN FORTRAN II AND IN BINARY FOR IBM 7094

464 FTN 1410 SPC SCHAPIRO SCO1/PHI,CHI,TWO THETAS FOR XRD-5 LWA
DATA GENERATED IN LINES WITHIN PLANES ALL OF WHICH INTERSECT IN ONE LINE

520 FORTRAN2 SPC LS HAMILTON MODE1/GONIOSTAT SETTING AND LS. LWA
CALCULATES GONIOSTAT ANGLES AND PERFORMS LEAST SQUARES ON OBSRVED ANGLES TO REFINE CELL CONSTANTS, ORIENTATION MATRIX, AND SCALE ZEROES FOR FOUR CIRCLES. PHI,CHI, AND TWO THETA CALCULATED FOR FIXED VALUE OF OMEGA WHICH NEED NOT BE ZERO. TESTED ON IBM7094.

7531 FORTRAN4 SPEC ALBA,DOME*VAC PESI/WEIGHTS FOR LS REFINEMENT LNA
THE PROGRAM ASSIGNS WEIGHTS FOR LEAST SQUARES REFINEMENT, AND PREPARES INPUT TAPE FOR MNQF, MNQC, MNQA. SEVERAL WEIGHTING SCHEMES AVAILABLE. TESTED ON 16K 7040.

505 FORTRAN SPEC BAUR MADELUNG CONSTANTS LNA
EWALD METHOD, ANY SYMMETRY, REPULSIVE AND VAN DER WAALS ENERGY(INVERSE POWER). CONTAINS SET OF SOLID ANALYTIC GEOMETRY SUBROUTINES FOR SYSTEMA TIC VARIATION OF ATOMIC POSITIONS.

5059FORTRAN R.HUBER 3DIM.CONVOLUTION MOLECULE METHOD LWA
THE PROGRAMM USES THE CONVOLUTION MOLECULE METHOD (W. HOPPE A.C. 10(1957) 750, R.HUBER A.C. (1965) IN THE PRESS)TO DETERMINE THE ROTATIONAL AND TRANSLATIONAL PARAMETERS OF A KNOWN PART OF A MOLECULE. THE PRGRAMM CONSISTS OF 3 PARTS 1.COMPUTATION OF THE STRUCTUREFACTORS OF THE CONVOLUTION MOLECULE 2. FOURIERSYNTHESIS 3.SEARCH FOR THE CORRECT MOLECULE PARAMETERS. WITH THE USE OF DATACARDS AND SUBROUTINES THE PROGRAMM WORKS WITH ALL SPACEGROUPS IN THE TRICLINIC, MONOCLINIC AND ORTHOROMBIC SYSTEMS)

7029 FORTRAN SPEC TOURNARIE 344E/MEAN MOLECULAR PLANE MPA

500 FORTRAN2 SPEC WILLIAMS,D.E. PACK2/MOLECULAR PACKING ANALYSIS LWA
CALCULATES AND MINIMIZES PACKING ENERGY AS FUNCTION OF MOLECULAR ORIENTATION, INTERNAL MOLECULAR ROTATION, AND LATTICE CONSTANTS BY STEEPEST DESCENT METHOD. ANY SPACE GROUP. CHECKED ON 20K IBM 7074.

7540 FORTRAN STAT DAMIANI,GIGLIO* DET SYM CENT,RAMACHANDRAN,SRINIVASAN LNA

7539 FORTRAN STAT DAMIANI,GIGLIO* DET SYM CENT,HOWELLS,PHILLIPS,ROGERS LNA
7538 FORTRAN STAT DAMIANI,GIGLIO* DETECTION SYMMETRY CENTRE,WILSON LNA
468 FTN 1410 STAT SCHAPIRO STAT1,2,3,4/ LWA
CALC. SCL AND DEBYE,C.D.F.,MEAN, AND VAR. OF E**2 FOR SUITABLE SUBSETS OF DATA. CALC. E,E**2,U,AND PLOT VS HKL
496 FORTRAN STAT YAKEL,H.L. ORSTAT,ORNL-TM-750/WILSON+HPR TESTS LWA
WILSON AVERAGING AND/OR STATISTICAL(HPR) TESTS FOR UP TO 3000 REFLECTIONS FORTRAN PROGRAM COMPILED AND TESTED ON IBM 7090 AND CDC 1604. AVAILABLE IN FORTRAN OR BINARY DECKS. 1604 TIME IS APPROX .5 SEC/REFL.
7031 FORTRAN4 THETA JAMARD BRAGG/GENERATOR FOR HKL,THETA,D,ETC. LWS
GIVEN UNIT CELL (ANY SYSTEM) AND WAVELENGTH, GENERATES HKL, THETA, D, Q(HKL) = U/D**2, IN ORDER OF INCREASING THETA. TAKES INTO ACCOUNT EXTINCTION RULES. TESTED ON 1107 UNIVAC.
533 FORTRAN2 TF SRIVASTAVA,SHO* VIBELL/ ANISO TF LPA
INVERTS AND DIAGONALIZES THERMAL MATRIX GIVING PRINCIPAL DIRECTIONS AND VIBRATIONAL AMPLITUDES. ALL NECESSARY INSTRUCTIONS ON COMMENT CARDS (NO SEPARATE WRITE-UP).
TESTED ON IBM 7090.
3042 FORTRAN2 THETA HALL CRYSTAL-COUNTER ORIENTOR LWA
HKL, TWO THETA, PHI, SIN THETA AND SIN TWO THETA ARE GENERATED FROM THE CELL DIMENSIONS

PROGRAMS LISTED UNDER ACTUAL MACHINE DESIGNATIONS

3053 ATLAS 2CDIR DARLOW J V LPA
USES STRUCTURE INVARIANTS METHOD WITH PROBABILITIES TO OBTAIN FROM LIST OF TRIPLE PRODUCTS POSSIBLE SETS OF SIGNS, EACH WITH A NUMBER GIVING THE ORDER OF PROBABILITY.
3052 ATLAS CONTOUR DOLLIMORE INCLUDED IN FR ABOVE LWA
3049 ATLAS FR DOLLIMORE SPACEGROUPS 1-74 NOT 43 OR 70 LWA
3070 ATLAS DP DIA, DREW FIFI/ DATA RECUD. WEISSENBERG
PART OF SYSTEM ATSYS (Q. V.)
STORES OUTPUT ON MAGNETIC TAPE.
3071 ATLAS DP DOL, DREW PLIP/ DATA REDUC. PRECESSION
PART OF SYSTEM ATSYS (Q. V.)
STORES OUTPUT ON MAGNETIC TAPE.
3075 ATLAS DP DREW KIKI/STORES DATA MAG TAPE
PART OF SYSTEM ATSYS (Q.V.)
STORES DATA ON MAG TAPE DIRECTLY FROM PLANES LIST ON 5-HOLE TAPE. WILL ALSO OUTPUT DATA ON CARDS FOR BUSING-LEVY 7090 LS AND THE X-RAY 63 SYSTEM
3067 ATLAS DP DREW MANIPULATION OF UP TO 3 DATA LISTS
ACCEPT UP TO THREE LPID DATA LIST
COMPARES COMMON REFLECTIONS, CORRELATES OR CALCULATES SCALES AND APPLIES THEM
3073 ATLAS DP DREW POLO/ SCALE ON DIFFERENT AXES
PART OF SYSTEM ATSYS (Q. V.)
SCRUTINIZES AND SCALES DATA ON TWO OR MORE AXES, TO FORM COMPLETE PLANES LIST. INCLUDES LS PROCEDURE FOR SCALING.
3059 ATLAS F DP MOORE,SHEFTER DP WITH INTERLAYER SCALING NNN
3074 ATLAS FR HARD, DREW PEPE/ FOURIER
PART OF SYSTEM ATSYS (Q. V.)
UP TO MONOCLINIC AND MANY ORTHORHOMBIC, THE REST EASIOY ADDED.
3058 ATLAS F FR SF C MOORE 3D FOURIER WITH CENTRIC SF CALC NNN
3077 ATLAS ID DIA, DREW ELSI/ DISTANCE AND ANGLE PGM
PART OF SYSTEM ATSYS (Q.V.)
CALCULATES BOND DISTANCES AND ANGLES, ALSO STANDARD DEVIATIONS.
3051 ATLAS ID DOLLIMORE INCLUDES BOND ANGLES LWA
3066 ATLAS ID E DREW DIST,ANGLS,S.D OF BOTH,ANY SYM,TRANS LWA
3063 ATLAS F ID JMS,SHFTER,MORE LS PLANE INCLUDED NNN
3072 ATLAS LC DIAMAND LSCD/ LS FIT POWD OR S.C. DATA
PART OF SYSTEM ATSYS (Q. V.)
CALCULATES LEAST SQUARES FIT ON POWDER OR SINGLE CRYSTAL DATA TO GIVE ACCURATE CELL DIMENSIONS. APPLICABLE TO ALL CRYSTAL CLASSES.
3056 FORTRAN LS E FARRAR FOR1/ HEX TET COHN LS ERROR TEST LPA
USES DIFFRACTOMETER, FILM DATA. CALCULATES LS USING COHEN LS METHOD WITH

WEIGHTING FACTOR, PERFORMS ERROR TEST ON EACH LINE. REJECTS ON INSTRUCTION. REPEATS LS ANALYSIS. UP TO 50 DIFFRACTION LINES SUITABLE FOR HEX OR TET. COMPILED ON 1620 60K AUTO-DIVIDE.

3057 ATLAS F LS LC BRACHER FORTRAN INPUT HKL AND THETA LDA

3064 ATLAS LS LC DIAMAND HKL PLUS FUNCTION OF THETA LWA

3076 ATLAS LS SF DIA, DREW BABA/ BLOCK DIAG LS
PART OF SYSTEM ATSYS (Q. V.)
SIMILAR TO ROLLETT MERCURY PROGRAM. BLOCK DIAG., MIXED ISOTROPIC AND ANISOTROPIC REFINEMENT.

3061 ATLAS F PATSUP MOORE BUERGER MINIMUM FUNCTION NNN

3078 ATLAS PLANE SPARKS, HUNT DIDO/ LS PLANE THRU GROUP OF ATOMS
PART OF SYSTEM ATSYS (Q.V.)
CALCULATES WEIGHTED LEAST-SQUARES PLANE THRU GROUP OF ATOMS.

3055 ATLAS ROTN FN HARDING ROTATION FUNCTION MPA
ROSSMANNS FUNCTION, ROTATES WEIGHTED RECIPROCAL LATTICE ON SELF, OR ON THAT OF SECOND CRYSTAL, AND EVALUATES COINCIDENCE. AUTOCODE.

3050 ATLAS SF DOLLIMORE MAY SUBDIVIDE POSITIONS LIST LWA

3054 ATLAS SF + FR HARDING FOURIER 7.8/WITH STRUCTURE FACTORS MPA
3D FR,BL SUMMATION, ANY MONOCLINIC SPACE GROUP, ORTHORHOMBIC ON REQUEST. MAY BE PRECEDED IN SAME RUN BY MODIFICATION OF F OR BY SF CALCULATION AND SELECTION OR WEIGHTING OF FO - AGREEMENT ANALYSIS GIVEN. LANGUAGE EMA.

3065 ATLAS SFLS DM DIAMAND MIXED REFINEMENT

3060 ATLAS F SFLS DM JMS,SHFTER,MORE BLOCK DIAGONAL NNN

4014 ATLAS 2SFRFRDF DARLOW J V,MAIN,DARLOW S F*/ LWA
CALCS SF. SCALES WITH F OBS USING ALL OR OUTER ONLY REFLEXIONS. GIVES R FOR ALL AND/OR OUTER TERMS. CALCS FR(OBS) AND/OR FR(CALC) AND/OR DF USING INNER, OUTER, OR ALL TERMS, ANY OR ALL OF 9 COMBINATIONS POSSIBLE, UNIQUE AREA ONLY. ANY DIVISION ALONG EACH AXIS. ANY SECTION OF PROGRAM MAY BE USED BY ITSELF. 2D ONLY.

3079 ATLAS SPEC DIAMAND DIAN/ DIHEDRAL ANGLES
PART OF SYSTEM ATSYS (Q. V.)
CALCULATES DIHEDRAL ANGLES, ETC. USEFUL FOR MODEL BUILDING.

3062 ATLAS F STAT MOORE WILSON PLOT NNN

3069 ATLAS SYSTEM DREW ATSYS/ ATLAS CRYSTALLOGRAPHIC SYSTEM
SEE UNDER ATSYS (SYSTEMS)

517 B 5000 LS FM GALLAHER/KAY TRANSLATION OF ORFLS LPA
TRANSLATION OF PROG.360 TO EXTENDED ALGOL FOR B 5000 (32K)

7018 BULL GET LP BASSI L AND LP CALC,SIN SQUARE THETA LWA
CALC. L AND LP FACTORS AND SINUS SQUARE THETA

7016 BULL GET LS BASSI LS.DM.64 PARAMETERS MAX LWA
LEAST SQUARES REFINEMENT, DM, 64 PARAMETERS MAXIMUM. NO TEMPERATURE FACTOR.

7017 BULL GET SF LP BASSI SF OR INTENSITIES,LP, N OR XRAYS LWA
SF OR INTENSITIES CALCULATIONS, N OR X RAYS, L OR LP FOR POWDERS, ALMOST ALL SPACE GROUPS. 16 ATOMIC POSITIONS MAX, 4096 ATOMS PER UNIT CELL MAX. LF PEPINSKY APPROX.

7015 BULLGAET D LP LF LAB.CALC.CNRS D,LP(WEIS,P,..),LF LWA
TRICLINIC. CALCULATES 1/D, L, AND LP FACTORS (N OR X RAYS)
FOR POWDERS, WEISSENBERG,.... CALCULATES LF LINEAR INTERPOLATION

5016 BULLGAET DP EXT IITAKA EXTINCTION COR FOR STRONG REFLECTION LWA
CORRECT F FOR EXTINCTION ASSUMING DARWINS EQ.I*=I/1'GI.WHERE I IS I OBS. G IS FOUND FOR THE GIVEN STRONG REFLECTIONS AND CALCULATES I* AND F FOR THE PLANES.

5017 BULLGAET DP TF IITAKA WILSON PLOT FINDS SCL AND TF LWA
GIVES DATA FOR WILSON PLOT. TF AND SCL FAC. IS CALCULATED BY LS IF THE WEIGHT FOR EACH ZONE IS ASSIGNED.

7013 BULLGAET FR 2 LAB.CALC.CNRS FOURIER SYNTHESIS 2 DIM. LWA
FOURIER SYNTHESIS 2 DIMENSIONS. STEPS FROM 1/100

5019 BULLGAET H 2THETA IITAKA LIST H,2THETA ETC IN A GIVEN REGION LWA
LISTS HKL,MULTIPLICITY,SIN THETA BY LAMDASQ.,2THETA ETC FOR THE PLANES WITHIN A GIVEN 2THETA MAX. HKL IS IN A DEFINITE ORDER EXCL.ABSENT REFLECTIONS.CALCULATION ONLY FOR ANY GIVEN ZONE OR A LAYER OR AN AXIS IS POSSIBLE.

5023 BULLGAET ID IITAKA ID BET GIVEN ATOMS ALSO BOND SEARCH LWA
ANY SYM.OPERATION INCLUDING LATTICE TRANSLATIONS,DEFINED FOR PARTICULAR SPACE GROUP IS APPLIED FOR ANY ATOM (IN ASYM UNIT). DISTANCES AND

ANGLES BETWEEN ANY SPECIFIED (OR NOT SPECIFIED) ATOMS ARE CALCULATED. IN ANGLE CALCULATION, IT IS POSSIBLE TO FIX ONE ATOM AS CENTER AND CALCULATE ALL POSSIBLE DISTANCES AND ANGLES AROUND IT.

5021 BULLGAET LC IITAKA FOR ALL XTL SYS BY LS INCL 3 SYST ER LWA
FINDS RECIPROCAL LATTICE CONST.(MAX 6 PARAMETERS) BY LS METHOD BASED ON INDEXED 2THETA OBS BY POWDER OR SINGLE TAKEN BY ANY WAVELENGTH. INDIVIDUAL WEIGHT FOR EACH OBS CAN BE PUT. SYSTEMATIC ERRORS UP TO 3 KINDS ARE INCLUDED. HKL, 2THETA OBS AND CAL TABLE IS PRINTED.

5020 BULLGAET LC TRANS IITAKA TRANSFORM LC IN BOTH DIRECTIONS LWA
GIVES BOTH CELL VOLUMES AT THE SAME TIME.

5018 BULLGAET LP,ABS IITAKA WEIS PREC FOR ANY LAYER,XTL SETTING LWA
WEIS., RETIGRAPH,OSC AND PREC. PHOTO CAN BE TREATED FOR ANY METHOD OF TAKING PHOTO,ANY CRYSTAL SETTING (AXIS) AND FOR ANY LAYER LINE. ABSORPTION CORRECTION BY INTERPOLATING THE STORED TABLE AND CAN BE APPLIED FOR SPHERICAL AND CYLINDRICAL SPECIMENS.

5015 BULLGAET LS 3 IITAKA TRI,MONO,ORTH,C,DM,ISOTF.EACH ATOM LWA
REFINES FOR F SQ.ALL DATA ARE STORED IN THE MACHINE.USES WEIGHTS BY HUGHES SYSTEM. THE WEIGHT CAN BE MODIFIED BY A FACTOR GIVEN BY EACH INPUT PLANE CARD. THE SHIFTS XYZB FOR EACH ATOM AND OVERALL SCALE FACTOR ARE OBTAINED BY DIAGONAL APPROX.THEY ARE MULTIPLIED BY GIVEN DAMPING FAC. (XYZ AND B SCL SEPARATELY). AT THE END OF EACH CYCLE SHIFTS,E.S.D.S, R ETC ARE LISTED. SPEED FOR TRI. 0.5N+0.28J+1.5 SEC/PLANE.N ATOM J KIND.

5024 BULLGAET PERP. D IITAKA FIND BEST PLANE,CALC. PERPENDIC. D LWA
TRICLINIC CASE. FINDS THE BEST PLANE THROUGH A GIVEN SET OF ATOMS BY LS METHOD AND CALCULATES THE PERPENDICULAR DISTANCES FROM ANY GIVEN ATOM. THE COEFFICIENTS OF THE EQUATION OF THE BEST PLANE ARE GIVEN WHICH ARE PROPORTIONAL TO THE MILLER INDICES OF THE PLANE.

7014 BULLGAET SF 2 3 LAB.CALC.CNRS SF DIRECT SUMMATION LWA
SF BY DIRECT SUMMATION, GIVEN COORDINATES OF EACH ATOM, HKL SET , AND LF. 1000 ATOMS, MAX VALUE OF H (OR K OR L) 100

5022 BULLGAET SF 3 FR2 IITAKA TRI MONO ORTH C FOLLOWED BY FR PROJ LWA
ISO. TF FOR EACH ATOM KIND. DATA FOR ANY FR OR DIF FR PROJ. ARE STORED DURING SF CAL. BUT SF INPUT IS FOR UNIQUE REF. R FAC. ETC ARE LISTED. FR CAL. CAN START AFTER SF FOR ANY PART OF THE CELL WITH ANY INTERVAL. OUT PUT PERMITS DIRECT CONTOURING. SF SPEED FOR TRI. 0.06N+0.52J+3 SEC/ PLANE. N ATOM J ATOM KIND.

7012 CAB 500 ID CNRS BELLEVUE ID,BOND ANGLES,TRICLINIC,ORTHORHOMB. LWA
INTERATOMIC DISTANCES AND BOND ANGLES FOR TRIPLETS OF ATOMS IN TRICLINIC AND ORTHORHOMBIC SYSTEMS

7004 CAB 500 LF 1/D2 CNRS BELLEVUE CALC LF,1/D SQUARE ALL SYSTEMS LWA
CALCULATES 1/D SQUARE AND LF, ALL SYSTEMS, HKL SET AND LF VALUES FOR DISCRETE VALUES OF 1/D BEING GIVEN. LF BY LINEAR INTERPOLATION

7011 CAB 500 LP CNRS BELLEVUE LP CALC,WEIS EQUI-INCL.H.ALL SYSTEMS LWA
IN ALL SYSTEMS, GENERATES HKL LIMITED BY REFLECTION SPHERE. FOR EACH HKL, GIVES 1/D SQUARE, AND LP FOR WEIS EQUI-INCL.

7002 CAB 500 LS 2 CNRS BELLEVUE LS 2 FOR DIFFERENT PLANE GROUPS.DM LWA
ONE PGM OF LS REFINEMENT FOR EACH OF PLANE GROUPS P2, PGG, PMG, CMM, PMM. REFINES ATOMIC COORDINATES, ISOTROPIC TF (THE SAME FOR ALL ATOMS), AND SCALE FACTOR. DM. MAX NUMBER OF ATOMS UNRELATED BY SYMMETRY 20. MAX NUMBER OF REFLECTIONS 300. 10 DIFFERENT ELEMENTS MAX.

7001 CAB 500 LS 3 CNRS BELLEVUE LS 3 FOR P212121 SPACE GROUP.DM LWA
LS REFINEMENT FOR P212121 SPACE GROUP, ON THE ATOMIC COORDINATES OF 20 INDEPENDENT ATOMS MAX. 300 REFLECTIONS MAX. LFS PROPORTIONAL TO A UNIQUE LF. DM.

7006 CAB 500 SCL TF CNRS BELLEVUE SCL AND TF WILSON METHOD LWA
SCALE AND TEMPERATURE FACTORS BY WILSON METHOD. 1400 VALUES OF EXPERIMENTAL INTENSITIES MAXIMUM.

7007 CAB 500 SF 2 CNRS BELLEVUE CALC SF 2 FROM AT.COORD. OF EACH AT. LWA
CALCULATES SF 2 FROM ATOMIC COORDINATES OF EACH ATOM, HKL AND CORRES-PONDING LFS BEING GIVEN. 40 ATOMS MAX. (OR 80 IF CENTERED). 4 DIFFERENT ELEMENTS MAX.

7009 CAB 500 SF 2 3 C CNRS BELLEVUE SF 2 3 TRICL C WITH ISOTROPIC TF LWA
CALCULATES SF 2 OR 3 FOR TRICLINIC CENTERED CELL. ISOTROPIC TEMPERATURE FACTOR IF NEEDED. HKL SET, 1/D SQUARE, AND LFS ARE GIVEN FROM ANOTHER PROGRAM.

7008 CAB 500 SF 3 CNRS BELLEVUE CALC SF 3 FROM AT.COORD. OF EACH AT. LWA

CALCULATES SF 3 FROM ATOMIC COORDINATES OF EACH ATOM, HKL AND CORRESPONDING LFS BEING GIVEN. 100 ATOMS MAX. (OR 200 IF CENTERED). 4 DIFFERENT ELEMENTS MAX.

7010 CAB 500 SF 3 C CNRS BELLEVUE SF 3C WITH INDIVIDUAL ISOTROPIC TF LWA
CALCULATES SF 3 FOR CENTERED CELL. ISOTROPIC TEMPERATURE FACTOR FOR EACH ATOM, IF NEEDED. HKL SET, 1/D SQUARE, AND LFS ARE GIVEN FROM ANOTHER PROGRAM.

7005 CAB 500 SPEC CNRS BELLEVUE F OBS FROM OPTICAL DENSITIES LWA
CALCULATION OF F OBSERVED AS SQUARE ROOT OF OPTICAL DENSITIES CORRECTED WITH LP FACTORS

7003 CAB 500 SPEC CNRS BELLEVUE NORMALIZES INTENSITIES FROM N FILMS LWA
PUTS ON THE SAME SCALE INTENSITIES FROM N FILMS. N MAX = 12. GIVES FOR EACH REFLECTION THE N VALUES ON SCALE OF FIRST FILM AND MEAN VALUE.

