I U Cr WORLD LIST

OF

CRYSTALLOGRAPHIC COMPUTER

PROGRAMS

FIRST EDITION
SEPTEMBER 1962

INTERNATIONAL UNION OF CRYSTALLOGRAPHY
COMMISSION ON CRYSTALLOGRAPHIC COMPUTING

Produced by photo-offset from a tabulator listing of IBM punched cards. The listing, and most of the card processing, was done at the MIT Computation Center, Massachusetts Institute of Technology, Cambridge, Massachusetts, U.S.A.

PRINTED BY V.R.B.. GRONINGEN, THE NETHERLANDS

I U CR WORLD LIST OF CRYSTALLOGRAPHIC COMPUTER PROGRAMS

FIRST EDITION
SEPTEMBER 1, 1962

INTERNATIONAL UNION OF CRYSTALLOGRAPHY
COMMISSION ON CRYSTALLOGRAPHIC COMPUTING

GENERAL DESCRIPTION

1. THE FORM OF LISTING OF CRYSTALLOGRAPHIC COMPUTER PROGRAMS WILL BE THAT USED PREVIOUSLY BY THE CRYSTALLOGRAPHIC COMPUTING COMMITTEE OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION. FOR EASE IN ASSEMBLY AND REVISION A FORMAT BASED ON IBM PUNCHED CARDS IS USED.

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. COMMENTS ON THIS SYSTEM AND SUGGESTIONS FOR EVENTUAL MODIFICATION ARE SOLICITED. HOWEVER, FOR THE TIME BEING, IT SEEMS ADVISABLE TO FREEZE THE SYSTEM IN THE FORM HERE DESCRIBED.

DAVID P. SHOEMAKER, EDITOR
MASS. INST. OF TECH.
CAMBRIDGE 39, MASS., USA

I U CR COMMISSION ON
CRYSTALLOGRAPHIC COMPUTING
G. A. JEFFREY, CHAIRMAN
T. HAHN
M. A. PORAJ-KOSHITS
D. ROGERS
D. P. SHOEMAKER

THE PROGRAM LISTINGS HERE GIVEN WERE COLLECTED BY THE REGIONAL AND MACHINE CORRESPONDENTS WHOSE NAMES ARE GIVEN BELOW, ACCOMPANIED BY THEIR ASSIGNED RANGES OF ACCESSION NUMBERS AND THEIR PRESENT ADDRESSES.

1 - 2999 D. SAYRE (CANADA AND U. S. A., AMER. CRYST. ASSN. LIST)
IBM CO., 590 MADISON AVENUE, NEW YORK 22, N. Y.

3001 - 3499 D. ROGERS (ZEBRA, AUSTRALIA, NEW ZEALAND, SOUTH AFRICA, U. K.)
IMPERIAL COLLEGE, U. OF LONDON, LONDON S.W.7, ENGLAND

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

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

5001 - 5999 T. HAHN (AUSTRIA, GERMANY, SWITZERLAND)
MINERALOG. INST., U. OF FRANKFURT, SENCKENBERG-ANLAGE 30, FRANKFURT/MAIN, 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 P. MERIEL (FRANCE, PORTUGAL, SPAIN)
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 D. SMITS (BELGIUM, NETHERLANDS)
MATH. INST., U. OF GRONINGEN, REITDIEPSKADE 4, GRONINGEN, NETHERLANDS

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

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

A	ACENTRIC (NON-CENTROSYMMETRIC) ONLY
ABS	ABSORPTION CORRECTIONS
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)
FM	FULL MATRIX
FPK	FOURIER PEAK SHAPE ANALYSIS
FR	FOURIER SYNTHESIS (2 OR 3 DIM)
FT	FOURIER TRANSFORM
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 FACTCRS