7526 CEP SF C AT GUERRI,BERTOLUZ MIN SF/ LWS

7527 CEP SF C 2 GUERRI,BENVENUT MIN F/ LWS

6008 DASK K2 FR 2 3 LARSEN F DASK 330D/GENL FR 3 DIM LWA
3-DIM FR PGM APPLICABLE TO ANY SPACE GROUP.
STRAIGHT OR DIFFERENCE FR AND BOUNDED PROJECTIONS POSSIBLE.

6009 DASK K2 SF MONDRUP DASK 330/GENL SF LWA
SF PGM, ANISOTROPIC TF, USES TRICLINIC FORMULAE.

4023 DEUCE DP SIME/SPEAKMAN LP TUNNELL CORR FOR WEISSENBERG MWA
P014/EQUI-INCLINATION WEIS DATA FOR A TRICLINIC CRYSTAL ARE CORRECTED FOR LP TUNNELL FACTORS. BASIC DEUCE GIVES 50 PLANES PER MINUTE. OUTPUT SUITABLE FOR ROLLETT SF SFLS FR PGMS.

4028 DEUCE FR ROLLETT/PETERS FR/3D BL GENL MWA
ALL SPACE GROUPS BUT MUST SUM OVER ALL REFLECTIONS WITH NON-NEGATIVE INDICES. NO LIMIT ON REFLECTIONS, SECTIONS MUST BE DONE IN PARTS IF MORE THAN 60 BY 80 POINTS. INTERVALS N/240.

4021 DEUCE FR 2 SIME/SPEAKMAN ELECTRON DENSITY IN GENERAL PLANE MWA
P028,029,030/PROGRAM COMPUTES FOURIER SECTION AT A GENERAL PLANE THRU A MONOCLINIC CELL USING THE METHOD OF TREUTING AND ABRAHAMS ACTA CRYST. 14, 190.

4049 DEUCE FR 3 DF SIME/SPEAKMAN DIFFERENTIAL SYNTH NPX

4020 DEUCE ID SIME/SPEAKMAN BOND LENGTH AND ANGLE MWA
P031,032/BOND LENGTHS AND ANGLES CALCULATED FOR UP TO 128 ATOMS AND CAN GENERATE FROM THESE TWELVE RELATED SETS OF 128 ATOMS.

4025 DEUCE PLANE WATSON/SPEAKMAN MEAN MOLECULAR PLANE DETERMINATION MPX
P069/ALPHACODE PROGRAM DETERMINES BEST PLANE THROUGH A SET OF ATOMS BY METHOD OF SCHOMAKER, ACTA CRYST. 12, 600. ATOMS CAN BE GIVEN ANY WEIGHT FOR THE LEAST SQUARES PROCESS. DISTANCES OF ALL ATOMS FROM THIS PLANE ARE ALSO OBTAINED.

4022 DEUCE R SCL SIME/SPEAKMAN SCALE AND DISCREPANCY FACTOR MWA
P019/BASIC DEUCE, SCL AND R FROM ROLLETT STYLE SF OUTPUT.

4029 DEUCE SF ROLLETT/PETERS SF/3D GENL ISOTROPIC MWA
ALL SPACE GROUPS NO LIMIT ON REFLECTIONS. PARAMETERS, F SCALE, POSITIONS, ISOTROPIC B FACTORS, CHEMICAL TYPES. UP TO 1664 ATOMS OF 16 TYPES.

4030 DEUCE SF LS ROLLETT/PETERS LS/3D BLOCK DM AT GENL MWA
ALL SPACE GROUPS, NO LIMIT ON REFLECTIONS. PARAMETERS, F SCALE, POSITIONS, ANISOTROPIC B FACTORS, CHEMICAL TYPES. UP TO 64 ATOMS OF 16 TYPES.

4024 DEUCE T/OMEGA SIME/SPEAKMAN CRUICKSHANK THERMAL ANALYSIS ACTA 9 MWX
P036,037,038,039/ALPHACODE AND GIP MONOCLINIC THERMAL ANALYSIS PGM. 1) TRANSFORMS COORDINATES, TEMP FACTORS TO ORTHOG MOLECULAR AXES. GIVES VALUES OF U SUB IJ FOR EACH ATOM (ACODE). 2) FORMS LS NORMAL EQTNS FOR DETN OF T AND OMEGA (ACODE). 3) INVERTS MATRIX, SOLVES FOR T AND OMEGA (GIP7). 4) DETERMINES STANDARD DEVIATIONS (ACODE).

5073 ER 56 ABS THURN ABSORB/WEIS,IRREG POLYHEDR CRYSTAL LWA
IT LC, EQU OF CRYST LIMITING PLANES, SF, OT CORRECTED SF

5007 ER 56 FR 2 THURN GENL, VARIABLE GRID, H, K UP TO 19 LWA
NEEDED FOR IT -- ABSOL VALUES OF STRUCT AMPLITUDES, PHASE ANGLES

5004 ER 56 FR 2 C KRUECKEBG,BERG. 2DIM ALL CENTROSYM SPACE GROUPS LPA

5005 ER 56 ID MATTES DIST. ANGLES BETWEEN SELECTED ATOMS LWA
ANY SYMMETRY. DISTANCES AND BOND ANGLES BETWEEN SELECTED ATOMS

5003 ER 56 LC BY LS SCHMID STRUCTUR E/ REFINEMENT OF LC BY LS LWA
GILT FUER ALLE KRISTALLKLASSEN. IT. WELLENLAENGE UND (UNGENAUE

LC ODER KOEFFIZIENTEN DER QUADRATISCHEN FORM) SOWIE (THETA ODER 4XTHETA ODER SINUSQUADRAT THETA) UND KENNZIFFER FUER KRISTALLKLASSE. OT. VERBESSERTE KOEFF. DER QUADR. FORM, E, LC VERBESSERT, (SINQUADRAT THETA FUER GEGEBENE (HKL)) GEMESSEN UND MIT NEUEM LC BERECHNET. BIS 200 THETAWERTE ZUGELASSEN.

5006 ER 56 LP WEIS MATTES WEIS LP FOR ANY LEVEL LWA
CALC OF SF, SQUARE OF SF, SIN THETA FROM EQUIINCLINATION WEIS'DATA

5001 ER 56 THETA+SF SCHMID STRUC. A/IN MILLER INDICES ARRANGED LWA
SINQUADRAT THETA UND KOMPLEXER SF FUER ALLE KRISTALLSYSTEME 3'DIM. BIS ZU 200 ATOME AUS 10 VERSCHIEDENEN ATOMSORTEN JE ELEMENTARZELLE ZUGELASSEN. AUSGABE IN LEXIGRAPHISCHER ANORDNUNG DER MILLER INDICES

5002 ER 56 THETA+SF SCHMID STRUCTUR B/ARRANGED INCREASING THETA LWA
FUER MONOKLINE UND HOEHERE SYMMETRIE ERHAELT MAN SINQUADRAT THETA, THETA UND KOMPLEXEN SF, DER GROESSE VON THETA NACH GEORDNET. BIS ZU 200 ATOME AUS 10 VERSCHIEDENEN ATOMSORTEN JE ELEMENTARZELLE SIND ZUGELASSEN. ERFASST WERDEN DIE MILLERINDICES H='9(1)+9, K=0(1)9, L=0(1)9.

6020 FACIT 2K ABS WERNER ABSP/PREC 3, XTALS OF ARBITR SHAPE LWA
AS ABSW FOR FACIT EXCEPT THAT CALC TIME IS C. N*M**3*0.018 SEC PER REFL

6019 FACIT 2K ABS WERNER ABSW/WEISS 3, XTALS OF ARBITR SHAPE LWA
CALULATES ABS FACTORS AND CORRECTS INTENSITIES. GAUSS METHOD FOR NUMERICAL INTEGRATION. N (MAX. 14) XTAL SURFACES. M**3 VOLUME ELEMENTS TO BE CHOSEN SO THAT M**3* (N+1) IS LESS THAN 8000. INPUT IS EQN. FOR - OR COORDINATES FOR THREE POINTS IN - EACH XTAL SURFACE, CELL DIMENSIONS, LINEAR ABSORPTION COEFFICIENT, WAVE LENGTH, HKL AND OBSERVED INTENSITIES. ABOUT N*M**3*0.009 SEC PER REFLECTION.

6029 FACIT 2K ABS-EXT WERNER ABSG/SEC EXTINCTION AND ABS MPA
GE SINGLE XTAL DIFFR DATA. AS ABSP FOR FACIT EXCEPT THAT CALCS. FOR SEC EXTINCTION CORR ARE INCLUDED. ABSG USES RESULT FROM PGM GALPI FOR FACIT

6034 FACITAGL DP NORRESTAM AUTO-GALPI/LP,WEIGHTS ETC. MPA
PGM GALPI MODIFIED FOR HANDLING RESULT FROM G.E. AUTOM. SINGLE XTAL DIFF.

6033 FACITAGL DP NORRESTAM GALPI/LP, WEIGHTS ETC. LWA
PGM CALCULATES LP, STATISTICAL WEIGHTS AND DIRECTION COSINES OF X-RAYS FOR G.E. MANUAL SINGLE X-TAL DIFFRACTOMETER RESULT. ANY SYMMETRY. 2THETA-THETA SCAN. RESULT USED BY PGM ABSG FOR FACIT

6030 FACITAGL E ASB/NORRESTAM STINTA/E IN ID LPA
PGM CALCULATES E IN ID FROM E IN COORDS AND LC FOR ANY SYMMETRY. ALL ATOMS ARE TREATED AS INDEPENDENT. USES RESULT FROM MODIFIED PGM VINTER-2

6014 FACIT FR 2 3 LIMINGA,OLOVSON PROFFS/ANY SYMM,GRID.REFL ANY ORDER. LWA

6016 FACIT ID LIMINGA,OLOVSON VINTER/DIST,ANGLES.ANY SYMMETRY. LWA

6026 FACIT 2K LF WESTMAN AFFE/LS FIT POLYNOM(SIN THETA)=LOG LF MPA

6017 FACIT LP WERNER PREC, LP FOR ANY LEVEL, H LWA

6024 FACIT 2K LP WESTMAN,ASBRINK LOPPA/LP OF INTENSITIES FROM WEIS MPA

6023 FACIT LS ASBRINK,BRANDEN LS/BLOCK-DM APPR,LAYER SCLS,ISOTR TFS LWA
SFLS (OR SF) PGM FOR ORTHORH SYMM AND LOWER. PGM REFINES F BY SHIFTING LAYER SCALEFACTORS COUPLED IN A MATRIX WITH AVERAGE VIBRATION PARAMTR, AND BY SHIFTING ATOMIC COORDS AND INDIV ISOTR VIBR PARAMTRS USING BLOCK DIAG MATRIX APPROXIMATION. PGM USES LF TABLES, PROVIDES THREE DIFFERENT WEIGHTING SCHEMES, HAS ACCELERATION DEVICES AND MAKES WEIGHT ANALYSIS. ACCIDENTALLY ABSENT REFLS, IF INCLUDED, ARE TREATED SEPARATELY.

6027 FACIT 2K P WERNER PR1/PI APPR KNOWN PTRN, REFINES LC LWA

6028 FACIT 2K P WERNER PR2/PI TRIAL-AND-ERROR,ORTHORH SYMM LWA

6015 FACIT SF H LIMINGA,OLOVSON STRIX/CALC SF+H FOR FR IT.ANY SYMM. LWA

6035 FACIT SFLSFMCS LUNDBERG,B.K.S. ROHAP/REF.OF PARAM.ISOM.REPL. PROT. LPA
METHOD DESCRIBED IN ACTA CRYST. (1965) 18, 576. SOON IN FORTRAN.

6032 FACITAGL SPC NORRESTAM AUTO-GIP/SPC GONIOSTAT MPA
PGM GIP MODIFIED FOR STEERING G.E. AUTOMATIC SINGLE XTAL DIFFRACTOMETER USING 2THETA-THETA SCAN. SCAN INTERVAL CALCULATED AS FUNCTION OF THETA

6031 FACITAGL SPC NORRESTAM GIP/SPC GONIOSTAT LWA
SPC FOR G.E. MANUAL SINGLE XTAL DIFFRACTOMETER. ANY SYMMETRY. H IN DESIRED OCTANT. EXTINCTION CONDITIONS MAY BE SPECIFIED

6513 LGP30 D LINEK*NKB FOR THETA INTERPOLATE IN TABLES NPA
INPUT ARBITRARY TABLES, LATTICE CONSTANTS. OUTPUT VALUES OF PHYSICAL FUNCTIONS FROM TABLES FOR EVERY HKL.

1 LGP30 DP KOENIG M-13 100/AVG WEISS OR PREC DATA, LP LWA

3 LGP30 FR 2 A KOENIG M-13 102/BL 1/64 ACENTR LWA
2 LGP30 FR 2 C KOENIG M-13 101/BL 1/64 CENTRO LWA
6512 LGP30 ID LINEK*NKB GENERAL FORMULA LWA
3514 KDF9 AUT A-C TEST HAMOR ACENTRIC-CENTRIC STATISTICAL TEST LWA
STATISTICAL TEST FOR CENTER OF SYMMETRY BY METHOD OF HOWELLS, PHILLIPS, AND ROGERS. TREATS HKL,HKO,HOL,OKL DATA SEPARATELY. AXIAL REFLECTIONS OMITTED. INPUT AS FOR ROLLETT SF LS PROGRAM.
3516 KDF9 AUT DP HAMOR,WATKIN LP TUNNELL CORR FOR WEIS DATA LWA
OT SUITABLE FOR ROLLETT SF LS PROGRAM. PROGRAM ALSO AVAILABLE TO CONVERT THIS OT TO FORM SUITABLE FOR CRUICKSHANK,SIME ALGOL PROGRAMS.
3517 KDF9 AGL FR 3 SIME GEN FR ALL SG INCL CONTOUR OT MPA
3518 KDF9 AGL ID MUIR,MCGREGOR MPA
3515 KDF9 AUT ID WATKIN,HAMOR INTRA-,INTER-MOLEC DIST AND ANGLES LPA
GIVEN ATOMIC COORDS AND EQUIVALENT POSITIONS (TRICLINIC,MONO, OR ORTHO) CALCULATES ALL INTRAMOLECULAR DISTANCES BELOW GIVEN LIMIT, AND INTER-MOLEC DISTANCES BELOW SECOND GIVEN LIMIT. ANGLE CALC. DETERMINED BY SAME LIMITS.
3513 KDF9 AUT PLANE HAMOR BEST PLANE THROUGH SET OF POINTS LWA
EQUATION OF PLANE THRU SPECIFIED POINTS SELECTED FROM INPUT COORDS CALCULATED BY METHOD OF SCHOMAKER ET AL, AND BLOW. OT INCLUDES DEVIATIONS OF SPECIFIED POINTS FROM PLANE, MEAN AND RMS DEV AND DIST OF OTHER POINTS FROM PLANE.
3512 KDF9 AGL SFLS CRUICK,SMITH JG ALL SG,AT,DISPERSIN,SCLS,DM OR FM,E MPA
4011 MERCURY DIRC WOOLFSON WOOLFSONS FOLLY/ LPA
DATA - SIGN RELS IN FORM OF TRIPLE PRODUCTS.
OUTPUT - ALL SETS OF SIGNS FOR WHICH SIGN RELS ARE VALID WITHIN PRESCRIBED LIMITS.
METHOD - AS DESCRIBED IN ACTA CRYST 10, 116.
TIME - DEPENDS ON PRESCRIBED LIMITS. (SEE ALSO PGM 4002, FOR 704.)
4031 MERCURY DP LAI/ROLLETT CORRELATE F-SQUARED LPA
GIVEN F-SQUARED FROM 2 SETS INTERSECTING LAYERS AND SCL FACTORS, PRODUCES AVERAGED DATA ON COMMON SCALE.
4038 MERCURY DP MAIR/ROLLETT CORRELATE AND SORT MWA
GIVEN F-SQUARED FROM 2 SETS INTERSECTING LAYERS AND SCL FACTORS, PRODUCES AVERAGED DATA ON COMMON SCALE. ANSWERS CAN BE SORTED BEFORE OUTPUT.
4032 MERCURY DP ROLLETT SORT HKL DATA MPA
GIVEN HKL DATA IN RANDON ORDER, PROVIDES DATA SORTED INTO ANY DESIRED ORDER OF INDICES.
4039 MERCURY E MAIR/ROLLETT BOND LENGTHS AND STANDARD DEVIATIONS
GIVEN POSITION AND VARIANCE MATRIX OUTPUT FROM 3-D LS, FINDS BOND LENGTHS AND THEIR STANDARD DEVIATIONS.
6002 MERCURY FR 2 KEILHAU NDRE-R2280/COSCOS OR SINSIN VERSION LWA
COMPUTES 2-DIM FR AS A SUMMATION OVER F (HKL) COSCOS-
OR F (HKL) SINSIN-TERMS ONLY. SPEC CASE OF PGM NDRE-R2281.
AXES SUBDIVISION 1/60. INPUT PGM NDRE BIP.
6003 MERCURY FR 2 KEILHAU NDRE-R2281/COSCOS + OR - SINSIN VERSN LWA
COMPUTES 2-DIM FR AS A SUMMATION OVER (A(HKL) COSCOS + OR -
B (HKL) SINSIN) TERMS. AXES SUBDIVISION 1/60. INPUT PGM NDRE BIP.
6004 MERCURY FR 2 KEILHAU NDRE-R2282/PLANE GROUPS 7,8 AND 12 LWA
COMPUTES 2-DIM FR AS A SUMMATION OVER A(HKL) COSCOS TERMS WHEN Q IS EVEN, B (HKL) SINSIN TERMS WHEN Q IS ODD, Q BEING H OR K OR H+K.
AXES SUBDIVISION 1/60. INPUT PGM NDRE BIP.
6005 MERCURY FR 2 KEILHAU NDRE-R2284/GENERAL VERSION LWA
COMPUTES 2-DIM FR AS A SUMMATION OVER TERMS A (HKL) COSCOS+B (HKL) SINCOS +C (HKL) COSSIN-D(HKL) SINSIN. AXES SUBDIVISION 1/60. INPUT PGM NDRE BIP.
6006 MERCURY FR 3 KEILHAU NDRE-R2285/230 OPTIMAL PGMS LWA
CONSTRUCTS OPTIMAL WORKING PGM VALID FOR THE SPACE GROUP IN QUESTION TAKING FULL ADVANTAGE OF COMPUTATIONAL SHORTCUTS MADE POSSIBLE BY SYMMETRY RELATIONS. WORKING PGM IS VERY CLOSE TO ABSOLUTE OPTIMUM. FINALLY PERFORMS 3-DIM FR. AXES SUBDIVISION 1/60. INPUT PGM NDRE DIP.
4046 MERCURY GEOMETRY ROLLETT ROTATE BOND MPA
GIVEN POSITIONS OF THREE ATOMS FORMING TWO BONDS, FINDS POSITION BY ROTATING ONE BOND ABOUT ANOTHER.
4047 MERCURY GEOMETRY SPARKS/ROLLETT LOCATE HYDROGEN ATOMS MWA
THREE ROUTINES WHICH PROVIDE COORDINATES FOR H ATOMS CALCULATED FROM

OTHER POSITIONS FOR ATOMS JOINED TO XH, XHH, XHHH GROUPS RESPECTIVELY.

4043 MERCURY GEOMETRY SPARKS/ROLLETT MOLECULAR AXES MWA
GIVEN ATOMIC POSITIONS AND WEIGHTS, FINDS CENTROID, AXES OF INERTIA (BY LATENT VECTOR ANALYSIS) AND COORDINATES REFERRED TO THESE AXES.

4045 MERCURY ID SPARKS/ROLLETT DISTANCES AND ANGLES MWA
GIVEN ATOMIC POSITIONS AND SYMMETRY OPERATIONS, PROVIDES ALL UNIQUE DISTANCES IN STRUCTURE BELOW GIVEN LIMIT, ALL ANGLES WITH LEGS BELOW SECOND LIMIT.

4012 MERCURY LC MAIN,WOOLFSON FROM WEIS DATA LPA
USES ALPHA 1 - ALPHA 2 SEPARATION FROM ZERO-LAYER WEIS. INPUT - INDICES WITH MEASURED SEPARATIONS, CAMERA CONSTANTS, ROUGH LC. OUTPUT - ACCURATE LC WITH E. ACCURACY ABOUT 1/2000.

4008 MERCURYP P H D SF PAULING,DOLLIMORE/RD1/CALC,SORT D, SF NPA
FOR GIVEN CELL, GENERATES HKL, CALCULATES D FOR ALL PLANES IN GIVEN SHELL, SORTS IN ORDER OF S, PUNCHES ANY OF D, 1/D, D2, 1/D2, S, S2, LAMBDA S, (LAMBDA S)2, THETA, 2THETA. FOR GIVEN STRUCTURE WILL PRODUCE F, I, ILP. ISOTROPIC TF ONLY, ANY SPACE GROUP.

4040 MERCURY PATSUP ABRHMSN,ROLLETT PATTERSON SUPERPOSITION 3D LPA
GIVEN 3-D PATTERSON FUNCTION, SYMMETRY OPERATIONS, TRANSLATES ORIGIN TO EACH OF UP TO 16 GRID POINTS, CALCULATES SPECIFIED FUNCTION OF COINCIDENT POINTS.

4048 MERCURY PK LOCN SPARKS/ROLLETT 19-POINT GAUSSIAN INTERPOLATION MWA
GIVEN 19 POINTS OF FO MAP PROVIDES PEAK POSITION AND HEIGHT. GIVEN FC (OR FO - FC) POINTS AS WELL AND INPUT POSITION CALCULATES N-SHIFTS AND BACK-SHIFTS. GIVES B-FACTOR ALSO IF AXES ORTHOGONAL.

4007 MERCURY LS2 FMAT CURTIS/BOWLER 29F/GENL 2D LS,FM,AT,N OR XRAY LWA
GENERAL 2-DIM SF + LS PGM, FULL MATRIX, ANISO. NEUTRON OR XRAY. INPUT PLANE GP NO, LC, LF, LIST OF HKF, PARAS, CONTROL CODE FOR EACH CYCLE. WEIGHT IS A FUNC OF F. OUTPUT PARAS, CHANGES, ERRORS, SF, AS REQD. WRITE-UP AERE-R3134 AMENDED BY CPN 52. SAME AS 7090 PGM LS2D,NO. UP TO 31 DISTINCT ATOMS, 85 PARAS REFINED, 500 PLANES, ON 24K MERCURY

4041 MERCURY R LAI/ROLLETT AGREEMENT ANALYSIS LPA
GIVEN F-OBS, F-CALC, FINDS SUMS OF MODULI OF F-OBS, F-CALC, F-OBS MINUS F-CALC, AND R FACTORS, FOR GROUPS INDICATED BY F-OBS, SIN THETA, AND INDEX VALUES.

4033 MERCURY SCLLAYRS ROLLETT LAYER SCL FROM RELATIVE F-SQUARED LPA
GIVEN F-SQUARED FROM LAYERS WHICH INTERSECT, FINDS SCL FACTORS TO PLACE LAYERS ON SAME SCL BY LATENT VECTOR ANALYSIS.

4035 MERCURY SF LS ROLLETT LS/3D BLOCK DM GENL MPA
ALL SPACE GROUPS. LIMIT OF 6000 REFLECTIONS, PARAMETERS, F SCALE, POSITIONS, ISOTROPIC B FACTORS, CHEMICAL TYPES. UP TO 96 ATOMS OF 16 TYPES.

4036 MERCURY SF LS ROLLETT LS/3D BLOCK DM AT GENL MWA
ALL SPACE GROUPS. LIMIT OF 6000 REFLECTIONS, PARAMETERS, F SCALE, POSITIONS, ANISOTROPIC B FACTORS, CHEMICAL TYPES. UP TO 96 ATOMS OF 16 TYPES.

4042 MERCURY TFANALYS SPARKS/ROLLETT MOLECULAR VIBN-LIBN TENSORS MWA
GIVEN ATOMIC POSITIONS, TF, AND WEIGHTS, FINDS AXES AND AMPLITUDES OF VIBRATION AND LIBRATION. LIBRATION AXES PASS THROUGH CENTRE OF MASS. OBSERVED AND CALCULATED ATOMIC VIBRATION TENSORS ALSO OUTPUT.

4044 MERCURY TFANALYS SPARKS/ROLLETT ATOM VIBRATION AXES MWA
GIVEN AT FOR ATOM, PROVIDES PRINCIPAL VIBRATION AXES AND AMPLITUDES BY LATENT VECTOR ANALYSIS.

4013 MERCURY 3ABSLP WOOLFSON EQUI-INCLINATION WEIS LWA
LIMITED TO CRYSTALS IN FORM PARALLELEPIPED WITH EDGES ALONG CELL DIRECTIONS. SIMPLE INPUT. OUTPUTS ABS CORRECTION, LP, PHILLIPS SPOT-SHAPE FACTOR, SIN THETA. TIME DEPENDS ON CRYSTAL SIZE - NORMALLY 2 SECS PER REFLECTION.

8518 M1B FR 2 NIIZEKI XTL2/GENL,A,C,GRID N/1000 LWA
TREATS ANY SPACE GROUP AS TRICLINIC. A OR C BY PGM PARAMETER. SIN TABLE LOOK UP. INPUT IS MATRIX OF F VALUES WITH PROPER END MARKS. GRID N/1000.

8515 M1B ID NIIZEKI DIST,ANGLES,ANY SYM LWA
PGM NEEDS INDICATIONS OF ATOMS BY PROPER NUMBERINGS. COMPUTES INTERATOMIC DISTANCE OF GIVEN PAIR OF NUMBERS OR ANGLE OF GIVEN TRIPLET OF NUMBERS.

8516 M1B LP ABS NIIZEKI XTL3/LP,ABS CORR HEX PRSM XTLS LPA
APPLICABLE TO EQUATOR REFLECTIONS FROM CRYSTAL WITH UP TO 6 SIDED PRISM

SHAPE. INPUT IS INDICES CRYSTAL OUTLINE SIN THETA/LAMDA AND ORIGINAL F SQUARED. PGM TAKES ANY NUMBER OF REPRESENTATIVE POINTS AND INTEGRATES BEAM PATHS.

8514 M1B SF 2 NIIZEKI XTL4/FOR 14 PLANE GROUPS LPA
SUBROUTINE GENERATES ATOMIC F VALUE OF EACH ATOM FOR EACH REFLECTION. PGM SELECTS ANY ONE OF FOURTEEN PLANE GROUPS BY PGM PARAMETER. USES ISOATOMIC TEMPERATURE FACTORS.

8517 M1B SPC NIIZEKI XTL1/GONIO STGS PO CONTROL TAPE LWA
NORMAL BEAM ANY LEVEL ANY ROTATION AXIS. INPUT IS CELL CONSTANTS WAVELENGTH AND MAXIMUM THETA. PGM GENERATES INDICES CALCULATES SETTINGS PHI UPSILON FOR RIGAKUDENKI SXG1 GONIOMETER FOR SINGLE CRYSTAL. ALSO PUNCH OUT CONTROL TAPE FOR AUTOMATIC MEASUREMENTS OF INTEGRATED INTENSITIES.

6529 NE 803B FR SASVARI*GERGELY FOR THE 2 DIM SGR P2, PGG, PGM, PMM LWA
THE FOURIER PROJECTION OR THE CORRESPONDING PATTERSON FUNCTION WILL BE COMPUTED DEPENDING ON A SPECIAL REFERENCE NUMBER GIVEN AMONG THE DATA. THE PROGRAMS (WRITTEN IN ACODE) WITH DIRECTIONS OF USE ARE PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

6531 NE 803 B FR TICHY 2,3 FOR S. G. P2/M, P21/C, C2/C LWA

6514 NE803 ID LINEK GENERAL FORMULA LWA

6525 NE 803B LP SASVARI*SANTA TRICL., MONOCL. AND ORTHORHOMB. LWA
ALL POSSIBLE VALUES OF (HKL) WILL BE COLLECTED ON THE BASIS OF THE SIN**2 THETA VALUES AND THE 1/LP COMPUTED FOR EQUI-INCLINATION WEISS. PHOTOGRAPHS WITH ROTATION AROUND ALL THREE AXES. THE PROGRAMS (WRITTEN IN AUTOCODE) WITH DIRECTIONS OF USE ARE PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

6533 NE 803 B LS TOMAN,OCENASKOVA*/C,E,ICA,R,SCL,TF FOR MONOCL.SP.GRPS LWA

6527 NE 803B SCL SASVARI ABSOLUTE AND UNITARY SCALE FACTORS LWA
THE DATA OF SCALE FACTORS FOR THE DETERMINATION OF ABSOLUTE AND UNITARY STRUCTURE FACTORS WILL BE COMPUTED. THE PROGRAM (WRITTEN IN ACODE) WITH DIRECTION OF USE IS PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

6530 NE 803B SF SASVARI*SANTA MONOCLINIC P21/C LWA
THE STRUCTURE FACTORS WITH OR WITHOUT ISOTROPIC TEMPERATURE CORRECTION WILL BE COMPUTED FOR VARIABLE NUMBER AND KIND OF ATOMS, GIVING AT THE END THE RELIABILITY FACTOR. ALSO THE STRUCTURE FACTOR FOR DIFFERENCE FOURIER CAN BE COMPUTED. THE PROGRAM (WRITTEN IN ACODE) WITH DIRECTION OF USE IS PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

6532 NE 803 B SPC TOMAN, TICHY* 3, NORMAL BEAM LWA

6526 NE 803B STAT SASVARI N(Z) FUNCTION FOR 2 AND 3 DIM DATA LWA
THE PROGRAM (WRITTEN IN ACODE) WITH DIRECTION OF USE IS PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

6528 NE 803B USF SASVARI LWA
THE UNITARY STRUCTURE FACTORS WILL BE COMPUTED FROM THE ABSOLUTE ONES ON THE BASIS OF THE TABULATED UNITARY SCALE FACTOR VALUES FI. THE PROGRAM (WRITTEN IN ACODE) WITH DIRECTION OF USE IS PUBLISHED (ENGLISH) IN ACTA CHIM. HUNG., 1964.

7048	PALLAS	FR	PROTAS CNRS BEL	PNAM ELECTRONIC DENSITY SECTIONS	MWA
7054	PALLAS	FR 2	RERAT CNRS BEL	P1	MWA
7049	PALLAS	ID	PROTAS CNRS BEL	ID,BOND ANGLES,ANY SYSTEM	MWA
7037	PALLAS	LS 2 A	MARCHAN CNRSBEL	PG1 REFIN.ATOM.COORD.ISOT.TR,SCL	MWA
7034	PALLAS	LS 2 C	FUERXER/LEROY	P2 REF.ATOM.COORD.ISOT.TF.SCL	MWA
7035	PALLAS	LS 2 C	PROTAS CNRS BEL	P6 REFIN.ATOM.COORD.ISOT.TF,SCL	MWA
7036	PALLAS	LS 2 C	PROTAS CNRS BEL	P6M REFIN.ATOM.COORD.ISOT.TF,SCL	MWA
7033	PALLAS	LS 2 C	SETI/CNRS	PGG PMG REFIN. AT COORD,TF,SCL	MWA
7042	PALLAS	LS 3 A	CHANOINE BEL	B21M REFIN.AT.COORD.ISOT.TR.SCL R	MWA
7040	PALLAS	LS 3 A	PROTAS CNRS BEL	P63 REF.ATOM.COORD.ISOT.TF,SCL	MWA
7039	PALLAS	LS 3 C	CHANOINE BEL	PNMA REF.AT.COORD.ISOT.TF,SCL	MWA
7055	PALLAS	LS 3 C	PROTAS CNRS BEL	I41/ACD REF.ATOM.COORD.INDIV.TF.SCL	MWA
7041	PALLAS	LS 3 C	PROTAS CNRS BEL	PNAM REFIN.AT.COORD.INDIV.ISO.TF,SCL	MWA
7038	PALLAS	LS 3 C	RERAT CNRS BEL	P21/NREF.AT.COORD.ISOT.TF.EA.AT.SCL	MWA
7056	PALLAS	PATSUP	RERAT CNRS BEL	PATT. SUPERPOS., USES FR P1 (7054)	MWA
7050	PALLAS	SF	FUER/LEROY CNRS	SF,R, FOR P1 AND P1BAR GROUPS	MWA
7046	PALLAS	SPEC	CHANOINE BEL	P2/M ELECTRONIC DENSITY COEFFS.	MWA
7045	PALLAS	SPEC	CHANOINE BEL	PMMM PATT.COEF.10 SECT.	MWA
7051	PALLAS	SPEC	FUER/LEROY CNRS	CALC ATOM SCATTERING FAC.FROM TABLE	MWA
7043	PALLAS	SPEC	FUER/LEROY CNRS	CALC 1/D SQUARE,LF ALL SYSTEMS	MWA

7044 PALLAS SPEC FUER/LEROY CNRS CALC 1/D SQUARE,SF,P1 AND P1BAR GRPS MWA
7053 PALLAS SPEC MARCHAN CNRS BEL SCL AND TF WILSON METHOD MWA
7052 PALLAS SPEC PROTAS CNRS BEL NORMALIZE INTENS)FROM N FILMS NMAX20 MWA
7047 PALLAS SPEC PROTAS CNRS BEL PNAM ELECTRONIC DENSITY COEFFS. MWA
8524 PC1 D IITAKA 1/D**2,2THETA(HKL) FOR ALL REFS LWA
INPUT, LC (OR RECIP. LC), WAVELENGTH, 2THETA MAX, EXTINCTION RULE.
OUTPUT, LISTS H,K,L,Q,2THETA OR SINTHETA/LAM. FOR ALL REFS (EXCLUDING ABSENT REFS) WITHIN GIVEN 2THETA MAX.
8520 PC1 DP LP IITAKA CORR EQUI WEISS LWA
LP CORRECTION FOR EQUIINC. WEISS. DATA. CORRECTS IOBS FOR ANY LAYER FOR A GIVEN AXIS (A OR B OR C).
8522 PC1 DP P IITAKA FIND NEAREST QCAL(HKL)FOR Q BY POWD. LWA
STORE REC.LC, TABLE OF QOBS BY POWDER PHOTO, QOBS MAX. CALCULATES QCAL FOR ALL HKL WITHIN QMAX AND FINDS THE NEAREST QOBS. TABULATES HKL, QCAL, QOBS, QOBS-QCAL.
8525 PC1 ID IITAKA BOND SEARCHING. NO ANGLE CALTD. LWA
CALCULATES DISTANCES BETWEEN TWO ATOMS ONE IN AN ASYM. UNIT AND OTHERS IN THE SAME UNIT OR OUTSIDE OF THE UNIT. THE ATOMIC COORDINATES ARE DERIVED BY SYM. OPERATIONS INCLUDING LATTICE TRANSLATIONS. MAX AND MIN DISTANCES CAN BE DEFINED AND ALL THE DISTANCES WITHIN THE RANGE ARE PRINTED OUT TOGETHER WITH THE SYM. OPERATION CODES AND THE COORDINATES.
8521 PC1 SF IITAKA MONOCL.C.ISOTF FOR EACH ATOM KIND LWA
FOR MONOCLINIC CENTRIC SPACE GROUPS. ATOMIC SCATTERING FAC ARE CALTED BY THE 2 TERM GAUSSIAN EXPANSION. INPUT TAPE, HKL, SINTHETA/LAM, (FOBS), OUTPUT TAPE, HKL, SINTHETA/LAM, (FOBS), FCAL. MAX N=38-2J. SPEED=0.2N+ 0.4J SEC/PLANE. N ATOMS J KINDS IN AN ASYM. UNIT.
8523 PC1 TABLE IITAKA MAKE SINTHETA**2 OR Q TABL.VS.2THETA LWA
MAKE SINTHETA**2(X10**5) OR QVALUE(X10**5) VS. 2THETA(X10**2) TABLES IN A CLEAR TABLE STYLE. STARTING AND ENDING 2THETA ANGLES CAN BE DEFINED. Q VALUES (1/D**2) ARE CALTED FOR ANY GIVEN WAVELENGTH.
3040 PDP 6 FR3 RAE IT=SFLS OT.OT FR/DIF LPA
A THREE PASS PROGRAM. FIRST PASS ACCEPTS OUTPUT FROM SLFS AND CONVERTS IT INTO A FORM SUITABLE FOR SECOND PASS WHICH EVALUATES A FOURIER OR DIFF. IN SECTIONS UP ANY AXIS AT INTERVALS MULTIPLES OF 120THS OF CELL EDGE. OUTPUT ON LINE LISTING AND TAPE. THIRD PASS ACCEPTS OUTPUT OF SECOND PASS AND CONTROUS FOURIER DIRECTLY ONTO A FAST CRT DISPLAY. PROGRAM LANGUAGE IS MIXED FORTRAN AND MACRO 6.
3039 PDP 6 SFLS RAE TRICL,MONOCL,ORTH,AT LPA
PROGRAM IS IN TWO PASSES. 1ST PASS CALCULATES SFS AND LEAST SQUARES SUMS. SECOND PASS INVERTS LEAST SQUARES MATRIX AND EVALUATES NEW PARAMETERS. AND STANDARD DEVIATIONS. INDIVIDUAL ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTORS MAY BE USED. ALLOWANCE MAY BE MADE FOR ANOMALOUS DISPERSION. THE BLOCK DIAGONAL APPROXIMATION IS USED. PROGRAM LANGUAGE IS FORTRAN.
3007 SILLIAC ABS LOVELL/FREEMAN ABS CORR FOR XTLS WITH PLANE FACES LWX
ABSORPTION FACTORS FOR CRYSTALS BOUNDED BY PLANE FACES. AVAILABLE FOR THREE-DIMENSIONAL EQUI-INCLINATION DATA
3009 SILLIAC ANGLES LOVELL/FREEMAN BOND ANGLES ONLY LWX
COMPUTES ALL ANGLES SUBTENDED AT A CENTRAL ATOM BY PAIRS OF ATOMS FROM A SPECIFIED GROUP.
3008 SILLIAC ID LOVELL/FREEMAN BOND DISTANCES ONLY LWX
COMPUTES ALL DISTANCES LESS THAN A SPECIFIED LIMIT WITHIN BASIC CELL AND 26 SURROUNDING CELLS. ALL SPACE GROUPS CAN BE HANDLED.
3010 SILLIAC SF 3ATN LOVELL/FREEMAN ALL SYMM N/XDIFF DOES 2*2 FOR SCLTF LWX
GENERAL STRUCTURE FACTPR PGM. AVAILABLE FOR ANY SYMMETRY. NEUTRON OR X-RAY DATA WITH ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTORS. GIVES R FACTOR AND DOES 2X2 MATRIX FOR AVERAGE TEMPERATURE FACTOR AND SCALE FACTOR.
6506 URAL 1 DP NOVAK E101/LP,ABS.CORR LPA
6505 URAL 1 SF LINEK,NVK,NADR E82/GENERAL FORMULA.ICA LPA
6507 URAL 1 STEREO LINEK*NVK FROM THREE FR2 A 3MODEL IS COMP. NPX
COMPUTATION OF THE CUBE ROOT OF PRODUCT OF RO(XY).RO(XZ).RO(YZ) IN EVERY (XYZ) FROM UNIT CELL.
8021 TR4-AGL 3 GEOM SMITS GRON-CH-9/MOLECULAR GEOMETRY LPA
BOND DISTANCES,BOND ANGLES,BEST PLANES,DISTANCES TO THESE PLANES
8022 TR4-AGL LP ABS VOS GRON-CH-10/ABS. CORR. LPA
LP AND ABS CORR.WEIS,PREC.+CAPILL,MAX.8X8X8 POINTS

8020 TR4AGL PROF BOOM POLYCHR.D-SCH,KON.NED.AKAD.WET.68B46 LPA
PROGRAM CALCULATES MONOCHROMATIC POINTFOCUS, POLYCHROMATIC POINTFOCUS, AND POLYCHROMATIC LINEFOCUS PROFILES FOR DEBYE-SCHERRER (PHOTOGRAPHIC) CYLINDRICAL POWDER CAMERAS FROM RADII AND ABSORPTIONCOEFFICIENTS OF SPEC IMEN AND MOUNTING CAPILLARY, PEAK WAVELENGTH, HALFWIDTH AND ASYMMETRY OF RADIATION USED, FOCUS WIDTH AND EMISSIVITY CURVE, AND CAMERA GEOMETRY, STORES PROFILE-COORDINATES ON MAGNETIC TAPE, PUNCHES INTERMEDIATE RESULTS IN PLOTTER-TAPE, INDICATES 'CORRECT' POSITIONS OF DIFFRACTION LINES. 23K.

6001 WGMATIC LP WEIS3 ROMMING CS-01/ LWA
LP OF INTENSITIES FROM WEIS ANY LAYER LINE. PRINTS SIN SQ THETA, CORRECTED INTENSITY, SQ ROOT OF CORRECTED INTENSITY.

8057 X1 8K DP RUTTEN-KEULEMAN OX4/DATA CONTROL MWA

8058 X1 8K DP RUTTEN-KEULEMAN OX5/AVERAGING DATA MAXES IT OX9 MWA

8055 X1 8K FR 3 RUTTEN-KEULEMAN OX8/PATSUP TRICL MONOCL RHOMBIC LWA

8056 X1 8K SCL DP RUTTEN-KEULEMAN OX3/LS-METH FROM DATA OF 2 AXES MWA

8054 X1 8K SFLS DM RUTTEN-KEULEMAN OX9/AT ALL SPACEGR 3X3POS 6X6AT LWA
DIFFERENT SCALE FACTORS ALL KINDS OF SPECIAL POSITIONS CAN BE TREATED WITHOUT PROGRAMMING.
GIVES INPUT FOR OX8 FOR RELIABLE REFLECTIONS.

3021 ZEBRA DP ROGERS ZK3/CONVERT F COSALPHA TO FA,FB MWA
CONVERTS TAPES WITH /F/, COSALPHA TO FA, FB AND MARKERS FOR USE WITH ZK1/2.

3022 ZEBRA DP ROGERS ZK5/OTHER OCTANTS LSW
PREPARES 3D DATA FOR ZK1/2 FROM ABBREVIATED FORMAT. AVAILABLE FOR BOTH PMMM AND P212121.

3037 ZEBRA DP SPC ROGERS ZK56/CENTROID DIFFR LINE MNA
EVALUATION OF SYMM FIXED-RANGE CENTROID OF DIFFRACTOMETER LINE (PIKE-WILSON METHOD).

3031 ZEBRA ENERGY ROGERS ZK35/DIPOLE ENERGY IN TRICLINIC LATT MNA
PROG FOR EVALTN OF DIPOLE INTERACTION ENERGY AS A FUNCTN OF RADIUS IN TRICLINIC LATTICE. USED FOR NYLON BUT GENERAL IN FORM.

8016 ZEBRA FITPLANE PALM 0-519/FIT PLANE THROUGH SET OF POINTS LWA

3023 ZEBRA FR OT VAN DER SLUIS ZK7/TRANSFORM FR OT LSW
OFFERS 3 MODES OF DISPLAY OF FR SUMS TO FACILITATE CONTOURING.

8008 ZEBRA FR 2 3 SMITS ZK2/C TRICL. GRID 1/256 LWS

8007 ZEBRA FR 2 3 SMITS,SCHOONE ZK1/C OR A, TRICL. GRID 1/256 LWS

8012 ZEBRA IT SMITS ZK23/PREPARES F-TAPES FOR ZK20,21,22 LWS

3012 ZEBRA,SC LIN REG RUDOLPH 2 LINE LS, E LWA
MAX 100 POINTS (WEIGHTS OPT), OT COEF LINEAR REGRESSION, VARIANCE

8015 ZEBRA LP ABS. PALM 0-500/F FROM I, EQUI-INCL WEIS LWA
CALC. F SQ, F, ABS.CORR. FOR SPHER. OR CYLINDR. SPECIMEN

8014 ZEBRA LP WEIS SMITS ZK /F FROM I, ANTI-EQUI INCL LWS
CALCULATES SIN THETA, SIN SQ THETA, F SQ AND F FROM INTENSITIES

8013 ZEBRA LP WEIS SMITS ZK43/F FROM I, EQUI-INCL WEIS LWS
CALCULATES SIN THETA, SIN SQ THETA, F SQ AND F FROM INTENSITIES

3018 ZEBRA,NC LS DATA BOONSTRA B05/PREPARES LS IT FROM PAT IT NPA
IT PAT TAPE ZK1,2. OT TAPE FOR IT LS ZK22. MANUAL CORRECTIONS NEEDED FOR CENTRAL LATTICE ROWS

8011 ZEBRA LS SCHOONE ZK22/INDIV ISOTROPIC TF, DIAGONAL REF LWS
INSERTS FOR VARIOUS SPACE GROUPS. MAX 64 ATOMS, 9 TYPES

3016 ZEBRA,NC MARGIN BOONSTRA B03/SHIFT TELEPRINTER MARGIN 10 SP NPA
SHIFT MARGIN OF TELEPRINTER OT 10 SPACES, EASILY CHANGED

3014 ZEBRA,SC P PISTORIUS, C. GI9/TAB P ACCORDING TO H NPA
AID TO PI. IT LC, OT OF P LISTED.ACC TO H. SUPERCEDED BY 704 PROG

3035 ZEBRA PI LOENE ZK51/RECOG ZONES IN POWDER DATA MPA
USES DE WOLFFS METHOD.

3036 ZEBRA PROF COR NEETHLING ZK54/STOKES CORRN FOR INST BROADENING LWS

3013 ZEBRA,SC PLANE RUDOLPH 3 PLANE LS THRU ATOM POS LWA
MAX 100 POINTS (WEIGHTS OPT), OT LS PLANE, IND, TOTAL DEVIATION
SUPERCEDED BY PROG MORGAN, QUEENS COLLEGE, DUNDEE

3017 ZEBRA,MC SF CORR BOONSTRA,SMITS B04/SPOT-SHAPE INC IN WEIS INT CORR NPA
GRON-CH-20 BY SMITS (WEIS INT TO CORR SF) MODIFIED TO INCLUDE SPOT-SHAPE FACTOR

3015 ZEBRA,NC SF STAT BOONSTRA B02/SF, SF**2 INC SCL FROM LS ZK22 NPA
DATA FOR STAT. IT FOR LS ZK22 USED TO LIST SF, SF**2 INC SCL

8009 ZEBRA SF A SMITS ZK20/A INDIV ISOTROPIC TF LWS

INSERTS FOR VARIOUS SPACE GROUPS. MAX 80 ATOMS, 13 TYPES.

8010 ZEBRA SF C SMITS ZK21/C INDIV ISOTROPIC TF LWS
INSERTS FOR VARIOUS SPACE GROUPS. MAX 80 ATOMS, 13 TYPES.

3033 ZEBRA SPC SMITS ZK41/SPC FOR C2/C MNA

3019 ZEBRA 1FRTRANS NEETHLING ZK70/1D FR TRANSFORMATION MNA
ACCEPTS 1000 ORDINATES, ADJUSTABLE SPECTRUM INTERVAL.

3027 ZEBRA 3 GEOM ROGERS ZK30/MOLECULAR BOND SCAN LSW
IDENTIFIES ALL INTERATOMIC DISTANCES WITHIN ASYMMETRIC LIMIT. ALSO GIVES ORTHOGONALIZED COORDS IN AU.