LP	LORENTZ-POLARIZATION CORRECTION
LS	LEAST SQUARES (ASSUMED TO BE 3 DIM UNLESS OTHERWISE INDICATED)
N	NEUTRON (DIFFRACTION)
OT	OUTPUT
P	POWDER CALCULATIONS
PATSUP	PATTERSON SUPERPOSITION, MINIMUM FUNCTION, ETC.
PI	POWDER INDEXING
PK	PEAK
PREC	PRECESSION
PROF	PROFILE
R	R FACTOR, AGREEMENT FACTOR
S	SPECIAL
SCL	SCALE FACTOR
SF	STRUCTURE FACTORS
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
TF	TEMPERATURE FACTOR
THETA	BRAGG ANGLE
WEIS	WEISSENBERG
2	TWO-DIMENSIONAL
3	THREE-DIMENSIONAL

MACHINE ABBREVIATIONS

ALWAC	(OREGON STATE UNIVERSITY, USA)
BULL GET	BULL TYPE GAMMA ET (FRANCE)
BULLGAET	BULL TYPE GAMMA AET (FRANCE)
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)
G-15	BENDIX
G-15D	BENDIX
KDC1	KYOTO (JAPAN) DAIGAKU DIGITAL COMPUTER
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
PC2	FACOM-202 (JAPAN)
TR4	TELEFUNKEN TR 4 (GERMANY)
PEG	FERRANTI PEGASUS (BRITAIN)
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
ZRA 1	(GERMAN DEMOCRATIC REPUBLIC)
Z22	ZUSE Z22 (GERMANY)
Z22R	ZUSE 22R (GERMANY)
1103	REMINGTON RAND UNIVAC
1620	IBM
2002	SIEMENS 2002 (GERMANY)
204	BURROUGHS
205	BURROUGHS
220	BURROUGHS
2203B	NEAC - 2203 BASIC UNIT (JAPAN)
6001	OLIVETTI ELEA 6001. K INDICATES 10000 DIGITS HIGH SPEED STORAGE.
628	IBM
650	IBM

701 IBM
704 IBM
7070 IBM
709 IBM
7090 IBM
NOTE -- IBM 709 AND 7090 ARE INTERCHANGEABLE IN NEARLY EVERY RESPECT EXCEPT SPEED. VIRTUALLY ALL IN EXISTENCE ARE 32 K.
9002 OLIVETTI ELEA 9002. K INDICATES 10000 DIGITS HIGH SPEED STORAGE.

PSEUDO-MACHINES (GENERAL PROGRAMMING LANGUAGES, 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)
AUTOCODE
FORTRAN FORMULA TRANSLATION (IBM)
FORTRAN2 FORTRAN II
MAD MICHIGAN ALGORITHMIC DECODER (RELATED TO ALGOL)

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.