3028 ZEBRA 3 GEOM ROGERS ZK31/INTERMOLECULAR CONTACTS SCAN LSW
IDENTIFIES ALL CONTACTS BETWEEN PARENT ASYMMETRIC UNIT AND NEIGHBORS WITH LENGTHS LESS THAN PRESCRIBED LIMIT.

3029 ZEBRA 3 GEOM ROGERS ZK32/MOLECULAR GEOMETRY LSW
GIVES BOND LENGTHS AND DIRN COSINES OF SPECIFIED BONDS, ANGLES BETWEEN STATED PAIRS OF BONDS, BEST PLANES (WITH OR W/OUT CONSTRAINTS), DISTANCES OF ATOMS FROM PLANES.

5034 Z22 R ER2 BRUHN

5035 Z22 R SF TOEPFER'BRUHN

5071 Z23 FOLD BRADACZEK,URBAN ELIM.LAV.SCATT.DET.ABSO.COEFF.CRYST. LWA
CALC. THEOR. CURVE I = ALPH.I(L) + (1 - ALPH)I(B)
I(B) = P(X) EXP(-UX) GAUSS I(L) = I(B) 1/B.B
PORT.LAV.SCAT. -- ANTL = ALPH.INT(I(L))/INT(I)
PARAMETERS -- ALPH, U, G G ELIM. PART. SIZE EFFECT
MEAS. CURVE COMP. WITH I
FOLD FOLDING INTEGRAL DETERMINATION

7568 Z23A 8K FR 3 2 ZELENKO,ZAKRAJS GENL,60 GRID MPA
FOR ZUSE Z23A, PAPER TAPE. ABS FRQ H,K,L LESS THAN 60. 2000 F(HKL), 8K. GENRALLY, ONE FR 3 DIMS WITH SYMMETRY ABOUT 3 DAYS.

5070 Z23 FT LEMM FT INTENS.LIQUIDS FOR ELIMIN.CUT-OFF LPA
CALCUL 1. R(RHO - RHO.ZERO) = F(S.ZERO)
2. R(RHO - RHO.ZERO) = F(R)
3. 4PI.R.SQU.RHO = F(R)

7567 Z23A 8K LS ZELENKO,LESJAK GENL,WITHOUT WEIGHTING FUNCTION MPA
FOR ZUSE Z23A, PAPER TAPE, ABS FRQ H,K,L LESS THAN 60.
2000 F(HKL), 8K. GENERALLY, FOR ONE ATOM IN 30 MINUTES.

7569 Z23A 8K SF ZELENKO,STALEC GENL MPA
FOR ZUSE Z23A, PAPER TAPE. ABS FRQ H,K,L LESS THAN 60. 2000F(HKL), 8K. GENERALLY, ONE SF IN 5 HOURS

5069 Z23 STAT LEMM STRUCT.ANAL.DISTR.FUNCT.1-ATOM.LIQ. LPA
CALCUL. SYNTHETIC RAD. DISTRIB. FUNCTIONS OF LIQUIDS FROM CHOSEN ASYMM. DISTANCE STATISTICS FOR THE NEAREST NEIGHBOR BY CONVOLUTION-POLYNOM.

6518 ZRA 1 FR 2 WEISS 003*043 LWA
FR2 WITH DIFFERENT SUBPROGRAMS FOR PATTERSON,DIFFERENCE,FR WEIGHTED ACCORDING TO ABSOLUTE VALUE OF SFOBS+SFCALC,AND OTHERS

6521 ZRA 1 ID WEISS 001*022 LWA
ID OT VALUES SMALLER THAN LIMIT

6517 ZRA 1 LP,THETA KRAUSE 000*012 LPA
SINE THETA + LP FOR EQUIINCLINATION WEIS

6522 ZRA 1 SF,A DENNER 002*121 LWA
SF+CONTRIBUTION OF SELECTED ATOMS/H/A

6515 ZRA1 SF,A,R KRAUSE 002*023 LWA
SF + COMPARISON WITH SFOBS/R/A

6523 ZRA 1 SF,C DENNER 002*111 LWA
SF+CONTRIBUTION OF SELECTED ATOMS/H/C

6524 ZRA 1 SF,C,R KRAUSE 002*012 LWA
SF + COMPARISON WITH SFOBS/R/C

6516 ZRA1 SF,C,R KRETSCHMER 002*211 LPA
SF/C/+COEFFICIENTS FOR DETERMINATION OF 3RD ATOM COORDINATE FROM KNOWN PROJECTION AFTER KUTSCHABSKY/MONATSBER/ D/DAW/7/1965/95+ACTA/1965/IN PRESS

6519 ZRA 1 STAT WEISS 000*306 LWA
STAT/HOWELLS ET AL ACTA 3,1950,210 FOR C-TEST

6520 ZRA 1 STAT WEISS 000*309 LWA
STAT/SRINIVASAN ACTA 13,1960,388 FOR C-TEST

8053 1103 FR 3 2 KEUNING, VONK* VOKAS/GRID N/10000 LWA

8052 1103 FRSORTER KEUNING, VONK* VOPRE/PREPARES FOURIER DATA TAPE LWA
8050 1103 LP KEUNING, VONK* VINTS/F FROM I LWA
7525 1103 2K PAT2 MARIANI FIAT INTP LANG PAT2 COS COS LWA
8051 1103 SF KEUNING, VONK* VALCO/SF,SCL,TF,R LWA
7524 1103 2K SF MARIANI FIAT INTP LANG SPACEGROUP 14 0 LEVEL LWA
493 1105 FR 2 MORROW 3/GRID N/50 LWA
494 1105 FR 3 MORROW 9/GRID N/360 NPA
495 1105 LP ABS MORROW 14/LP OSC-ROT,WEISSENBERG,ABS 6PTGAUS NPA
492 1105 SF MORROW 2/GEN SF 100ATOMS ANISO TEMP FACTORS LWA
446 1604 FR 2 3 BLOUNT/DAHL* FOURIER/FAST,GENERAL,BL,GRID N/240 LWA
APPLICABLE TO ANY SPACE GROUP THRU ORTHORHOMBIC (EXCEPT THOSE WITH D-GLIDE). USES UNIQUE REFLECTIONS ONLY. REGULAR OR DIFF FOURIER. VARIABLE OUTPUT FORMAT. PROGRAM IN CDC FORTRAN-63 AND CODAP-1 FOR USE WITH COOP MONITOR SYSTEM.
447 1604 FR3 SF BLOUNT/DAHL* PREFOUR/SF+FR WITHOUT SCRATCH TAPE LWA
SAME AS FOURIER BUT ALSO INCLUDES SF AND LS SCALE FACTOR CALCULATIONS. UP TO 4000 INDEPENDENT REFLECTIONS STORED INTERNALLY. MAX 100 ATOMS IN ASYMMETRIC UNIT, OTHERS GENERATED BY SYMMETRY CARDS.
392 1604AFT2 SPEC BROWN G M ANALYZE/FIT OF F**2 CALC AND OBS LPA
COMPUTES RATIO AVG F**2 OBS/CALC FOR RANGES OF F**2 OR OF INTENSITY EITHER CALC OR OBS OR FOR RANGES OF (SIN THETA/LAMBDA)**2. ALSO COMPUTES R FACTOR, AVG DELTA/SIGMA, ETC. INPUT TAPE FROM XFLS (AC 389) OR BMFLS (AC 390).
387 1604 STEREO JOHNSON C K ORTEP/THERMAL ELLIPSOID PLOT PROGRAM LWA
UTILIZES PLOTTER SUCH AS CALCOMP TO PLOT BALL-AND-STICK CRYSTAL STRUCTURE FIGURES IN STEREO WITH THERMAL ELLIPSOIDS OR CIRCLES ON THE ATOMIC SITES. MAIN PROGRAM IS IN FORTRAN II. IBM 7090 OR CDC 1604 MACHINE ORIENTED PLOT ROUTINES ARE LIBRARY TYPE WITH MINOR MODIFICATIONS. 32K MACHINE REQUIRED.
523 1620T20K ABS JOHNSON/PATT* COMPUTES TRANSMISSION FACTORS LWA
PROGRAM FOR CRYSTAL GROUND AS AN ELLIPSOID OF REVOLUTION. FOR G. E. GONIOSTAT TRANSMISSION FACTORS ARE COMPUTED AS A FUNCTION OF THETA AND CHI, FOR WEISSENBERG DATA AS A FUNCTION OF THETA AND LAYER LINE.
292 1620 SPS ABS BS MAC/MOSELEY ABS FOR GONIOSTAT.
294 1620 SPS AT CEN MAC/LACHER AT. CENTERS FROM 3-FR.
285 1620 40K D H HAENDLER,COONEY 12/TETRAGONAL D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN, UP TO ANY GIVEN Q VALUE.
312 1620,704 D H LP MEYER,MUELLER D SPACE,HKL,PHI,CHI,LP,EXTINCTIONS LPA
INPUT-TITLE CARD, CELL DATA, INSTRUCTION CARD. GENERATES INDICES WITH CHOICE OF EXTINCTIONS ACCORDING TO BUERGER (P83) CALCULATES D SPACINGS TOGETHER WITH TRIG. FUNCTIONS. PHI, CHI FOR 3D ORIENTATION,LP AVAILABLE
461 1620 20K D H PI PIPPY/AHMED* (HKL) + D(HKL) IN SPECIFIC SPHERE LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. GENERATES INDICES AND COMPUTES SPACINGS FOR ALL REFLEXIONS WITHIN ANY PART OF SPECIFIC SPHERE.
277 1620 40K D P HAENDLER 2/ORTHORHOMBIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN, UP TO ANY GIVEN Q VALUE.
279 1620 40K D P HAENDLER 4/MONOCLINIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM RECIPROCAL CELL DATA FOR HKL VALUES FROM 000 TO NNN UP TO ANY GIVEN Q VALUE.
283 1620 40K D P HAENDLER 9/FACE-CENTERED CUBIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN, WITH HKL ALL EVEN AND ALL ODD UP TO ANY GIVEN Q VALUE.
530 1620 40K D P HAENDLER 8/SIMPLE CUBIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN UP TO ANY GIVEN Q VALUE.
531 1620 40K D P HAENDLER 10/BODY-CENTERED CUBIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN, WITH H+K+L EVEN, UP TO ANY Q VALUE.
284 1620 40K D P HAENDLER 11/HEXAGONAL D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM UNIT CELL DATA FOR HKL VALUES FROM 000 TO NNN.
287 1620 40K D P HAENDLER 14/TRICLINIC D SPACINGS LWA
CALCULATES Q(HKL), SQUARE OF SIN THETA, D(HKL) FROM RECIPROCAL CELL DATA FOR HKL VALUES FROM 000 TO NNN UP TO ANY GIVEN Q VALUE.

456 1620 40K DF 3 AHMED GENERAL 3-D DIFFERENTIAL SYNTHESIS LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. CALCULATES ELECTRON DENSITY, 3 FIRST AND 6 SECOND DERIVATIVES, FRACTIONAL SHIFTS AND PEAK CENTRES FOR UP TO 40 OR 50 ATOMS IN ONE PASS. ANY SPACE GROUP.

7545 1620 20K DF 3 GIGLIO GENERAL,FAST,AT MOST 32 ATOMS LNA

7546 1620 20K DF E GIGLIO STANDARD DEVIATIONS FROM DF LNA

454 1620 20K DP WEIS GABE/AHMED INTENSITY ESTIMATE REDUCTION LWA
USES CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. APPLIES SCL, LP, ABS TO WEISSENBERG MEASUREMENTS. FO SQ MAY BE SHARPENED.

525 1620T20K DP WEIS MINKIN/PATT* WEISSENBERG DATA REDUCTION LWA
CALCULATES STRUCTURE FACTORS FROM WEISSENBERG EQUI-INCLINATION DATA. CORRECTS FOR ABSORPTION BY INTERPOLATION FROM TABLE PRODUCED BY PGM 523.

458 1620 20K E AHMED COORDS S.D. SUMS + AGRMT ANALYSIS LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. EVALUATES SUMS FOR S.D. OF ELECTRON DENSITY AND COORDS, R, SCALE. APPLIES TF CORRECTION. GIVES DETAILED ANALYSIS OF SF ERRORS. ANY SPACE GROUP.

497 1620-2 FR BRYDEN 2,3-DIM FOURIER SUM. CARD OUTPUT. LPA
COMPUTES 2 AND 3-DIM. FOURIER SERIES AT 120 DIV PER CELL EDGE, OR SUB-MULTIPLE OF 120. CARD INPUT AND OUTPUT.

8045 1620C20K FR VDHELM,KING* ERA210/FOURIER LWA
CARD VERSION OF PROGRAMME 354

485 1620 20K FR2 HALL,SHIONO* SPS,CARD, GRID N/100 LWM
TRICLINIC,MONOCLINIC,ORTHORHOMBIC, NO LIMIT ON 1ST INDEX,LESS THAN 31 FOR 2ND. ANY NO. OF REFLEXIONS. IA,MF FEATURES.IBM LIBR. 8.4.005

400 1620 SPS FR2 SVETICH 012/112 GEN PROJ,N/200,PATT,F,DELTA F LWA
20K OR MORE, AUTO DIV. AVAILABLE W OR W/O INDIRECT ADD,PLEASE SPECIFY CARD I/O

354 1620T20K FR3 VDHELM/PATT* GRID 1/100,OUTPUT NUM.OR ALPHAPLOT LWA
THE PROGRAM CALCULATES ONE SECTION AT A TIME. THE SORTING ORDER OF THE DATA ON THE INPUT TAPE DETERMINES ON WHICH AXIS THE SECTIONS ARE MADE. THERE IS A CHOICE OF A NUMERIC TYPOUT, DIRECT ALPHA NUMERIC TYPOUT ON THE APPROXIMATE SCALE OF THE UNIT CELL AND A POSSIBLE OUTPUT ON TAPE. THERE ARE NO SPACE GROUP LIMITATIONS.

370 1620 FR 3 2 AHMED GENERAL 3-D OR 2-D, GRID N/120 LWA
GENERAL 3-D OR 2-D FOURIER. FOR 1620 WITH 40K OR 20K DIGITS, CARD I/O, AUTOMATIC DIVIDE+ INDIRECT ADDRESSES. INTERVALS OF N1,N2,N3/120. EMPLOYS THE DATA CARDS PRODUCED BY THE SF PROGRAM.

486 1620 20K FR3 HALL,SHIONO* SPS,CARD, GRID N/100 LWM
TRICLINIC,MONOCLINIC,ORHTORHOMBIC, NO LIMIT ON 1ST INDEX,LESS THAN 31 FOR 2ND. ANY NO. OF REFLEXION IN ANY ORDER. IA,MF FEATURES. IBM LIBR.8.4.006 ALSO ALPHABETIC PLOTTING PROG. FOR CONTOURING, IBM LIBR. 8.4.007

401 1620 SPS FR PCH SVETICH 220/225/240/250 FOURIER PCH OUT LWA
CC SS SC CS TABLE EXPANS AND PCH OUT FROM 1 QUAD CC SS SC CS TABLES IN STORAGE PCH 1,2 OR 4 QUAD OF THESE OR SUMS CC-SS OR SC+CS AND ADD ANY PREVIOUS PARTIAL CALC X1 OR X2 IN 20THS 25THS 40THS 50THS TO CONTOUR DIRECTLY ON 402 OR 407 PRINTOUT. AVAILABLE W OR W/O INDIRECT ADDR PL SPEC

371 1620T20K FRSORTER VDHELM/PATT* PREPARES FOURIER DATA TAPE LWA
THE PROGRAM PREPARES FOURIER AMPLITUDES FROM OUTPUT OF SFLS PROGRAM. IT REARRANGES THE TERMS IN EACH AMPLITUDE ACCORDING TO THE DESIRED SORTING ORDER. IT TAPESORTS THE AMPLITUDES.

8047 1620C20K FRIT KING ERA235/CONVERSION ERA302 OT ERA210 IT LWA
TREATS SF OUTPUT FOR SPACE GROUP SYMMETRY.

524 1620T20K GONIO DP JOHNSON/PATT* G.E. GONIOSTAT DATA REDUCTION LPA
CONPUTES STRUCTURE FACTORS FROM DATA MEASURED WITH THE G.E. GONIOSTAT APPLIES ABSORPTION CORRECTIONS BY INTERPOLATION FROM TABLE PRODUCED BY PGM 523. OUTPUT IS IN FORM SUITABLE FOR INPUT INTO PGM 372.

280 1620 40K H HAENDLER,COONEY 5/INDICES TRANSFORMATION LWA
CONVERTS ANY SET (A) OF HKL VALUES TO SECOND SET (B) IF MATRIX OF TRANSFORMATION FOR SET A TO SET B IS GIVEN.

281 1620 40K H HAENDLER,COONEY 6/REVERSE INDICES TRANSFORMATION LWA
CONVERTS ANY SET (B) OF HKL VALUES TO SECOND SET (A) IF MATRIX OF TRANSFORMATION FOR SET A TO SET B IS GIVEN.

8042 1620 H D KING ERA119/HKL + SIN ,HETA/LAMBDA LPA

499 1620-2 ID BRYDEN INTERATOMIC DISTANCES AND ANGLES MPA
COMPUTES INTERATOMIC DISTANCES AND ANGLES IN ALL CRYSTAL SYSTEMS. CARD INPUT AND OUTPUT.

490 1620 20K ID CHU,SHIONO SPS,CARD,ALL DISTANCES,ANY SYM. LWM
CALCULATE ALL DISTANCES LESS THAN A LIMIT. DIV,MF,TNF,IA FEATURES. ALL ANGLES AROUND AN ATOM BY 2ND PROG. IBM LIBR. 8.4.008

526 1620T20K ID JOHNSON/PATT* INTERATOMIC DISTANCES AND ANGLES LWA
NO RESTRICTIONS ON LATTICE SYMMETRY. UP TO EIGHT SYMMETRY-RELATED EQUIVALENT UNITS CAN BE SPECIFIED. ASYMMETRIC UNIT MAY CONTAIN ONE TO 48 ATOMS. LIMITS FOR DISTANCES AND ANGLES ARE SPECIFIED BY OPERATOR.

459 1620 20K ID (1) PIPPY/AHMED* BOND LENGTHS, ANGLES, E.S.D.S LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. CALCULATES BONDS AND/OR ANGLES BETWEEN SPECIFIED ATOMS IN GIVEN LIST OF COORDS. CAN COMPUTE E.S.D.S FOR ANY ANGLE, AND ANY BOND EXCEPT IN TRICLINIC CELLS.

460 1620 ID (2) AHMED INTER + INTRAMOLECULAR DISTANCES LWA
40K, OR 20K WITH MODIFICATIONS. CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. FROM A LIST OF ATOMIC COORDS OF ONE MOLECULE, IT COMPUTES ALL BOND LENGTHS WITHIN A GIVEN LIMIT, ALL BOND ANGLES, GENERATES POSITIONS OF EQUIVALENT MOLECULES AND SCANS ALL INTERMOLECULAR DISTANCES.

278 1620 40K LC HAENDLER,COONEY 3/DIRECT LATTICE FROM RECIPROCAL LWA
CALCULATES DIRECT LATTICE PARAMETERS FROM RECIPROCAL LATTICE PARAMETERS INCLUDES ANGLE FUNCTIONS AND VOLUMES.

288 1620 40K LC HAENDLER,COONEY 16/RECIPROCAL LATTICE FROM DIRECT LWA
CALCULATES RECIPROCAL LATTICE PARAMETERS FROM DIRECT LATTICE PARAMETERS INCLUDES ANGLE FUNCTIONS AND VOLUMES.

289 1620 40K LC HAENDLER,COONEY 19/AXIAL TRANSFORMATION LWA
CONVERTS 3-DIMENSIONAL COORDINATE SYSTEM (A) TO SYSTEM B, GIVEN THE MATRIX OF TRANSFORMATION FOR (A) TO (B). WILL CONVERT RECIPROCAL OR DIRECT CELLS.

455 1620 40K LF AHMED LF AND WILSON PLOT LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. COMPUTES SIN SQ THETA AND LF FOR MAX. OF 10 F-CURVES. EVALUATION OF TF AND SCALE BY WILSON PLOT OPTIONAL. PREPARES INPUT TO PROGRAM NO. 369.

8044 1620C20K LF KING ERA121/SUBTABULATION LWA
INTERPOLATES PUBLISHED LF TABLES TO GIVE TABLES AT ANY DESIRED INTERVAL USES INDIRECT ADDRESSING

488 1620 20K LF SHIONO SPS,CARD,4 POINT INTERPLN. LWM
F VS. SIN OR SIN/LAMBDA TABLE OF DESIRED INTERVAL FROM LIT.VALUES. DIV.MF,TNF,IA FEATURES. IBM LIBR. 8.4.003

498 1620-2 LP BRYDEN CORR INT FROM EQUI-INCL WEISS LPA
CORRECTS EQUI-INCLIN WEISS PHOTOS FOR LP AND FOR UPPER-LAYER SPOT EXTEN BY THE METHOD OF PHILLIPS. CARD INPUT AND OUTPUT.

489 1620 20K LP SHIONO SPS,CARD,NORMAL-B./EQUI-INCLIN. LWM
WITH OR WITHOUT EXTENDED SPOT CORRECTION BY PHILLIPS.DIV,MF,IA FEATURES IBM LIBR. 8.4.002

527 1620T20K LS OT IT JOHNSON/PATT* LS SUMS SOLVER - PARAMETER SHIFTER LPA
PARAMETER CORRECTIONS ARE COMPUTED BY SOLVING LEAST SQUARES SUMS WHICH ARE PART OF OUTPUT FROM PGM 372. NEW PARAMETER TAPE IS PREPARED FOR INPUT INTO ANOTHER CYCLE OF LEAST SQUARES WITH PGM 372.

521 1620 40K PI HAENDLER,COONEY POWDER INDEXING PROGRAM LWA
FROM ACTA CRYST., 16,1243(1963), BASED ON ITO METHOD

7547 1620 20K R DAMIANI FAST,R FOR SYSTEMATIC TRANSLATION MNA
AND ROTATION IN THE SPACE OF ONE OR MORE ASYMMETRIC UNITS.THE NUMBER OF REFLEXIONS IS 120 AT MOST

3048 1620 60K R MASLEN AGREEMENT ANALYSIS LWA
R-FACTOR IS CALCULATED FOR SPECIFIED INCREMENTED RANGES OF FOBS,SIN THETA SQUD.,H,K,ANDL. SLOWER FT2 VERSION FOR 20K MACHINE AVAILABLE

8048 1620C20K SCL TF KING ERA256/PATTERSON SHARPENER LWA
WILSON PLOT FOR SCL/TF. CALCULATES NORMALIZED STRUCTURE FACTORS AND COEFFICIENTS OF SHARPENED PATTERSON. USES INDIRECT ADDRESSING.

402 1620 SPS SF CAUGHLAN 400/410 PARAMETER GEN AND SF CALC LWA
20K OR MORE, AUTO DIV. CALC SF W ISO TEMP FACTOR. ANY SPACE GROUP

8043 1620 SF KING ERA164/TRICL PPA

487 1620 20K SF SHIONO SPS,CARD, TRI,MONO,ORTHO LWM
INDIV.ISOTROPIC. UP TO 150 ATOMS ONE PASS, ANY AXIAL SETTING, ANY NO. OF REFLEXIONS. DIV.IA,MF,TNF FEATURES. IBM LIBR. 8.4.004

403 1620 SPS SF SVETICH 402/STRUCTURE FACTOR RESCALE LWA
20K OR MORE, AUTO DIV

7544 1620 20K SF 3 DAMIANI FAST,ISOTROPIC AND ANISOTROPIC TF MNA

NO GENERAL,AVAILABLES SPACE GROUPS 1,2,7,8,14 INTERNATIONAL TABLES

8046 1620C20K SF LS KING ERA302/BLOCK DIAGONAL LS LPA
TRICLINIC,MONOCLINIC,ORTHORHOMBIC SPACE GROUPS. PARAMETERS = FSCALE, POSITIONS,ISOTROPIC TF. UP TO 68 ATOMS OF 9 TYPES IN ASYMMETRIC UNIT USES INDIRECT ADDRESSING.

457 1620 40K SFLS MAIR/AHMED LS REFINEMENT. BLOCK DIAGONAL. LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. COMPUTES SF AND ACCUMULATES LS TOTALS. GIVES NEW VALUES FOR ATOMIC COORDS, ISO AND/OR ANISOTROPIC TEMPERATURE PARAMETERS, R, BONDS, ANGLES. ALL SPACE GROUPS

369 1620 SF R SCL AHMED SF+R+SCL ALL SPACE GRPS. VERY FAST LWA
SF R SCL. 1620 WITH 40K DIGITS, CARD I/O, AUTOMATIC DIVIDE + INDIRECT ADDRESSES. CALCULATES SF FOR ALL SPACE + PLANE GRPS. ALSO R + SCL. MAX. OF 50 ATOMS, 10 F-CURVES. ISOTROPIC T.F. AT PRESENT. VERY FAST.

355 1620T20K SPC H JOHNSON/PATT* GONIOSTAT SETTINGS LWA
G. E. GONIOSTAT ANGULAR SETTINGS FOR TRICLINIC OR HIGHER SYMMETRY. REQUIRES A REFLECTION AT CHI NINETY. OUTPUT SEQUENCE ARRANGED TO MINIMIZE DUPLICATE ANGLE SETTINGS.

462 1620 20K SPC H LP PIPPY/AHMED* (HKL) + GONIOSTAT SETTINGS + 1/LP LWA
CARD I/O, AUTOMATIC DIVIDE, INDIRECT ADDRESSES. GENERATES INDICES AND CALCULATES PHI, CHI, 2THETA, AND 1/LP FOR ALL REFLEXIONS WITHIN ANY PART OF SPECIFIC SPHERE IN RECIPROCAL SPACE. ALL SYSTEMS.

8049 1620C20K SPC H KING ERA270/GONIOSTAT SETTER LPA
GONIOSTAT SETTINGS AND LP FOR ALL REFLEXIONS IN GIVEN SPHERE. USES INDIRECT ADDRESSING.

5062 1620FTN2 SPEC SEGMUELLER SIMULTANEOUS BRAGG REFLEXIONS LWA
COMPUTES AZIMUTHS OF SIMULTANEOUS BRAGG REFLEXIONS (UMWEGANREGUNG) FOR ALL POSSIBLE PAIRS OF LATTICE PLANES FOR A GIVEN MAIN REFLEXION IN CUBIC AND HCP CRYSTALS. 40K.

5011 2002 DIR BEITINGER-HOP* SIGN DET WITH DOUBLE PATT FUNCTIONS LXA

5027 2002 FR 2,3 HILDEB,HAHN* GEN VERS BL GRID VARIABLE LWA
FOR 2002 WITH PUNCHED CARD ACCESSORIES. SECTIONS PARALLEL A,B IN HEIGHTS Z. SIZE AND DENSITY OF GRID IN A,B AND Z-VALUES MAY BE SPECIFIED BY USER. ANY SYM. IT VIA CARDS, ONE FOR EACH H,K,L COMBINATION,SORTED ON L,K,H. OT ON DIRECT PRINTER. (SEE PGM NO. 5009)

5053 2002 FR 2,3 PLEHWE,BAERNIG* BL. A OR C. FR 3 OR SECTIONS OR PRO- MWA
JECTION OR PROJECTED SLABS PARALLEL X,Y. SIZE AND DENSITY OF GRID MAY BE SPECIFIED BY USER. BLK POSSIBLE. IT AND OT VIA TAPE. 5000 WORD MAGNETIC CORE AND 10000 WORD DRUM MEMORY NECESSARY.

5056 2002 H PLEHWE,BAERNIG* H FOR THE 14 BRAVAIS LATTICES WITHIN MWA
GIVEN LIMITING SPHERE, CALCULATION OF Q-VALUES FOR GIVEN RECIPROCAL LC AND SORTING BY INCREASING Q. OT HKL AND 4THETA OR SQARE OF SIN(THETA) OR 2SIN(THETA) OR D.

5057 2002 ID PLEHWE,BAERNIG* DISTANCES AND ANGLES BETWEEN MWA
SPECIFIED ATOMS ARE CALCULATED. ANY SYMMETRY.

5054 2002 SF 3 PLEHWE,BAERNIG* A OR C OR INSERTS FOR SPACE GROUPS. MWA
UNLIMITED NUMBER OF REFLEXIONS, UP TO 333 ATOMS AND 20 LF TABLES. INDIVIDUAL ISOTROPIC TF, IF NEEDED. R AND SCL, IF FO-VALUES ARE GIVEN. IT AND OT VIA TAPE.

5055 2002 LP WEIS PLEHWE,BAERNIG* LP CORRECTION FOR EQUI-INCLINATION MWA
WEIS DATA FOR ANY LAYER ABOUT ANY DIRECTION UVW. IT RECIPROCAL LC, ZETA UVW, HKL AND INTENSITY. OT SF AND SQUARE OF SF.

267 205 EL DARWIN, SMITH TB71/RADIAL DISTR FUNCTION LWM

269 205 EL DARWIN, SMITH TB102/LEAST SQU REFINEMENT LWM

266 205 FR 2 EVANS/BURROUGHS TB59/PROJECTIONAL FOURIERS LWM
PROGRAM DEVELOPED BY US GEOLOGICAL SURVEY AND DISTR BY BURROUGHS CORP. OUTPUT IS ON 407 TABULATOR.

114 205 FR 3 MARSH,EICHHORN TB22/FOURIER AND VECTOR MAPS LWM
GENERAL FOURIER SYNTHESIS ACCORDING TO BEEVERS-LIPSON PRINCIPLE, IN UP TO 76-TH CELL EDGE FOR ALL SPACE GROUPS. PRINTS FIGURE FIELD DIRECTLY, NEGATIVE VALUES IN RED. PERMITS FORMATING FOR OBLIQUE CELLS AND APPROXIMATE RATIO OF EDGES.

111 205 H EICHHORN TB19/LATTICE POINT GENERATION LWM
PROGRAM GENERATES ALL POSSIBLE INDEX COMBINATIONS WITHIN GIVEN LIMITING SPHERE, SUBJECT TO SPACEGROUP CONSTRAINTS. PRINTS LIST OF PERMITTED (HKL) WITH THEIR SINESQUTHETA VALUES.

112 205 ID E EICHHORN TB20/BONDS,ANGLES AND ERRORS LWM
GIVEN ATOMIC POSITIONS WITH THEIR ESD VALUES, COMPUTES ALL BONDS THAT ARE LESS OR EQUAL TO SUPPLIED MAXIMUM VALUE. CALCULATES MOST PROBABLE ERROR OF DISTANCES. THEN COMPUTES REQUIRED ANGLES AND THEIR MPE.

113 205 LP 3 EICHHORN TB21/LP FOR PRECESSION LWM
PROGRAM COMPUTES LP FACTORS ACCORDING TO WASER FORMULA, THEN PROCESSES INTENSITIES AND PRINTS LIST OF (HKL),RAW INT, FSQU, F AND SINESQUTHETA.

115 205 LP 3 EICHHORN TB23/LP OSCILLATION-ROTATION-WEISSBG LWM
PROGRAM USES DIRECT EXPRESSION FOR LP FACTOR, HAS OPTION FOR ROTATION-OSCILLATION OR WEISSENBERG EQUI-INCLINATION CASE. PROCESSES RAW INT DATA AND FURNISHES LIST OF (HKL). INT, F, FSQU AND SINESQUTHETA.

260 220 DF EICHHORN TB58A/P-BAR-ONE DIFF SYNTH LWM
COMPLETE MATRIX WITH INDIVIDUAL ANISOTROPIC DEBIJE-WALLER FACTORS. PROGRAM CAN BE OVERLAID FOR OTHER CENTRIC SPACEGROUPS. DEPENDING UPON SYSTEM MAKEUP CAN ACCOMODATE UP TO 99 ATOMS OF UP TO 8 SCATTERING TYPES. NO RESTRICTION ON NUMBER OF REFLEXIONS.
PROGRAMS TB 58B THROUGH G DOVETAIL INTO TB 58A.

298 220 DP SILVERTON X-2A/LP + PREP DATA TAPE FOR =117 LPA

265 220 FR 3 HOOGSTEEN,EICHH TB58G/FOURIER AND VECTOR MAPS LWM
PROGRAM CONTAINS SCHOMAKER-SHARPENING SUBROUTINE FOR PATTERSON VECTOR MAPS. OUTPUT IS ON 407 TABULATOR. GRID INTERVALS UP TO 1/100 OF EDGE.

300 220 FR 3 SILVERTON X-4C/ADAPTATION PROG 2 TO 3 LPA
PRELIM. 1D SUMMN. FOR ANY MONOCLINIC CENTRIC SP GP.
TO ADAPT HOOGSTEEN 2D PROG. FOR 3D

264 220 H S EICHHORN TB58F/UNIT CELL AND LATTICE POINT GEN LWM
FIRST COMPUTES RECIPROCAL CELL FROM DIRECT CELL, OR VICE-VERSA. THEN GENERATES, SUBJECT TO SPACEGROUP CONSTRAINTS, ALL POSSIBLE (HKL) WITHIN GIVEN LIMITING SPHERE.

261 220 ID E EICHHORN TB58B/POSITIONS,BONDS,ANGLES AND ESD LWM
PROGRAM FIRST COMPUTES ESD FOR ATOMIC POSITIONS ACCORDING TO CRUICKSHANK EXPRESSION, THEN COMPUTES DISTANCES AND ANGLES AND THEIR MPE.

262 220 LF EICHHORN TB58C/PREP OF SCATT CURVES LWM
CURVEFITS GENERALLY SUPPLIED (INT.TABLES,ETC) LITTLE F TO YIELD A SET OF PUNCHED CARDS AS STANDARD INPUT FOR TB 58A.

116 220 LF S EICHHORN TB41/HARTREE WAVEFIELD TO LITTLE F LWM
INPUT TO PROGRAM ARE SELFCONSISTENT FIELD WAVEFUNCTIONS WITH P AS FUNCTION OF R IN BOHR RADII. ROUTINE INTEGRATES WAVEFUNCTIONS PER SHELL, MULTIPLIES INDIVIDUAL VALUES BY ELECTRON OCCUPANCY, TOTALS FOR ALL SHELLS AND PRINTS ATOMIC SCATTERING FUNCTION AT INTERVALS OF 0.02 IN SINETHETA OVER LAMBDA. INTEGRATION PROCEDURE IS BY OVERLAP-CURVEFITTING.

263 220 LP 3 EICHHORN TB58E/LP OSCILLATION-ROTATION-WEISSBG LWM
PROGRAM USES DIRECT EXPRESSION FOR LP FACTOR, HAS OPTION FOR ROTATION-OSCILLATION OR WEISSENBERG EQUI-INCLINATION CASE. PROCESSES RAW INT DATA AND FURNISHES LIST OF (HKL), INT, F, FSQU AND SINESQUTHETA.

268 220 LS S HEBERT/BURR TB97/LS PLANE WASER-MARSH METHOD LWM
PROGRAM WILL ACCEPT A MAXIMUM OF 50 POINTS, WILL FIRST ORTHOGONALIZE POSITIONS AND THEN COMPUTE OPTIMUM LEAST SQUARES PLANE.

297 220 SPC SILVERTON X-1/GONIOSTAT SETTINGS LPA

7563 6001 1K AT MUSATTI SHIFTS OF AT LPA
CALCULATES THE SHIFTS OF ANISOTROPIC THERMAL PARAMETERS FROM OBS AND CALC DERIVATIVES BY NARDELLI-FAVA METHOD. THIS METHOD MAKES CALCULATION INDEPENDENT OF THE NUMBER OF REFLECTIONS.

7565 6001 1K AT SD ANDREETTI ANISOTROPIC THERMAL PARAM SD LPA
CALCULATES SD OF ANISOTROPIC THERMAL PARAMETERS BY CRUICKSHANK FORMULAE.

7561 6001 1K DF 2 3 MUSATTI GEN 2 AND 3D DF LPA
CALCULATES THE ELECTRON DENSITY, 3 FIRST DERIVATIVES AND 6 SECOND DERIVATIVES AT ASSUMED ATOM POSITIONS (NO RESTRICTIONS ON NUMBER OF REFLECTIONS AND OF POSITIONS) AND THE ATOMIC SHIFTS FOR OBS AND CALC DATA IN ORTHORHOMBIC, MONOCLINIC, AND TRICLINIC SPACE GROUPS.

7566 6001 15 DP ANDREETTI LS PLANE POL COORD BONDS ANGLES LPA
CALCULATES WEIGHTED PLANE THROUGH GIVEN POINT USING LS METHOD, AND DETERMINES STATISTICAL SIGNIFICANCE OF DISTANCES FROM THIS PLANE. CALCULATES POLAR COORDS. FOR REPRESENTATION OF ATOMIC ENVIRONMENTS. GIVEN ATOMIC POSITIONS WITH THEIR E.S.D. VALUES, COMPUTES ALL BOND DISTANCES THAT ARE LESS THAN OR EQUAL TO SUPPLIED MAXIMUM VALUE, AND ALL POSSIBLE ANGLES. E.S.D. OF BOND DISTANCES AND ANGLES ARE CALC.

WITH DARLOW FORMULAE.

7506 6001 1K DP PANATT/LOMBARD* RESCALING FOR SF LWM

7509 6001 1K DP PREC PANATTONI,ZANO* LP LF THETA LWA

7512 6001 3K DP SCLTF PANATTONI,ZANO* WILSON PLOT RESCALING LWA

7507 6001 1K DP WEIS PANATTONI,ZANO* LP LF THETA LWA

7502 6001 1K FR 2 A PANATT/DEGRIF* FR BLK LWM

7501 6001 1K FR 2 C PANATT/DEGRIF* FR BLK LWM

7503 6001 1K FR 3 PANATT/LOMBARD* FR BL CENTRIC/ACENTRIC LWM

7554 6001 1K FPK DOMENICI,ZUCCA FPK AND STOKES CORRECTION LWA
CONVERTS THE 2 THETA DATA IN FUNCTION OF S, PERFORMS FOURIER INVERSION OF THE EXPERIMENTAL PEAK SHAPE AND OF THE STANDARD PEAK, GIVES AVERAGE CRYSTALLITE SIZE AND THE CORRECTED PEAK SHAPE BY FURTHER INVERSION.

7553 6001 1K FT DONENICI,ZUCCA FT FUNCT.R,S MAX,CORR.TERM.EFFECTS LWA
CONVERTS THE 2 THETA DATA IN FUNCTION OF S, 2 WAVE LENGTHS ACCEPTED, PERFORMS FOURIER INTEGRAL AS FUNCTION OF R AND/OR S MAX, CORRECTS TERMINATION EFFECTS BY EXTRAPOLATION.

7555 6001 1K ID DOMENICI,MIGLIO RDF,PERFECT CRYSTAL,MULTI ATOMS NPA
GIVES A LIST OF THE INTERATOMIC DISTANCES FROM R = 0 TO R = 15 ANGSTROMS, ARRANGED ACCORDING TO THE NUMBER AND TYPE OF COORDINATED ATOMS. PRESENTLY ABBREVIATED FOR SIMPLE CASES.

7558 6001 LP DOMIANO SPOT EXTEN. LP CORR 3 AXES LPA
CALCULATES LORENTZ POLARIZATION AND REFLECTION SPOT EXTENSION CORRECTIONS FOR REFLECTIONS TAKEN ABOUT 3 AXES.

7556 6001 LS C PANATT/GRUB LS/3D BLOCK 3X3 6X6 1X1 AT LWA
ALL SPACE GROUPS, NO LIMIT ON ATOMS AND REFLECTIONS, PARAMETERS,POSITIONS

7564 6001 1K PARAM SD MUSATTI POS PARAM SD LPA
PROGRAM CALCULATES STANDARD DEVIATIONS OF ELECTRONIC DENSITY AND OF FIRST AND SECOND DERIVATIVES AND OF POSITIONAL PARAMETERS ON A GIVEN ATOMIC PEAK.

7559 6001 SCL LS DOMIANO LS SC FAC DETN FOR MAX18LAYERS 2AX LPA
CALCULATES INTERLAYER SCALING FACTOR FOR TWO AXES DATA BY LEAST SQUARES FROM EIGENVALUES AND EIGENVECTORS OF SYMMETRIC MATRIX UP TO ORDER 18. CALCULATES SCALED AND AVERAGED INTENSITIES FOR REFLECTIONS OBS ON MORE THAN ONE LAYER.

7511 6001 3K SCLTF LS PANATTONI,ZANO* RESCALING SF LWA

7504 6001 1K SF 3 A PANATT/DEGRIF* LWM

7505 6001 1K SF 3 C PANATT/DEGRIF* LWM

7562 6001 1K SFRS R MUSATTI SF RESC AND R DETN LPA
RESCALES SF AND CALCULATES R FOR ALL REFLECTIONS OR FOR SINGLE LAYERS.

7560 6001 1K TF LS ANDREETTI SCL AND TF BY LS FROM WLP LPA
SCALE AND TEMPERATURE FACTORS ARE CALCULATED FROM THE LEAST-SQUARES STRAIGHT LINE.

34 650 ABS SANDS ABCOR/PLOTS ABS COR TEMPLATE FOR WEIS

5029 650 DP BARTL SCL AND OVERALL TF (WILSON'TEST) LWA
PREPARES DATA FOR WILSON'PLOT. K AND B MUST BE EVALUATED GRAPHICALLY. PROGRAM THEN APPLIES SCL AND TF TO LP'CORRECTED INTENSITIES.

5028 650 DP BARTL PL AND ABS CORRECT FOR EQUI WEIS LWA
CORRECTS I OBS FOR LP'FACT. ABSORPTION
CORRECTION BY MEANS OF TABLE OF A(SIN THETA)
SUPPLIED BY USER COMPUTES ALSO SIN THETA.
APPLICABLE FOR EQUIINCLINATION WEIS. (MONOCLINIC AND HIGHER SYM).

185 650 DP BROWN/LINGFTR*/5306 WILSON PLOT, SCL AND TEMP FACTOR MWA
LIMITED TO MONOCLINIC OR TRICLINIC SYMMETRY

180 650 DP BROWN,STEWART/LINGFTR*/530X DATA REDUCTION LWA
5301,5302/FORM FACTOR INTERPOLATION AND STORAGE FOR DATA REDUCTION
5303/DATA REDUCTION, LP 3 WEIS, MONOCLINIC SYMMETRY AND HIGHER
5304/DATA REDUCTION, LP 3 WEIS, ALL SYMMETRIES
5305/DATA REDUCTION, LP 2 PREC, MONOCLINIC SYMMETRY AND HIGHER

5036 650 DP DIETRICH X1/SHARPENING (VARIABLE FUNCTION) MWA
IT CONSTANTS FOR SHARPENING FUNCTION. OT OF (5040) OR (5041)
OT (5040) OR (5041) CARDS RESPECTIVELY, CONTAINING SHARPENED FO

5041 650 DP DIETRICH X10/INTERPOLAT SCAT FAC,CORREL LAYERS MWA
IT SCL FOR LAYER, UP TO 10 FORM FACTOR TABLES FROM LITERATURE (WIDE INTERVALS, SIN THETA/LAMBDA, F), OT OF (5040) COMPLETED BY PUNCHING ABS FACTOR AND WEIGHT, AND/OR OT OF (5039)
OT FOR (5040)'CARDS INDICES, SIN**2 THETA/LAMBDA**2, WEIGHT, FO, UP TO

10 SCATTERING FACTORS (ACCURATE LOGARITHMIC INTERPOLATION)
FOR (5039)'CARDS SAME AS ABOVE EXCEPT WEIGHT AND FO
5042 650 DP DIETRICH X11/SELECTS DATA, SCALES, 1ST SUMM FR MWA
IT 1 CARD WITH 30 STATEMENTS ABOUT WANTED TYPE OF SYNTHESIS, GRIDS AND LOWER AND UPPER LIMITS FOR X,Y,Z, SUMMATION ORDER, CONDITIONS FOR THE SELECTION AND PROCESSING OF DATA. 1 CARD WITH 21 FURTHER STATEMENTS (CHANGABLE DURING RUN) ABOUT CONDITIONS FOR SELECTION AND PROCESSG OF DATA. OT OF (5037) OR (5038) OR/AND PREVIOUS OT OF (5042)FOR ADDITION
OT COMPLETE AND OPTIMAL IT FOR FR'PROGR (5047) FOR SECTION OR PROJECTION EXTRA CARD CONTAINING CHECK TOTALS, LARGEST COEFFICIENT
5044 650 DP DIETRICH X13/N(Z)'TEST MWA
IT LIMITS OF RECIPROCAL SPACE OF DATA, 2 STATEMENTS FOR AUTOMATIC SELECTION OF (OVERLAPPING) RANGES OF SIN**2 THETA/LAMBDA**2, SCL, OT OF (5040) OR (5041)
OT N(0.1)TO N(1.0)AND MEAN VALUES OF FO**2 AND SIN**2 THETA/LAMBDA**2 FOR ALL RANGES OF THE LATTER. MEAN VALUES OF N(Z) AND DIFFERENCES TO THEORETICAL VALUES FOR ACENTRIC AND FOR CENTERED STRUCTURE
5046 650 DP DIETRICH X15/SELECTS DATA,PRODUCE IT FOR(118) MWA
IT 8 STATEMENTS FOR SELECTION OF DATA AND TYPE OF SYNTHESIS WANTED,F000, VOLUME OF CELL, 2 SCL ONE OF WHICH CAN BE CHANGED DURING RUN, OT OF (5040), (5037) OR (5038)
OT COMPLETE IT FOR (118)
2 EXTRA CARDS CONTAINING MAXIMUM AND MINIMUM VALUES OF OT
181 650 DP ABS STEWART/LINGFTR*/5308 ABSORPTION CORRECTION MPA
LIMITED TO ZERO LEVEL WEIS DATA, RECTANGULAR CRYSTAL CROSS SECTION
5040 650 DP LP DIETRICH X9/CORRECTS EQUIINCL WEIS INT,SQ ROOT MWA
IT WAVE LENGTH, EQUIINCLINATION ANGLE, OT OF (5039), COMPLETED BY PUNCHING INTENSITIES
OT INDICES, SIN**2 THETA/LAMBDA**2, FO, FO**2, 1/LP, SQUARE ROOT OF LP
324 650 DP LP SHIONO INTENSITY CORR. WEISSENBERG MWA
BASIC 650. EQUI-INCL WEISS. PRINCIPAL OR NON-PRINCIPAL AXES ROTN
329 650 DP PATS SHIONO SHARPENED PATTERSON COEF PGM170,171 LWA
BASIC 650
5038 650 DP R DIETRICH X6/SCALES FO. AO,BO,FO-FC,AO-AC,BO-BC MWA
IT OT OF (5037)
OT INDICES, FO,FC, FO-FC. FOR SYMMETRY P1 ALSO AO, BO, AO-AC, BO-BC
3 ADDITIONAL CARDS CONTAINING 2 TYPES OF R AND MAXIMUM AND MINIMUM VALUES OF MAIN OT
325 650 E SHIONO STAND.DEV OF ELECTRON DENSITY ETC LWA
BASIC 650
302 650 FPK LP DEANGELIS/COHEN BL/FOURIER ANAL.OF PEAK SHAPES,STOKES LWA
COMPUTE OR READ IN SIN AND COS COEFF. OF ANNEALED PEAK. COMPUTES SIN AND COS STOKES CORR. COEFF. OF BROADENED PEAK AND VALUES OF SIN/COS. CORRECTS FOR VARIATIONS OF ANGULAR FACTORS ACROSS PEAK. OUTPUT 31 COEFF. AT 1/2 HARMONIC INTERVALS AND 9 COEFF. AT 1/4 INTERVALS FOR ALL PEAKS.
508 650 FR 2 BAUR GENL PROJ CC SS CS SC LWA
650 WITH INDEX REG, VARIABLE GRID.
356 650 FR PCH JENSEN CC SS SC CS TABLE EXPANS AND PCH OUT LWA
FROM 1 QUAD CC SS SC CS TABLES ON DRUM PCH 1 2 OR 4 QUAD OF THESE OR SUMS CC-SS OR SC + CS AND ADD ANY PREVIOUS PARTIAL CALC X2 OR X3 IN 20THS 25THS 40THS 50THS CONVENIENT TO CONTOUR DIRECTLY ON 402 OR 407 PRINT OUT
5047 650 FR 2 DIETRICH X22/GENERAL,FAST, WITH( ) SECTIONS MWA
IT OT OF (5042) AND EVENTUALLY OT OF PREVIOUS RUN OF (5047) FOR ADDITION
OT 1 HEADING' AND CHECK'CARD. SYNTHESIS (7 VALUES PER CARD)
170 650 FR 2 SHIONO,HELLNER,WOLFEL/GENL PROJ CC SS CS SC, N/250 MWA
FOURIER PROJECTION ALSO FOR PGM 171. FOR BASIC 650 OR WITH IXA, IAS AND UP TO 4 TAPES OR IXA, IAS, TAPES AND ON-LINE 407
172 650 FR2 JENSEN ENL PROJ,N/200,PATT,F,DELTA F LWA
171 650 FR 3 SHIONO FOURIER,PATT,DIFFERENCE N/60 MWA
MONOCL,ORTHO. USE OUTPUT OF PGM 176. PGM 170 USED FOR 2ND,ORD SUMS. IXA, IAS, UP TO 5 TAPES, ON-LINE 407(OPTIONAL).
198 650 FR3 JENSEN GENL,N/1000XN/200,PATT,F,DELTA F LWA
174 650 FR 3 DF SHIONO DIFFERENTIAL SYNTH LWM
MONOCL,ORTHO. USE OUTPUT OF PGM 176. BASIC 650 OR WITH IXA,IAS, 1 TAPE.
5039 650 H DIETRICH X8/LATTICE POINT GENERATION MWA
IT A*,B*,C*,ALPHA*,BETA*,GAMMA*,MAXIMUM OF SIN THETA/LAMBDA,TYPE OF DATA

WANTED (1,2,3 DIMENSIONAL, INDICES,FOR WHICH ALSO NEGATIVE VALUES HAVE TO BE CONSIDERED)
OT INDICES, SIN**2 THETA/LAMBDA**2. NO POINTS RELATED BY FRIEDEL LAW

290 650 H SVETICH 2010/LIMITING SPHERE REFLNS T.M.O LWA
PROGRAM CALCULATES AND PUNCHES ALL INDEPENDENT REFLECTIONS IN LIMITING SPHERE OF REFLECTION FOR TRICLINIC MONOCLINIC AND ORTHORHOMBIC SYSTEMS SECOND SETTING ONLY FOR MONOCLINIC SYSTEMS

183 650 HYDROGEN STEWART,LINGFTR*/5105 H COORDS,BOND LENGTHS,ANGLES LWA
CALCULATES BOND LENGTHS AND ANGLES, GENERATES HYDROGEN POSITIONS FOR TERMINAL AND CHAIN TETRAHEDRAL, TRIGONAL, TERMINAL, OR H-BONDED ATOMS FOR SPECIFIED ATOM-HYDROGEN DISTANCES, MONOCLINIC OR HIGHER

221 650 ID LINGFTR*,BROWN/5112 INTERMOLECULAR DISTANCES LWA
GENERATES AND STORES RELATED ASYMMETRICAL UNITS SPECIFIED AND CALCULATES ALL INTER- AND INTRA-ATOMIC DISTANCES WITHIN MIN-MAX SPECIFIED LIMITS

184 650 ID SHIONO DIST,ANGLES,S.D. OF ANGLE, ANY SYM LWA
BASIC 650

220 650 ID STEWART,LINGFTR*,BROWN/5102 BOND LENGTHS, ANGLES LWA
CALCULATES BOND LENGTHS AND ANGLES BETWEEN SPECIFIED ATOMS WHOSE COORDINATES ARE STORED IN MEMBORY, MONOCLINIC OR HIGHER SYMMETRY

327 650 LF SHIONO 4 POINT INTERPOLATION, PGM 176 LWA
650 WITH IXA., ON-LINE 407(OPTIONAL) PREPARES ATOMIC F TABLE

133 650 PABSPROF MUSILBEUTHOMAS GOODYEARATOMICREPORTGATDM829DECK806 LWA
PROGRAM WRITTEN FOR IBM 650 TO CALCULATE COMBINED ABSORPTION AND RADIAL DIVERGENCE CORRECTIONS FOR DEBYE-SCHERRER POWDER DIFFRACTION LINES. PROCEDURE THAT OF TAYLOR AND SINCLAIR)PROC. PHYS. SOC. LONDON,57, 1945) FOR DIVERGENT RADIATION. MACHINE CALCULATION TIME ABOUT TWO AND ONE-HALF HOURS. INPUT DATA. SAMPLE RADIUS, TARGET TO SAMPLE DISTANCE, CAMERA RADIUS, MEASURED 2Θ, LINEAR ABSORPTION COEFFICIENT OF SAMPLE. PROGRAM OUTPUT IS RELATIVE INTENSITY VS. 2Θ, REFERENCED TO TRUE 2Θ POSITION.

509 650 LP BAUR PREC ANY LEVEL LPA
650 WITH INDEX REG AND FLOAT.PT., ANY SYMMETRY.

182 650 PLANE STEWART/LINGFTR*/5103 LEAST SQUARES PLANE LWA
CALCULATES LS PLANE FOR MONOCLINIC AND HIGHER SYMMETRY, RESTRICTED TO TOTAL OF 98 ATOMS AND 0.0035A MIN PLANE-ORIGIN DISTANCE

218 650 R SCL BROWN,STEWART/LINGFTR*/440X FO DATA RESCALING LWA
4400,4401/FO RESCALING AND STATISTICS PROGRAMS
4402/APPLIES OVERALL ISOTROPIC TEMP FACTOR CORRECTION BEFORE RESCALING

5043 650 SCL TF DIETRICH X12/WILSON PLOT MWA
IT LIMITS OF RECIPROC. SPACE OCCUPIED BY DATA,2 STATEMENTS FOR AUTOMATIC SELECTION OF AND OVERLAPPING OF INTERVALS OF SIN**2 THETA/LAMBDA**2, OT OF (5041)
OT ALL POINTS OF WILSON PLOT, SCL AND TF CALCULATED BY FITTING STRAIGHT LINE TO THE POINTS BY LS

5037 650 SF AT DIETRICH X5/CALCULATES ALSO SCL MWA
IT COORDINATES OF UP TO 200 ATOMS, CONSTANTS FOR UP TO 58 AT AND FOR UP TO 42 ISOTROPIC TF, SYMMETRY (P1 OR P-1), OT OF (5041)
OT INDICES, WEIGHT, FO, FC. FOR SYMMETRY P1 ALSO AC, BC, AC/FC, BC/FC EXTRA CARD SCL (CALCULATED BY LS OF WEIGHTED FO-FC)

177 650 SF AT 3 BROWN,JENSEN,LINGFTR*,STEWART/400X,420X/ LWA
4000,4010/PARAMETER LOADING AND GENERATION PROGRAMS
4001,4002/AT 2 ONLY WITH PARTIAL CONTRIB, MAX 100 ATOMS, 8 TYPES
4201/AT 3 AND DISPERSN CORRECTIONS, MAX 100 ATOMS, 8 TYPES, ANY ORDER

176 650 SF AT 3 SHIONO TRICL,MONOCL,ORTHO,8 KIND, 50 UNIQ LWA
ISOTROPIC OR ANISOTROPIC. BASIC 650 OR WITH IXA OR WITH IXA, IAS.

235 650 STAT ALDEN,STOUT* 1420/UNIT SF, WILSON + HPR STAT TESTS LPA

5031 650 STAT BARTL VARIANCE'TEST LWA
COMPUTES SPECIFIC VARIANCE FROM F SQUARED,PUT ON ABSOLUTE SCALE BY WILSON TEST.

5030 650 STAT BARTL N(Z)'TEST LWA
PREPARES DATA FOR N(Z)'PLOT.

219 650 TF STEWART/LINGFTR*/4500 TF CORR BY LST SQ LWA
CALCULATES LST SQ ISOTROPIC TEMP FACTOR AND SCALE FACTOR CORRECT FROM OUTPUT OF STRUCT FACTOR PROGRAMS (IUCR 177) FOR FO RESCALING (IUCR 218)

326 650 TF SHIONO ANISOTROPIC TF FROM PGM 174,176 LWA
BASIC 650. USE OUTPUT OF PGM 174

328 650 TF UNIF SHIONO WILSON PLOT, UNITARY SF LPA
650 WITH IXA,IAS, ON-LINE 407.

233 704 DIR WOOLFSON MULTIPLE SOLUTION DIRECT METHOD
DIRECT SIGN DETERMINATION USING METHOD OF STRUCTURE INVARIANTS AND Z-TEST -- MULTIPLE SOLUTION RESULTS DISPLAYED AS FOURIER MAPS. WRITTEN IN FORTRAN.

5025 704 8K FR 2,3 HILDEB,HAHN* GENER VERS BL GRID VARIABLE LWA
CALCULATES SECTIONS PARALLEL A,B IN HEIGHTS Z. SIZE AND DENSITY OF GRID IN A,B AND Z'VALUES MAY BE SPECIFIED BY USER. C AND A BY SENSE SWITCH. ANY SYM.IT HALF REC LATT, ONE CARD PER HKL COMBINATION, SORTED ON L,K,H. IT AND OT VIA TAPE.

118 704 8K FR 2 3 SLY,SHOEMAKER* MIFR1/GENL,FAST,BL,GRID N/120 LWA
SAP PROGRAM BEEVERS-LIPSON PRINCIPLE FAST TABLE LOOK-UP. APPLICABLE TO ANY SPACE GROUP THRU ORTHORHOMBIC BY SELECTION OF SYMMETRY CARDS. INPUT IS ONE CARD EACH UNIQUE REFLECTION. CARDS ARE SORTED ON INDICES AND PUT ON TAPE. STRAIGHT OR DIFFERENCE FOURIER POSSIBLE. VARIABLE FORMAT OUTPUT SHEETS PERMITS DIRECT CONTOURING. CALC UP TO 100,000 TERM POINTS PER SEC ON 32K 704. OPERATES ON 32K 709 WITH COMPATIBILITY. HAS BEEN REWRITTEN FOR BIM 709/7090 (PGM 357).

301 704 4K LC MOZZI,NEWELL RM1/THRU MONO, STD CALIBRATED LS DETN LWA
DETERMINES LATTICE CONSTANTS FOR MONOCLINIC AND HIGHER SYMMETRY SYSTEMS BY LEAST SQUARES METHOD UTILIZING AN ITERATIVE PROCEDURE9 DESIGNED FOR DIFFRACTOMETER MEASUREMENTS CALIBRATED BY USING A STANDARD AND THEREFORE NO EXTRAPOLATION FUNCTIONS ARE INCLUDED9 COMPUTES D VALUES FOR REQUESTED (HKL) SETS.

4002 704FT28K 2DIRC WOOLFSON,SPARKS LWM
INPUT DATA -- LC AND SF OR INTENSITIES. OUTPUT - FR FOR ACCEPTABLE SETS OR SIGNS. 7 PACKS OF CARDS RUN CONSECUTIVELY. REQUIRES OPERATOR INTERVENTION AT SOME POUNTS. USES PRINCIPLES DESCRIBED IN ACTA CRYST 10,116/11,277/11,393.

397 7040-44 FR3 HARRIS,D.R. ERFR3/MAP LPA
SUBSTANTIAL REVISION OF ERFR2 FOURIER OF SLY-SHOEMAKER-VAN DEN HENDE, BASICALLY A FAP TO MAP CONVERSION. CHANGES INCLUDE SOME ADDITIONAL OPTIONS AND TAPE ASSIGNMENT CHANGES WITHOUT REASSEMBLY.

383 7070 AUC COORD SCHAPIRO GENERATES ADDTL AT COORDS

381 7070 AUC FTN CLAY SHIONO MCEWEN FT FOR LAYER STRUCTURE(CLAY) LWA
FOR CLAY MINERALS. REF. KOLLOID Z.,149,96(1956).

511 7070 AUC FR2 A CHU,MCMULLAN MONOCLINIC A OR C PROJECTION LWA
USE OUTPUT OF PGM.330. 10K, 2 CHNL. ON-LINE 7500,7400 OR TAPE-1401

512 7070 AUC FR3 A CHU,MCMULLAN MONOCLINIC CENT/NONCENT. LWA
USE OUTPUT OF PGM330. 10K,2 CHNL. ON-LINE 7500,7400 OR TAPE-1401 SYSTEM NUMERIC OR ALPHABETIC OUTPUT FOR DIRECT PLOTTING

331 7070 ID CHU DIST.ANGLE,S.D.OF ANGLE, ANY SYM. LWA
FORTRAN, 10K(5K), 7400, 7500

332 7070 ID CHU INTER-,INTRA-MOLECULAR DIST.ANY SYM LWA
FORTRAN, 10K(5K), 7400, 7500

382 7070 FTN PLANE CHU ANY SYM. 50 ATOMS MAX. LWA

330 7070 SF 3 SHIONO TRICL,MONOCL,ORTHO LWS
10K(5K) CORE,7400,7500,2 CHNL 2 TAPE. INDIV ISO TF. 13 KIND,1500 ATOMS AVAILABLE THROUGH GUIDE

510 7070 AUC SF3 AT SHIONO SFIIA/ANY SYM. 460 ATOMS LWA
10K, 2 TAPES(2 CHNL.)CAN BE USED WITH ON-LINE 7400,7500 OR TAPE-1401 SYSTEM WITHOUT CHANGE.

338 7090 ABS BURNHAM GNABS/CORR FOR XLS OF ARBITRARY SHAPE LWA
FORTRAN2, AND FAP (NO IT-OT), SUBROUTINES FOR EQUI-INCL WEIS GEOMETRY. EASILY MODOFIED FOR GONIOSTAT GEOMETRY. 6010 + 13482 (COMMON) LOCATIONS. CHOICE OF 64, 216, 512 INTEGRATION POINTS. LIMITS - 25 XTL FACES (NO REENTRANT ANGLES), 25 RECIPROCAL LATTICE LEVELS.

5065 7090 FT2 ABS SCHULTZERHONHOF BN-ABS/ABS LWA
MODIFIED VERSION OF BUSING OR-ABS (PGM 362). IT FROM BN-ST1, OT FOR BN-ST2. RUNS INDEPENDENTLY OR WITH BN-X-64.

8018 7094 CONTOUR ANZENHOFER PLOT OF FOURIER MAPS. LWA
PREPARES A MAGNETIC INPUT TAPE FOR AN AUTOMATIC PLOTTING DEVICE. PARTS OF THE PROGRAM THAT DEPEND ON THE PLOTTER USED ARE INDICATED.

519 7090 45K CONTOUR CHERIN,MARTIN PLOTS CONTOURS,LOCATES MAXIMA MPA
PROGRAM PLOTS THE RESULTS OF A FOURIER SYNTHESIS IN THE FORM OF CONTOURS.

THE POSITIONS OF THE MAXIMA ARE DETERMINED PLOTTED. PROGRAM REQUIRES 40757 OCTAL STORAGE POSITIONS.WRITTEN IN FORTRAN

368 7090 CONTOUR VAN DEN HENDE ERSCP/OT ERFR2 TO TAPE FOR SCOPE NNX
TAKES THE BINARY OT FROM ERFR2 AND PRODUCES A BINARY TAPE WHICH CAN BE USED TO PRODUCE CONTOUR MAPS ON AN OSCILLOSCOPE.

49 709,7094 D H Q L* WOLTEN CALC ABOVE +THETA FROM LC,FT2,9PROGS LWA
2 OT LISTS, ORDERED ON H AND ON D

5058 7090 FT2 D,P KASPER,SCHMDMT* DWPULV/D,THETA FROM P LWA
DWPULV CALCULATES SIN,D,1/D**2,1/D AND CORRECTIONS BY K-ALPHA 1-2 SPLITTING FOR POWDER FILMS ACCORDING TO THE ASYMMETRIC METHOD. RELIABLE REFLEXES ARE DISTINGUISHED AND USED TO CALCULATE THE LENGTH OF THE FILM.

406 709,7094 D Q WOLTEN TABLES D,Q VS 2THETA INCR 0.01DEG LWA

8017 7094 DIR ANZENHOFER HARKER-KASPER INEQUALITIES LPA
INEQUALITIES OF THE TYPE 1-6 (SEE AC 3,436) CAN BE EVALUATED.THE PROGRAM IS USED AS PART OF A SYSTEM FOR APPLICATION OF DIRECT METHODS.

475 7094 32K DP CETLIN,B.B. CALCS SF AND STD LPA
FORTRAN PROGRAM TO COMPUTE AVERAGE VALUES FOR EACH STRUCTURE FACTOR WITH OBJECTIVE STANDARD DEVIATIONS.

303 709 DP PALENIK 14701/ PREP BIN DATA TAPE LNA
PREP BINARY DATA TAPE FOR INPUT INTO ALL PROGRAMS THREE POINT INTERPOLATION FOR SCATTERING FACTOR CAN ALSO BE USED TO CORRECT WEISSENBERG DATA ANY AXIS OR LEVEL

5063 7090 FT2 DP SCHULTZERHONHOF BN-X-64/SF,LP,ABS,SCL,FR,DF,LS FM,R,S LWA
SYSTEM FOR RUNNING CRYSTALLOGRAPHIC PROGRAMS TOGETHER.(CHAIN) CONTAINS PGMS.BN-ST1,BN-ABS,BN-ST2,BN-LSQ,BN-FSY AND SOME SMALL PGMS. FOR DP. ALL IT-OT CARDS OR TAPE. EACH PROGRAM MAY ALSO BE RUN INDEPENDENTLY. COMPARE ALSO DESCRIPTIONS OF BN-ST1,BN-ABS,BN-ST2,BN-FSY + BN-LSQ.

5066 7090 FT2 DP,SCL SCHULTZERHONHOF BN-ST2/DP,SCL BY WILSON STAT OR SPEC. LWA
IT FROM BN-ST1 AND BN-ABS.CORRECTS SF WITH ABS FROM BN-ABS(MAY BE OMITTED BY SWITCH),CALCULATES SCL BY SUBROUTINES(WILSON-STAT OR SYMMETRY). OT FOR BN-FSY FOR PATTERSON AND FOR BN-LSQ. MAY ALSO BE RUN WITH BN-X-64.

8019 7094 EL DALLINGA LEAST SQUARES GASDIFFR. INTENSITIES LWA
REFINEMENT OF MOLECULAR COORDINATES AND TEMPERATURE FACTORS.TWO TYPES OF CONSTRAINTS CAN BE USED A) LINEAR EXPRESSIONS INVOLVING 1,2 OR 3 INTERATOMIC DISTANCES, B) SCALE FACTOR AND TEMP.FACTORS MAY BE KEPT CONSTANT (SEE REC.TRAV.CHIM.83,789(1964)

7027 7094 II FM E S TOURNARIE 310D/OPTIMAL LINEAR AJUSTMENTS LWA

322 7090/709 FPK IBERS 27 PT. LS 10 PARAMETER GAUSSIAN FIT LNA
PROGRAM TAKES 27 POINT INPUT FROM MAP AND FITS THESE DATA WITH A 10 PARAMETER GAUSSIAN FUNCTION. AXES NEED NOT BE ORTHOGONAL NOR INTERVALS EQUAL. OUTPUT INCLUDES PEAK CENTER, HEIGHT, GAUSSIAN CONSTANTS. 7090 TIME IS 3 SECONDS/PEAK. WRITE UP AVAILABLE IN FORM OF FORTRAN LISTING WITH COMMENT CARDS. COMPILATION IS LEFT TO USER.

491 7090 FPK SANBORN LINE PROF ANAL LPA
LINE PROFILE FOURIER ANALYSIS. PROGRAMS IN FORTRAN BY KELLER AND SEGMULLER (REV SCI INST 34,684-8(1963)) FOR 1620 MODIFIED AND ADAPTED TO 7090. INPUT IS STEP SCAN FIXED COUNT DATA. CORRECTIONS APPLIED FOR BACKGROUND, ATOMIC SCAT FACTOR, LP FACT, ABSORPTION. OUTPUTS ARE CENTROID, VARIANCE, FOURIER COEFFICIENTS.

128 7094 FR 2 3 BRYDEN 2 AND 3 DIM FOURIER SUM. LPA
COMPUTES 2 AND 3 DIM. FOURIER SUMMATIONS BY A TABLE LOOK-UP PROCESS. THREE TAPE UNITS ARE USED TO SORT AND STORE DATA.

391 7090 FR3 CNTR LEVY,ELLISON* XFOUR/FOURIER SYNTH, CONTOURS PK POS LPA
MINOR MODIFICATION OF A. ZALKIN PROG. FORDAP. OPTIONS FOR FOURIER, PATTERSON, DIFFERENCE AND PARTIAL DIFFERENCE MAPS. SEARCH FOR POSITIVE AND NEGATIVE PEAK POSITIONS. CONTOUR MAPS ON CATHODE RAY PLOTTER. MOSTLY FORTRAN 2, PARTLY FAP.

357 7090 32K FR 3 2 SLY,SHO,HENDE* ERFR2/GENL,FAST,BL,120 GRID (MIFR1) LWA
MODIFICATION OF MIFR1 (PGM 118) FOR IBM 709/7090, 32K REQUIRED. GENERALLY SIMILAR, BUT WITH SOME ADDED CONVENIENCE FEATURES. FAST TABLE LOOKUP. ANY SPACE GROUP TRICLINIC MONOCLINIC ORTHORBOMBIC BY SELECTION OF SYMMETRY CARDS. INPUT IS ONE CARD EACH UNIQUE REFLECTION. CARDS ARE SORTED ON INDICES AND PUT ON TAPE. STRAIGHT OR DIFFERENCE FOURIER POSSIBLE. VARIABLE FORMAT OUTPUT SHEETS PERMIT DIRECT CONTOURING. CALCULATES UP TO 300,000 TERM POINTS PER SECOND. CAN BE RUN ON IB FORTRAN MONITOR SYSTEM.

THE SUPPLY OF ERFR2 MANUALS IS EXHAUSTED, BUT A COPY OF THE MANUAL HAS BEEN DEPOSITED AS ADI DOCUMENT NO 8933 WITH THE AMERICAN DOCUMENTATION INSTITUTE, U. S. LIBRARY OF CONGRESS, WASHINGTON 25, D. C. A COPY MAY BE OBTAINED BY CITING THE DOCUMENT NUMBER AND REMITTING $17.50 FOR PHOTOPRINTS OR $5.50 FOR MICROFILM. ADVANCE PAYMENT IS REQUIRED. MAKE CHECKS OR MONEY ORDERS PAYABLE TO **CHIEF, PHOTODUPLICATION SERVICE, LIBRARY OF CONGRESS**.
NOTE -- AN UPDATED VERSION OF THE PROGRAM FOR THE IBM 7094 IS MIFR2A (Q. V.).

534 7094 FR 3 2 SHOEMAKER,KATZ MIFR2A/ GENERAL FOURIER LPA
MODIFIED VERSION OF SLY, SHOEMAKER, VAN DEN HENDE ERFR2 7090 CRYSTALLOGRAPHIC FOURIER PROGRAM (Q. V.). CONTAINS ADDITIONALLY A RESCALING FEATURE TO AUTOMATICALLY CORRECT TOO HIGHLY SCALED INPUT DATA. PROGRAM IS IN FAP LANGUAGE, SOURCE PROGRAM AVAILABLE BY SENDING MAGNETIC TAPE TO D. P. SHOEMAKER, M. I. T.

394 7090 FT2 FR3 SPEC BROWN G M COMFO/3D COMPOSITE, SQ. MESH LPA
COMPUTES PARALLEL SECTIONS THRU CENTERS OF ATOMS ON SQUARE MESH. SECTIONS MAY HAVE ANY ORIENTATION. INPUT TAPE FROM XFLS (AC 389) OR BMFLS (AC 390). FOR SPECIAL PURPOSES, NOT GENERAL USE (SLOW).

408 7094 FR SPEC DONNAY,TAKEDA JH-ORTFR/DIRECT PRINT UNDEFORMED MAP LPA
CALCULATES FR SERIES AT THOSE POINTS WHERE COMPUTER PRINTS THEM, WE CAN DRAW CONTOURS ON DIRECT PRINT-OUT. WEITTEN IN FORTRAN FOR MONOCL. C, HOL PROJECTION AND SECTION, BUT BE EASILY GENERALIZED DESCRIPTION TO APPEAR IN *SCIENCE*.

453 709 FTN FT OCKEN*WAGNER RADIAL DISTRIBUTION FUNCTION LWA
COMPUTES RDF FROM MEASURED X-RAY SCATTERING OF LIQUIDS

503 709 FT2 FT OCKEN/YCC RDF OF LIQUIDS LWA
X-RAY DATA CORRECTED FOR POLARIZATION. RESULTS NORMALIZED TO ABSOLUTE UNITS. SI(S) FUNCTION GENERATED. RDF DETERMINED BY CALCULATION OF THE FOURIER SINE COEFFICIENTS OF SI(S) USING FILON'S METHOD. STORAGE, 9K.

5067 7090 FT2 FS,DF SCHULTZERHONHOF BN-FSY/FS,DF,PATTERSON. BL. LWA
SYSTEM OF FS PGMS.ALL SPACEGROUPS.RUNS INDEPENDENTLY OR WITH BN-X-64. IT POSSIBLE FROM BN-ST2 FOR PATTERSON, FROM BN-LSQ FOR FS OR DF. REFLECTIONS NEED NOT TO BE SORTED.BLK.

412 IBM7094 GENERAL STEWART*HIGH X-RAY-63/SYSTEM FOR IBM 709-7094-(DC) LWA
SEE ALSO UNDER X-RAY-63 ENTRY IN LIST FOR MORE DETAIL

363 7090 FT2 ID E BUSING*LEVY ORFFE/FORTRAN FUNCTION AND ERROR LWA
USED INDEPENDENTLY OR WITH ORFLS. COMPUTES THE FOLLOWING FUNCTIONS OF CRYSTAL PARAMETERS WITH THEIR STANDARD ERRORS- DISTANCES, ANGLES, DIHEDRAL ANGLES, RMS PRINCIPAL THERMAL DISPLACEMENTS, ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR DEFINED BY USER, RMS RADIAL THERMAL DISPLACEMENT, DISTANCE CORRECTED FOR THERMAL MOTION. WRITTEN IN FORTRAN 2.

473 7094 32K IT DP ABRAHAMS,CETLIN PEXRAD INPUT/AUTO DIFFR CONTROL TAPE LPA
FORTRAN PROGRAM TO ARRANGE VALUES OF H,K,AND L,BY LTH LAYERS, IN OPTIMUM ORDER, TO CONTROL CRYSTAL AND COUNTER SGTTINGS ON BELL TEL. LABS. PROGRAMMED ELECTRONIC X-RAY AUTOMATIC DIFFRACTOMETER (PEXRAD). TO BE USED IN CONJUNCTION WITH PEXRAD OUTPUT AND F**2 PROG.

515 7090 IT/OT/DP ABRAHAMS/CETLIN PEXRAD AUTOMATIC DIFFRACTOMETER PRGM LWA
FORTRAN PROGRAM TO CONTROL OPERATION OF AUTOMATIC DIFFRACTOMETER + CHECK ITS PERFORMANCE. STATISTICAL ANALYSIS OF EQUIVALENT STRUCTURE FACTORS GIVES MEAN STRUCTURE FACTOR AND STANDARD DEVIATION .

451 7090 LC BURNHAM LCLSQ/LS REFINEMENT OF LC LWA
FORTRAN2, + FAP (NO IT-OT) SUBROUTINES, 5173 + 1900 (COMMON) LOCATIONS (+ USER SUBROUTINES). LS REFINEMENT OF LC FOR ANY XTL SYSTEM. USES INDEXED SINGLE-XTL OR POWDER DATA. ALLOWS REFINEMENT OF 9 OR LESS SYSTEMATIC CORRECTION TERMS, E.G. ABSORPTION, SHRINKAGE, ETC. USER PROGRAMS TRIGONOMETRIC FORM OF CORRECTION TERMS WITH POSSIBILITY OF 5 DIFFERENT FORMS. PROVISIONS FOR WEIGHTING.

518 7094 LC BY LS2 OTTE,ESQUIVEL HEXAG LC BY NEW LS-2 FROM D-S PATTERN LWA
A NEW LS METHOD FOR PRECISE DETERMINATION OF HEXAGONAL LC FROM D-S(DEBYE-SCHERRER)PATTERNS. USES REITERATIVE PROCESS AND CORRECTION FACTOR WHICH,UNLIKE COHEN S (REV SCI INSTR,1935)VARIES LINEARLY WITH EXTRAPOLATION FN. PROVISION MADE FOR VARYING XRAY WAVE LENGTH AND WEIGHTING FACTOR.

47 7094 FT2 LC AND E VOGEL,KEMPTER* HERTA-2/PREC REFINMT OF LATTICE PARAM LWA
A CONVERGENT ITERATIVE TECHNIQUE (R.E.VOGEL AND C.P.KEMPTER,ACTA CRYST.

14,1130(1961)),WITH EXACT STATISTICAL WEIGHTS ASSIGNED TO THE OBSERVED POINTS IS USED TO DETERMINE LATTICE PARAMETERS AND THEIR STANDARD DEVIATIONS FOR THE CUBIC,HEXAGONAL,RHOMBOHEDRAL(ON HEXAGONAL AXES),TETRAGONAL ,ORTHORHOMBIC, AND MONOCLINIC SYSTEMS FROM DEBYE-SCHERRER,SYMMETRICAL BA3K REFLECTION,OR DIFFRACTOMETER DATA (FOUR EXTRAPOLATION FUNCTIONS).

130 7094 LP BRYDEN CORR. EQUIINCL. WEIS. INT. LPA
CORRECTS EQUIINCLINATION WEISSENBERG INTENSITIES FOR LP FACTORS, AND FOR UPPER LAYER LINE SPOT EXTENSION BY THE METHOD OF PHILLIPS.

310 709 LP PALENIK 14708/ANY SPACE GROUP LNA

320 7090 32K LP ABS H VAN DEN HENDE ERBR2/LP AND ABSN CORR,SHARPENING LPA
ERBR2 CORRECTS FOR LP AND ABSORPTION. NORMAL-BEAM AND EQUI-INCLINATION. CYLINDRICAL OR SPHERICAL SPECIMENS. ALSO SHARPENING FOR B POSSIBLE. GENERATION OF INDICES OPTIONAL, ALSO ADDITIONAL OUTPUT IN FORMAT OF SLY-SHOEMAKER FOURIER PROGRAM. MAY BE USED WITH 704 ALSO WITH MINOR CHANGES.

513 7090FT2 LP SMITH D K WEIS OR PREC LP CORR LPA
ALSO SCALES INTERSECTING SECTIONS BY LS FIT AND GIVES OT FOR SF CALC.

8527 7090 LS ASHIDA LSQALLTB/BLOCK-DM FORTRAN 2 AND 4 LWA
BLOCK-DM LS. AT,E,DISPERSION. 4*4 OR 9*9 FOR EACH ATOM. 2*2 FOR SCL AND OVERALL TF. ANY SPACE GROUP. 60 ATOMS. 5000 REFLECTIONS.

8530 7090 LS ASHIDA LSQAL/BLOCK-DM. FORTRAN 2 AND 4 LWA
BLOCK-DM LS. AT,E,DISPERSION. 4*4 OR 9*9 FOR EACH ATOM, 2*2 FOR SCL AND OVERALL TF. ANY SPACE GROUP. 60 ATOMS. 5000 REFLECTIONS.

361 7090 FT2 LS BUSING*LEVY ORGLS/GENL LS TO FIT ARBITRARY FUNCT. LWA
PERFORMS LEAST SQUARES FIT OF ANY FUNCTION DEFINED BY USERS SUBROUTINE. DERIVATIVE CALCULATION PROGRAMMED OR NUMERICAL. OBSERVATIONS WEIGHTED UNITY OR INDIVIDUALLY. TRIAL PARAMETERS TO BE VARIED ARE SPECIFIED FOR EACH JOB. COMPARISON OF CALCULATED AND OBSERVED FUNCTION PUT OUT BEFORE EACH CYCLE AND AFTER LAST. ADJUSTED PARAMETERS AND STANDARD ERRORS PUT OUT AFTER EACH CYCLE. CORRELATION MATRIX PUT OUT. MATRIX INVERTER IS FAP FOR 704, 709, OR 7090. VERSION ENTIRELY IN FORTRAN IS ALSO AVAILABLE.

5068 7090 FT2 LS SCHULTZERHONHOF BN-LSQ/LS,FM,R,TF,SIGN LWA
MODIFIED VERSION OF SCHERINGER LS. IT FROM BN-ST2. OT FOR BN-FSY(FS,DF). RUNS INDEPENDENTLY OR WITH BN-X-64.

360 7090 FT2 LS AT FM BUSING*LEVY ORFLS/FORTRAN LEAST SQUARES, SF,FM,AT LWA
STRUCTURE FACTOR LEAST SQUARES. ANY SPACE GROUP. VARIABLES ARE SCALE FACTORS, NEUTRON SCATTERING FACTORS, ATOM MULTIPLIERS, ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS. FULL MATRIX LEAST SQUARES. GENERAL OR UNIT WEIGHTS. REFINEMENT BASED ON F OR F SQUARED. ARBITRARY SELECTION OF PARAMETERS VARIED. 32K MEMORY USUALLY REQUIRED. USES NO TAPES FOR STORAGE. MATRIX INVERTER IS FAP FOR 704, 709, OR 7090. VERSION ENTIRELY IN FORTRAN IS ALSO AVAILABLE.

399 7090/94 LS BM AT VAN DEN HENDE LLXR6/BLOCK DIAGONAL LEAST-SQUARES LWA
LLXR6 ALLOWS ANISO AND ISO TEMP FACTORS, GENERAL WEIGHTING AS WELL AS DIFFERENTIAL SYNTHESIS WEIGHTING. IT WILL VARY 10 PARAMETERS FOR 176 ATOMS SIMULTANEOUSLY FOR ALL 230 SPACE GROUPS. CAN BE USED FOR STRUCTURE FACTOR CALC ALSO. SIMPLE CONTROLS ALLOW MORE THAN 20 OPTIONS. NEUTRON DATA ARE ALLOWED, ANOMALOUS SCATTERING IS TAKEN CARE OF. OUTPUT FOR ERFR2 FOURIER PROGRAM MAY BE WRITTEN. SUPERSEDES ERBR1. VERY FAST.

384 7090 LS FM GANTZEL,SPARKS,TRUEBLOOD/UCLALS1/REVN OF PGM 228
FULL-MATRIX LEAST SQUARES REFINEMENT OF SUITABLE TRIAL CRYSTAL STRUCTURES. REFINES UP TO 137 UNIQUE PARAMETERS, WITH UP TO 2100 UNIQUE F(HKL). EVERYTHING IS STORED IN HIGH-SPEED MEMORY. A CONSIDERABLE REVISION OF PROGRAM 228.

308 709 LS FM PALENIK 14706/ ANY ACENTRIC SPACE GROUP LNA
FULL MATRIX LEAST SQUARES ANY ACENTRIC SPACE GROUP USES UNIQUE DATA ONLY LIMIT OF 30 ATOMS FOR SF PART AND 18 ATOMS WITH ANISOTROPIC TEMPERATURE PARAMETERS FOR LEAST SQUARE PART RECYCLE CHANGING ONLY VECTOR OR VECTOR AND MATRIX

309 709 LS FM PALENIK 14707/ ANY CENTRIC SPACE GROUP LNA
SAME AS 14706 EXCEPT FOR CENTRIC SPACE GROUPS

317 709 LS H FM GTZL,SPKS/TRBD* UCLALS1/137 PAR,ISO OR AT, 2100 REFL LPA
UCLALS1/ ALL 2100 REFL DATA STORED IN MEMORY. NON-LIMITED ARE NO. OF CYCLES, S. G., SPEC POSNS. ROOM TO ADD VARIOUS SUBPROGRAMS SUCH AS DISTANCE-ANGLE, R BY CLASSES, DELETION, E.S.D., ETC. MODIFICN TO READ IN AND PROCESS ONE REFL AT A TIME EASILY PERMITS INF DATA AND 152 PARAMS

4001 7090FT2 LS2 FMAT CURTIS/GILMARTIN/LS2D/GENL 2D LS,FM,AT,N OR XRAY LWA
GENERAL 2-DIM SF + LS PGM, FULL MATRIX, ANISO. NEUTRON OR XRAY. INPUT PLANE GP NO, LC, LF, LIST OF HKF, PARAS, CONTROL CODE FOR EACH CYCLE. WEIGHT IS A FUNC OF F. OUTPUT PARAS, CHANGES, ERRORS, SF, AS REQD. WRITE-UP AERE-R3134 AMENDED BY CPN 52. SAME AS MERCURY PGM. NO. 29F (ENTRY NO. 4007). UP TO 50 DISTINCT ATOMS, 100 PARAS REFINED, 1000 PLANES, ON 32K 7090.

311 709 M SQ DIS PALENIK 14709/MEAN SQ. DISPLACEMENTS LNA

516 7090 OT/DP BERNSTEIN,J.L. ANOMALOUS DISPERSION PROGRAM LWA
FORTRAN PROGRAM CORRECTS OBSERVED STRUCTURE FACTORS OF A CENTRO-SYMMETRIC CRYSTAL FOR ANOMALOUS DISPERSION. PROGRAM USED WITH ONE OR TWO ATOMS DISPERSIVE. ONE CARD OBTAINED FOR EACH REFLECTION. CARDS PUNCHED IN FORMAT OF INPUT CARDS OF ORFLS

474 7094 32K OT DP ABRAHAMS,CETLIN PEXRAD OUTPUT/CALCS SF AND ERRORS LPA
FORTRAN PROGRAM TO INTEGRATE INTENSITY FROM BETA-ALPHA PROFILE,MAKE ALL CORRECTIONS AND COMPUTE STRUCTURE FACTORS,INDICATING ALL ERRORS.

514 7090FT2 P SMITH D K POWD/ COMPUTES POWDER INTENSITIES LWA
INCLUDING LP, MULTIPLICITY, AND ABSORPTION FOR ANY SYMMETRY

304 709 PATT SUM PALENIK 14702/ 3D PATTERSON MONOCLINIC LNA
WILL PRODUCE A SHARPENED OR UNSHARPENED PATTERSON WITH OR WITHOUT THE ORIGIN PEAK 3D LIMIT OF 2000 REFLECTIONS

305 709 PATT SUM PALENIK 14703/ 3D PATTERSON ORTHORHOMBIC LNA
SAME AS 14702 EXCEPT FOR ORTHORHOMBIC SPACE GROUPS

3041 7090 FT2 ROTF ROSSMANN GRF2/ROTATION FUNCTION*ALL SP.GRPS LWA
USES INTENSITIES TO FIND ANGULAR RELATIONSHIPS BETWEEN MOLECULES OR SUB UNITS WITHIN THE SAME ASYMETRIC UNIT OR IN DIFFERENT CRYSTAL MODIFICATIONS(ROSSMANN,BLOW ACTA 1962,VOL15,P.24)

7026 7094 II S DP TOURNARIE 308B/OPTIMAL SMOOTHING MWA

404 709,7094 SF,ICA WOLTEN CALC FROM LC AND AT PAR FT2 LWA
OT SAME AS PROG 49 PLUS SF,ICA

306 709 SF FR PALENIK 14704/ACENTRIC THRU ORTHORHOMBIC LNA
CALC SF AND USE SIGNS FOR FOURIER CALC BASED ON SIMPLFIED FORMS IN INTL TABLE USES ONLY THE UNIQUE INPUT ANY INTEGER VALUE OF 120 CAN BE USEDFOR FOURIER INTERVAL

307 709 SF FR PALENIK 14705/ CENTRIC THRU ORTHORHOMBIC LNA
SAME AS 14704 EXCEPT FOR CENTRIC SPACE GROUPS

8326 7090 SF FR SASADA,ASHIDA SFFR/SF,FR IN SUCCESSION FORTRAN2 LWA
CALCULATES SF AND FR. APPLICABLE TO TRI,MONO,ORTHO.
100 ATOMS, 3000 REFLECTIONS

316 709 SF H FR GANTZEL/TRBD* UCLANC1/ SEE ABSTR FOR LIMITATIONS LPA
UCLANC1/ ANY SG, 100 ATOMS, ANISO OR ISO B. FOR FOURIER, EQUIV DATA GEN FOLLOWS SF (WILL NEED PATCHES FOR CERTAIN SG). MAX INDEX PROD LIMITED TO ABOUT 2700 (SOON 5500) BECAUSE INTERNAL SORTING. NO. OF 4-TERM SUMS (HKL WITH ALL SIGNS FOR KL) LIMITED TO 1500. WRITTEN FOR NON-CENTROSYM(EASY MODIF FOR 2400 CENTROSYM 4-TERM SUMS).

5064 7090 FT2 SF,LP SCHULTZERHONHOF BN-ST1/SF,LP,THETA LWA
IT FROM WEIS OR COUNTER.CALCULATES SF,LP,FILM CORRECTIONS,THETA, OT FOR BN-ABS AND BN-ST2. MAY ALSO BE RUN WITH BN-X-64.

291 709 FT2 SF 2 NORTH SF2/2/FAST 2-DIMENSIONAL LWA
2-DIM. STRUCTURE FACTORS, PLANE GROUPS 1 - 9, SYMMETRY SPECIFIED BY PLANE GROUP NO. + 2 SELECTOR SYMBOLS, UNLIMITED NO. OF ATOMS, ISOTROPIC TEMP. FACTORS

315 709 SPC N SHOEMAKER,C+D PRPLOT/SMOOTH AND PLOT SPECROM DATA LPA
709 VERSION OF PGM 122

393 7090 FT2 SPEC BROWN G M EDIT/F SQUARE TABLE FOR PUBLIC. LPA
MINIMIZES CUTTING AND PASTING. SETS UP TABLE IN MULTICOLUMN FORMAT WITH NUMBERS OF LINES AND COLUMNS VARIABLE. INPUT TAPE FROM XFLS (AC 389) OR BMFLS (AC 390). FOR EXAMPLE, SEE R. D. ELLISON AND H. A. LEVY, ACTA CRYST. IN PRESS, 1965.

480 7094 SPEC DUCHAMP,MARSH*,ETAL/CRYRM/COMPLETE CRYSTALLO. SYSTEM LWM
CONTROL SYSTEM AND SUBPROGRAMS FOR INITIAL DATA REDUCTION(LP,SCALING,ETC) STRUCTURE-FACTOR LEAST SQUARES(SPACE GROUP SPECIFIC,ALL SPACE GROUPS,FM, BLOCK MATRIX,AT,ETC.),FOURIER(DIFFER,GEN.PLANE,2 OR 3,TO-SCALE MAPS), DISTANCES,ANGLES,L.S.PLANES,AUTOMATIC DIFFRACTOMETER CONTROL,LATTICE CONSTANT DETERMINATION,PUBLICATION LIST,TEMP. ELLIPSOIDS,STATISTICAL PHASING. PROVIDES FOR VERY LARGE PROBLEMS.

230 709 SPEC SPKS,BURKE/TRBD UCLAMO1/MOLEC ORIENTN,PGG,PGM,PG LPA
UCLAMO1/ EVALUATES A SORT OF R FOR A SPECIFIC ORIENTATION OF A MOLECULE OF KNOWN GEOMETRY TRANSLATED OVER A GIVEN PROJECTION. THREE ANGULAR PARAM TO BE SPECIFIED (FROM OTHER CONSIDERATIONS). MINIMA ARE PLAUSIBLE POSNS

231 709 SPEC SPARKS/TRBD* UCLAMOLS1/5 PAR LS OF 230 FOR PGG LPA
UCLAMOLS1/ REFINES THE FIVE APPROX PARAMS FROM 230 ONLY FOR PLANE GROUP PGG BY LS (THREE ANGLES, TWO POSITIONS)

405 709,7094 SPEC WOLTEN CALC INTERPLANAR ANGLES FROM LC,FT2 LWA

448 IBM7094 SPEC,DP LEDLEY,DAYH,JSTEW/AUTOMATIC SCAN DIFF FILM TO CORE MEMNPA
DIFFRACTION FILM OPTICAL DENSITIES ARE SCANNED AUTOMATICALLY INTO THE CORE MEMORY OF AN IBM 7094 USING THE =FIDAC= FLYING SPOT SCANNER. EACH DIFFRACTION SPOT IS COVERED BY SEVERAL HUNDRED SCANNER POINTS. INTEGRATED INTENSITY OF SPOTS IS OBTAINED BY FORTRAN AND FAP OPERATIONS ON THE DENSITIES OF SPOT AND BACKGROUND POINTS.

407 7094 SPEC LC TAKEDA,DONNAY JH-TRXL63/TRANSF. XL. SETTING LPA
TRANSFORMS CELL DIMENSION, SPACE-GROUP SYMBOL TO A CONVENTIONAL SETTING OF *CRYSTAL DATA*. RHOMBOH.-HEXAG. TRANSF.,, REORIENTATION OF ORTHOR.,, CELL REDUCTION OF MONOCLI. AND TRICLI.. USES SAME INPUT FORMAT. WRITTEN IN FORTRAN AND FAP(SOME SUBROUTINE).

388 7090 STEREO JOHNSON C K ORTEP/THERMAL ELLIPSOID PLOT PROGRAM LWA
UTILIZES PLOTTER SUCH AS CALCOMP TO PLOT BALL-AND-STICK CRYSTAL STRUCTURE FIGURES IN STEREO WITH THERMAL ELLIPSOIDS OR CIRCLES ON THE ATOMIC SITES. MAIN PROGRAM IS IN FORTRAN II. IBM 7090 OR CDC 1604 MACHINE ORIENTED PLOT ROUTINES ARE LIBRARY TYPE WITH MINOR MODIFICATIONS. 32K MACHINE REQUIRED.

232 709 TF AT CLTR,GTZL/TRBD* UCLATO1/RIGID BODY, TRANS AND LIBR LPA
UCLATO1/ OK FOR ANY AXIAL SYSTEM. USES CRUICKSHANK RIGID BODY APPROX INPUT ANISOT B'S AND ATOMIC POSNS. OUTPUT PARAMS INDIVID ATOMIC VIBR ELLIPSOIDS, T, OMEGA, AND ESD'S, AND DELTA U(IJ)

ACCESSION NUMBER INDEX

FOLLOWING EACH ACCESSION NUMBER THE FIRST FIVE CHARACTERS OF THE MACHINE ABBREVIATION AND THE FIRST TWO CHARACTERS OF THE FUNCTION ABBREVIATION ARE GIVEN, TO FACILITATE FINDING THE PROGRAM IN THE MAIN LIST.

FROM 1ST ED.
1 LGP30 DP
2 LGP30 FR
3 LGP30 FR
34 650 AB
47 7094 LC
49 709,7 D
111 205 H
112 205 ID
113 205 LP
114 205 FR
115 205 LP
116 220 LF
118 704 8 FR
120 FORTR DP
128 709 FR
130 709 LP
133 650 PA
170 650 FR
171 650 FR
172 650 FR
174 650 FR
176 650 SF
177 650 SF
180 650 DP
181 650 DP
182 650 PL
183 650 HY
184 650 ID
185 650 DP
198 650 FR
218 650 DP
219 650 TF
220 650 ID
221 650 ID
225 FORTR AB
226 FORTR LC
230 709 SP
231 709 SP
232 709 TF
233 704 DI
235 650 ST
236 ALGOL D
237 ALGOL SF
238 ALGOL LP
239 ALGOL S
240 ALGOL H
241 ALGOL LC
242 ALGOL TF
243 ALGOL LF
244 ALGOL LP
245 ALGOL S
246 ALGOL PR
247 ALGOL E
248 ALGOL DF
249 ALGOL DF
250 ALGOL DF
251 ALGOL DF
252 ALGOL LS
253 ALGOL LS
254 ALGOL SF
255 ALGOL SF
256 ALGOL FR
257 ALGOL SC
258 ALGOL SC
259 ALGOL SC
260 220 DF
261 220 ID
262 220 LF
263 220 LP
264 220 H
265 220 FR
266 205 FR
267 205 EL
268 220 LS
269 205 EL
277 1620 D
278 1620 LC
279 1620 D
280 1620 H
281 1620 H
283 1620 D
284 1620 D
285 1620 D
287 1620 D
288 1620 LC
289 1620 LC
290 650 H
291 709 F SF
292 1620 AB
294 1620 AT
297 220 SP
298 220 DP
300 220 FR
301 704 4 LC
302 650 FP
303 709 DP
304 709 PA
305 709 PA
306 709 SF
307 709 SF
308 709 LS
309 709 LS
310 709 LP
311 709 M
312 1620, D
313 FORTR LS
314 FORTR SP
315 709 SP
316 709 SF
317 709 LS
320 7090 LP
322 7090/ FP
324 650 DP
325 650 E
326 650 TF
327 650 LF
328 650 TF
329 650 DP
330 7070 SF
331 7070 ID
332 7070 ID
338 709 3 AB
344 FORTR FR
345 FORTR N,
354 1620T FR
355 1620T SP
356 650 FR
357 7090 FR
360 7090 LS
361 7090 LS
362 FORTR AB
363 7090 ID
368 7090 CO
369 1620 SF
370 1620 FR
371 1620T FR
381 7070 FT
382 7070 PL
384 7090 LS

NEW, 2ND ED.
385 FORTR N
386 FORTR LC
387 1604 ST
388 7090 ST
389 FORTR LS
390 FORTR LS
391 7090 FR
392 1604A SP
393 7090 SP
394 7090 FR
395 FORTR FT
396 FORTR ID
397 7040- FR
398 FORTR SF
399 7090/ LS
400 1620 FR
401 1620 FR
402 1620 SF
403 1620 SF
404 709,7 SF
405 709,7 SP
406 709,7 D
407 7094 SP
408 7094 FR
409 ALGOL ID
410 ALGOL LS
411 FORT2 GE
412 IBM70 GE
413 X-RAY GE
414 X-RAY SF
415 X-RAY LS
416 X-RAY LS
417 X-RAY LS
418 X-RAY FR
419 X-RAY CO
420 X-RAY PK
421 X-RAY DP
422 X-RAY SP
423 X-RAY DI
424 X-RAY ST
425 X-RAY SP
426 X-RAY ST
427 X-RAY LC
428 X-RAY TH
429 X-RAY WE
430 X-RAY SP
431 X-RAY FR
432 X-RAY PA
433 X-RAY ID
434 X-RAY ID
435 X-RAY ST
436 X-RAY LS
437 X-RAY SP
438 X-RAY DP
439 X-RAY DP
440 X-RAY DP
441 X-RAY DP
442 X-RAY DP
443 X-RAY DP
444 X-RAY SP
445 X-RAY SP
446 1604 FR
447 1604 FR
448 IBM70 SP
449 FT2 CO
450 FORTR AB
451 7090 LC
452 FORTR PA
453 709 F FT
454 1620 DP
455 1620 LF
456 1620 DF
457 1620 SF
458 1620 E
459 1620 ID
460 1620 ID
461 1620 D
462 1620 SP
463 FTN 1 LC
464 FTN 1 SP
465 FTN 1 DP
466 FTN 1 AB
467 FTN 1 LP
468 FTN 1 ST
469 FTN 1 LS
470 FTN 1 ID
471 FTN 1 ID
472 FTN 1 DE
473 7094 IT
474 7094 OT
475 7094 DP
476 FORTR DP
477 FORTR LS
478 FORTR FR
479 FORTR ID
480 7094 SP
481 FORTR PI
482 FORTR PI
483 FORTR PI
484 FORTR PI
485 1620 FR
486 1620 FR
487 1620 SF
488 1620 LF
489 1620 LP
490 1620 ID
491 7090 FP
492 1105 SF
493 1105 FR
494 1105 FR
495 1105 LP
496 FORTR ST
497 1620- FR
498 1620- LP
499 1620- ID
500 FORTR SP
501 FORTR LC
502 BALGO TH
503 709 F FT
504 FORTR FR
505 FORTR SP
506 FORTR ID

507 FORTR LP
508 650 FR
509 650 LP
510 7070 SF
511 7070 FR
512 7070 FR
513 7090F LP
514 7090F P
515 7090 IT
516 7090 OT
517 B 500 LS
518 7094 C
519 7090 CO
520 FORTR SP
521 1620 PI
522 FORTR SP
523 1620T AB
524 1620T GO
525 1620T DP
526 1620T ID
527 1620T LS
528 FORTR LS
530 1620 D
531 1620 D
532 FORTR ID
533 FORTR TF
534 7094 FR
535 FORTR PI

FROM 1ST ED.
3007 SILLI AB
3008 SILLI ID
3009 SILLI AN
3010 SILLI SF
3012 ZEBRA LI
3013 ZEBRA PL
3014 ZEBRA P
3015 ZEBRA SF
3016 ZEBRA MA
3017 ZEBRA SF
3018 ZEBRA LS
3019 ZEBRA 1F
3021 ZEBRA DP
3022 ZEBRA DP
3023 ZEBRA FR
3027 ZEBRA 3
3028 ZEBRA 3
3029 ZEBRA 3
3031 ZEBRA EN
3033 ZEBRA SP
3035 ZEBRA PI
3036 ZEBRA PR
3037 ZEBRA DP

NEW, 2ND ED.
3039 PDP 6 SF
3040 PDP 6 R3
3041 7090 RO
3042 FORTR TH
3043 FORTR LP
3044 FORTR DE
3045 FORTR ID
3046 FORTR ID
3047 FORTR PL
3048 1620 R
3049 ATLAS FR
3050 ATLAS SF
3051 ATLAS ID
3052 ATLAS CO
3053 ATLAS 2C
3054 ATLAS SF
3055 ATLAS RO
3056 FORTR LS
3057 ATL F LS
3058 ATL F FR
3059 ATL F DP
3060 ATL F SF
3061 ATL F PA
3062 ATL F ST
3063 ATL F ID
3064 ATLAS LS
3065 ATLAS SF
3066 ATLAS ID
3067 ATLAS DP
3068 ATSYS SY
3069 ATLAS SY
3070 ATLAS DP
3071 ATLAS DP
3072 ATLAS LC
3073 ATLAS DP
3074 ATLAS FR
3075 ATLAS DP
3076 ATLAS LS
3077 ATLAS ID
3078 ATLAS PL
3079 ATLAS SP

3512 KDF9 SF
3513 KDF9 PL
3514 KDF9 A-
3515 KDF9 ID
3516 KDF9 DP
3517 KDF9 FR
3518 KDF9 ID

FROM 1ST ED.
4001 7090F LS
4002 704FT 2D
4007 MERCU LS
4008 MERCU P
4011 MERCU DI
4012 MERCU LC
4013 MERCU 3A
4014 ATLAS 2S
4020 DEUCE ID
4021 DEUCE FR
4022 DEUCE R
4023 DEUCE DP
4024 DEUCE T/
4025 DEUCE PL
4028 DEUCE FR
4029 DEUCE SF
4030 DEUCE SF
4031 MERCU DP
4032 MERCU DP
4033 MERCU SC
4035 MERCU SF
4036 MERCU SF
4038 MERCU DP
4039 MERCU E
4040 MERCU PA
4041 MERCU R
4042 MERCU TF
4043 MERCU GE
4044 MERCU TF
4045 MERCU ID
4046 MERCU GE
4047 MERCU GE
4048 MERCU PK
4049 DEUCE FR

5001 ER 56 TH
5002 ER 56 TH
5003 ER 56 LC
5004 ER 56 FR
5005 ER 56 ID
5006 ER 56 LP
5007 ER 56 FR
5011 2002 DI
5012 ALGOL FR
5014 ALGOL SF
5015 BULLG LS
5016 BULLG DP
5017 BULLG DP
5018 BULLG LP
5019 BULLG H
5020 BULLG LC
5021 BULLG LC
5022 BULLG SF
5023 BULLG ID
5024 BULLG PE
5025 704 8 FR
5027 2002 FR
5028 650 DP
5029 650 DP
5030 650 ST
5031 650 ST
5034 Z22 R ER
5035 Z22 R SF
5036 650 DP
5037 650 SF
5038 650 DP
5039 650 H
5040 650 DP
5041 650 DP
5042 650 DP
5043 650 SC
5044 650 DP
5046 650 DP
5047 650 FR

NEW, 2ND ED.
5048 ALGOL AB
5049 ALGOL ID
5050 ALGOL SF
5051 ALGOL AB
5052 ALGOL LP
5053 2002 FR
5054 2002 SF
5055 2002 LP
5056 2002 H
5057 2002 ID
5058 7090 D,
5061 FORTR PA
5062 1620F SP
5063 7090 DP
5064 7090 SF
5065 7090 AB
5066 7090 DP
5067 7090 FS
5068 7090 LS
5069 Z23 ST
5070 Z23 FT
5071 Z23 FO
5072 ALGOL P
5073 ER 56 AB
5074 FORTR PR

FROM 1ST ED.
6001 WGMAT LP
6002 MERCU FR
6003 MERCU FR
6004 MERCU FR
6005 MERCU FR
6006 MERCU FR
6008 DASK FR
6009 DASK SF
6014 FACIT FR
6015 FACIT SF
6016 FACIT ID
6017 FACIT LP
6019 FACIT AB
6020 FACIT AB
6023 FACIT LS
6024 FACIT LP
6026 FACIT LF

NEW, 2ND ED.
6027 FACIT P
6028 FACIT P
6029 FACIT AB
6030 FACIT E
6031 FACIT SP
6032 FACIT SP
6033 FACIT DP
6034 FACIT DP
6035 FACIT SF
6036 ALGOL H
6037 ALGOL LS
6038 ALGOL DP
6039 ALGOL LS
6040 ALGOL RE
6041 ALGOL ID

FROM 1ST ED.
6505 URAL SF
6506 URAL DP
6507 URAL ST
6512 LGP30 ID
6513 LGP30 D
6514 NE803 ID

NEW, 2ND ED.
6515 ZRA1 SF
6516 ZRA1 SF
6517 ZRA 1 LP
6518 ZRA 1 FR
6519 ZRA 1 ST
6520 ZRA 1 ST
6521 ZRA 1 ID
6522 ZRA 1 SF
6523 ZRA 1 SF
6524 ZRA 1 SF
6525 NE 80 LP

6526 NE 80 ST
6527 NE 80 SC
6528 NE 80 US
6529 NE 80 FR
6530 NE 80 SF
6531 NE 80 FR
6532 NE 80 SP
6533 NE 80 LS

FROM 1ST ED.
7001 CAB 5 LS
7002 CAB 5 LS
7003 CAB 5 SP
7004 CAB 5 LF
7005 CAB 5 SP
7006 CAB 5 SC
7007 CAB 5 SF
7008 CAB 5 SF
7009 CAB 5 SF
7010 CAB 5 SF
7011 CAB 5 LP
7012 CAB 5 ID
7013 BULLG FR
7014 BULLG SF
7015 BULLG D
7016 BULL LS
7017 BULL SF
7018 BULL LP

NEW, 2ND ED.
7020 FORTR LC
7021 FORTR 2S
7022 FORTR N
7023 FORTR EL
7024 FORTR PR
7025 FORTR FT
7026 7094 S
7027 7094 FM
7028 FORTR S
7029 FORTR SP
7030 FORTR FT
7031 FORTR TH
7032 FORTR PI
7033 PALLA LS
7034 PALLA LS
7035 PALLA LS
7036 PALLA LS
7037 PALLA LS
7038 PALLA LS
7039 PALLA LS
7040 PALLA LS
7041 PALLA LS
7042 PALLA LS
7043 PALLA SP
7044 PALLA SP
7045 PALLA SP
7046 PALLA SP
7047 PALLA SP
7048 PALLA FR
7049 PALLA ID
7050 PALLA SF
7051 PALLA SP
7052 PALLA SP
7053 PALLA SP
7054 PALLA FR
7055 PALLA LS
7056 PALLA PA

FROM 1ST ED.
7501 6001 FR
7502 6001 FR
7503 6001 FR
7504 6001 SF
7505 6001 SF
7506 6001 DP
7507 6001 DP
7509 6001 DP
7511 6001 SC
7512 6001 DP
7524 1103 SF
7525 1103 PA
7526 CEP SF
7527 CEP SF

NEW, 2ND ED.
7528 FORTR LS
7529 FORTR LS
7530 FORTR LS
7531 FORTR SP
7532 FORTR SF
7533 FORTR SC
7534 FORTR FR
7535 FORTR DP
7536 FORTR LP
7537 FORTR SC
7538 FORTR ST
7539 FORTR ST
7540 FORTR ST
7541 FORTR ID
7542 FORTR LS
7543 FORTR HY
7544 1620 SF
7545 1620 DF
7546 1620 DF
7547 1620 R
7548 ALGOL LS
7549 ALGOL LS
7550 ALGOL SP
7551 ALGOL PI
7552 ALGOL SF
7553 6001 FT
7554 6001 FP
7555 6001 ID
7556 6001 LS
7557 ALGOL DP
7558 6001 LP
7559 6001 SC
7560 6001 TF
7561 6001 DF
7562 6001 SF
7563 6001 AT
7564 6001 PA
7565 6001 AT
7566 6001 DP
7567 Z23A LS
7568 Z23A FR
7569 Z23A SF

FROM 1ST ED.
8007 ZEBRA FR
8008 ZEBRA FR
8009 ZEBRA SF
8010 ZEBRA SF
8011 ZEBRA LS
8012 ZEBRA IT
8013 ZEBRA LP
8014 ZEBRA LP
8015 ZEBRA LP
8016 ZEBRA FI

NEW, 2ND ED.
8017 7094 DI
8018 7094 CO
8019 7094 EL
8020 TR4AG PR
8021 TR4-A 3
8022 TR4-A LP
8023 ALGOL SF
8024 ALGOL LS
8025 ALGOL PD
8026 ALGOL SF
8027 ALGOL PI
8028 ALGOL FR
8029 ALGOL SF
8030 ALGOL PI
8031 ALGOL ST
8032 ALGOL DP
8033 ALGOL ST
8034 ALGOL DI
8035 ALGOL DI
8036 ALGOL ST
8037 ALGOL ST
8038 ALGOL ST
8039 ALGOL AB
8040 ALGOL SP
8041 ALGOL TF
8042 1620 H
8043 1620 SF
8044 1620C LF
8045 1620C FR
8046 1620C SF
8047 1620C FR
8048 1620C SC
8049 1620C SP
8050 1103 LP
8051 1103 SF
8052 1103 FR
8053 1103 FR
8054 X1 8 SF
8055 X1 8 FR
8056 X1 8 SC
8057 X1 8 DP
8058 X1 8 DP
8059 ALGOL DP
8060 ALGOL ST
8061 ALGOL ST

FROM 1ST ED.
8514 M1B SF
8515 M1B ID
8516 M1B A
8517 M1B SP
8518 M1B FR
8520 PC1 DP
8521 PC1 SF
8522 PC1 DP
8523 PC1 TA
8524 PC1 D
8525 PC1 ID

NEW, 2ND ED.
8526 7090 SF
8527 7090 LS
8528 ALG SF
8529 ALG FR
8530 7090 LS

APPENDIX -- IBM 360 (FORTRAN 4) PROGRAMS

THE FOLLOWING PROGRAMS ARRIVED TOO LATE TO BE LISTED IN PROPER SEQUENCE WITH THE OTHER PROGRAMS IN THIS COLLECTION, BUT ARE JUDGED SUFFICIENTLY IMPORTANT TO MERIT INCLUSION IN THIS APPENDIX --

536 360 FT4 D H PIPPY / AHMED NRC-21/D FOR POWDER MEASUREMENTS LWA
GENERATES THE INDICES AND CALCULATES D(HKL) WITHIN THE SELECTED SPACE OMITS PROHIBITED REFLNS. AND SORTS ON D.

537 360 FT4 DIR HALL / AHMED NRC-4/SYMBOLIC ADD'N PROCEDURE (C) LWA
ESTIMATES THE STRUCTURE FACTOR PHASES OF CENTROSYMMETRIC STRUCTURES USING SYMBOLIC ADDITION (SIGMA-2) METHODS.

538 360 FT4 DP AHMED*,HUBER NRC-2/DP + GENER'N OF THE LISTS' TAPE LWA
GENERATES THE LISTS' TAPE NEEDED FOR STRUCTURE ANALYSIS WITH ALL THE NRC PROGRAMS. ALSO REDUCES DIFFRACT'R AND WEISS'G DATA, INTERPOLATES ON F-CURVES, ASSIGNS WEIGHTS TO FOBS, APPLIES SHARPENING FUNCTION.

539 360 FT4 FR 3 2 AHMED NRC-8/FOR DISTORTED+UNDISTORTED NETS LWA
COMPUTES THE FR SUMS (A) ALONG LINES PARALLEL TO THE UNIT-CELL AXES, OR (B) AT THE GRID PTS. OF A SQ. NET SUPERIMPOSED ON THE SECTIONS OF THE UNIT-CELL. THE RESULTS IN (B) ARE PRINTED TO CORRECT MAP SCALE.

540 360 FT4 ID PIPPY,AHMED* NRC-12/INTRA-,INTER-MOLR. D + ANGLES LWA
SCANS THE GIVEN COORDS. FOR BONDS, DERIVES THE EQUIVALENT ATOMIC POSITIONS, SCANS FOR INTERMOLECULAR CONTACTS, CALCULATES THE ANGLES, AND GIVES SUMMARY OF THE COORDINATION AROUND EACH ATOM. CALCULATES ESD'S.

541 360 FT4 SF LS AHMED NRC-10/BLOCK DIAGONAL LWA
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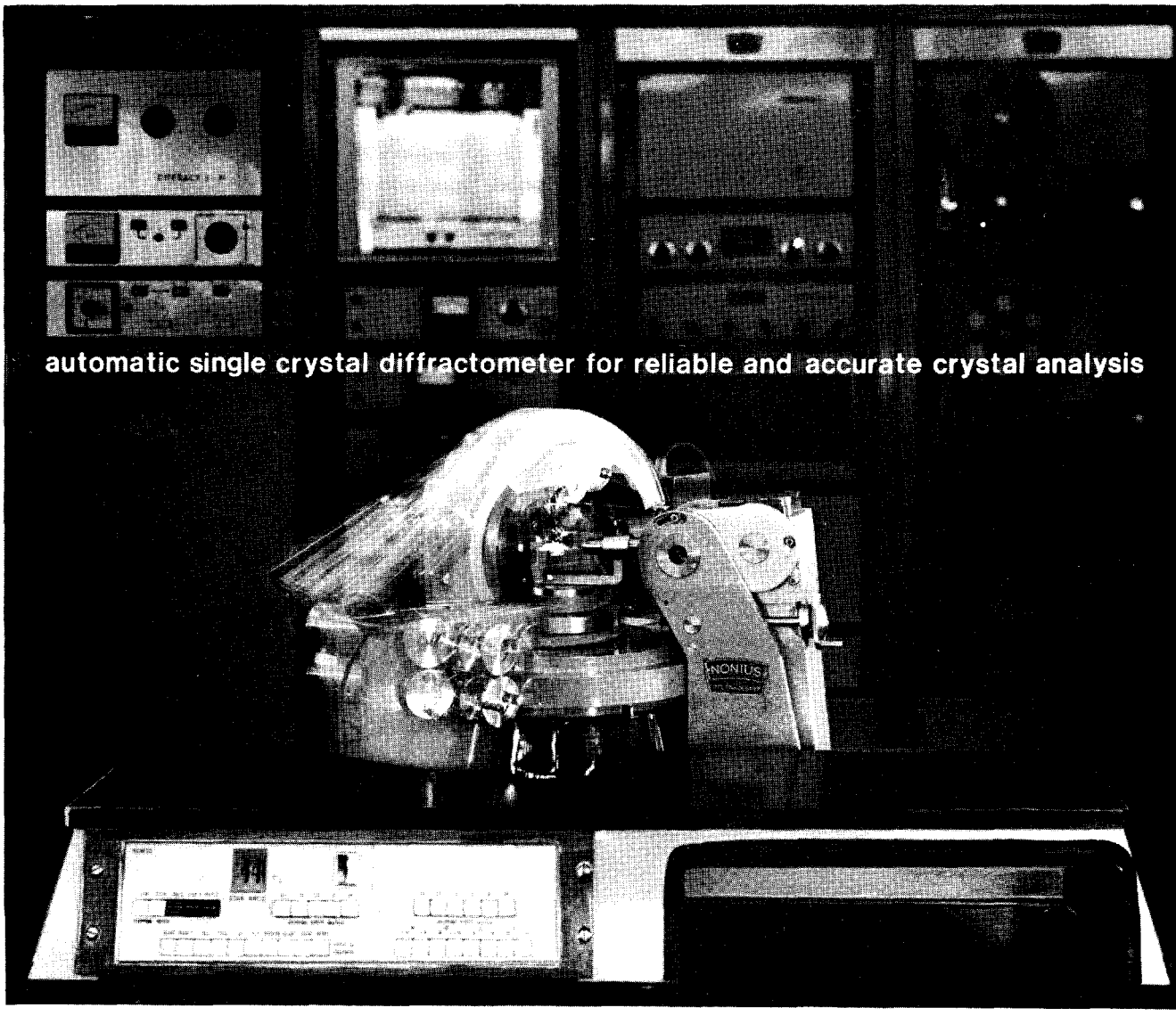

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