AUTHOR/PROGRAMMER INDEX

ABRAHAMS, S. C., BELL TELEPHONE LABORATORIES, MURRAY HILL, NJ
ABRAHAMSSON, S., INST. OF MEDICAL BIOCHEMISTRY, UNIV. OF GOTEBORG, SWEDEN
ABRAHMS, SEE ABRAHAMS, S. C.
ABRHMSN, SEE ABRAHAMSSON, S.
AHMED, F. R., NATIONAL RESEARCH COUNCIL, OTTAWA, CANADA
ALDEN, R. A., DEPT CHEM, UNIV. OF WASHINGTON, SEATTLE 5, WASH.
ALLEN, S., METALLURGY DEPT., MIT, CAMBRIDGE, MASS.
ANZENHOF. SEE ANZENHOFER
ANZENHOFER,K., MPI. EIWEISSFORSCHUNG, MUENCHEN, LUISENSTR. 39, GERMANY
APPEL, K., QUANTUM CHEMISTRY GROUP, UNIV. OF UPPSALA, UPPSALA, SWEDEN
ASB, SEE ASBRINK, S.
ASBRINK, S., INST. INORG. AND PHYS. CHEM., UNIV. OF STHLM., STOCKHOLM VA, SWEDEN
BAEHR, S., DAW-STRUKTURFORSCHUNG, BERLIN, GDR
BAENZIGER, N. C., IOWA UNIVERSITY, IOWA CITY, IOWA
BALLARD,MISS J.V., PHYS.DEPT., COLLEGE OF SCI. AND TECH., MANCHESTER 1, ENGLAND
BARTL,H.,MIN.INST.UNIV. FRANKFURT,SENCKENBERG ANLAGE 30, GERMANY
BASSI, G., CENTRE D*ETUDES NUCLEAIRES DE GRENOBLE, GRENOBLE, ISERE, FRANCE
BEITINGER, E., MUENCHEN-OTTOBRUNN, FA. BOELKOW, FINKENSTR. 15, GERMANY
BENOFFI ANDREA, OLIVETTI, VIA CLERICI 4, MILANO, ITALY
BENVENUT, SEE BENVENUTI P
BENVENUTI P, CSCE, SERVIZIO CALCOLI, LUNGARNO, PACINOTTI 16, PISA, ITALY
BERG., SEE BERGERHOFF
BERGERHOFF,G., CHEM. INST. UNIV.,BONN, GERMANY
BERTOLUZ, SEE BERTOLUZZA C
BERTOLUZZA, C, CSCE, SERVIZIO CALCOLI, LUNGARNO, PACINOTTI 16, PISA, ITALY
BEU, K. E., GOODYEAR ATOMIC, BOX 628, PORTSMOUTH, OHIO
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

BONNER, R. U., SHELL DEVELOPMENT CO., EMERYVILLE, CALIF.
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.
BRANDEN, C.I., DEPT. OF CHEMISTRY, UNIV. OF UPPSALA, UPPSALA, SWEDEN
BROWN, B. W. CHEM. DEPT., EVERETT JUNIOR COLLEGE, EVERETT, WASH.
BRUHN, RECHENINSTITUT PROF HAACK, TU BERLIN
BRWN, SEE BROWN, B. W.
BRYDEN, J. H., 2430 VASSAR PL., COSTA MESA, CAL.
BUJ, SEE BUJOSA, A.
BUJOSA, A., I.B.M., S.A.E., SERRANO 5, MADRID 1, SPAIN
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
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
CHAND, SEE CHANDROSS, R.
CHANDROSS, R., DEPT. OF CHEM., MIT, CAMBRIDGE, MASS.
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.
COONEY, W. A., SEE HAENDLER, H. M.
CORFIELD, P., DURHAM COLLS SCIENCE LABS, SOUTH RD, DURHAM, ENGLAND
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
DARLOW, S. F., PHYS. DEPT., COLLEGE OF SCI. AND TECH., MANCHESTER 2, ENGLAND
DEANGELIS,R J,DEPT.MATERIALS SC.,TECH INST., NORTHWESTERN UNIV.,EVANSTON,ILL.
DE GRIFFI ELENA, OLIVETTI, VIA CLERICI, MILANO, ITALY
DEGRIF, SEE DE GRIFFI ELENA
DELF, B. W., PHYS. DEPT., UNIVERSITY COLLEGE, CARDIFF, WALES
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.
DOLLIMORE,JEAN, CHEM. DEPT., UNIVERSITY COLLEGE, GOWER ST., LONDON W.C.1,ENGLAND
EDSTRAND, M., FORSKN. AVD., A.B. BOFORS NOBELKRUT, BOFORS, SWEDEN
EHRLICH,H.W.W.,ICI LTD,HEAVY ORG. CHEMICALS DIV, THE FRYTHE,WELWYN,HERTS,ENGLAND
EICHHORN, E. L., BURROUGHS CO., PASADENA, CALIFORNIA
FENN, R. H., ROYAL INSTITUTION, 21 ALBEMARLE ST., LONDON W. 1, ELGNALD
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
GANTZEL, PETER K. , DEPT CHEM, UNIV OF CALIF, LOS ANGELES 24, CALIF
GILMARTIN,MRS J.,AERE HARWELL, DIDCOT, BERKS, ENGLAND
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
GRUBISS, SEE GRUBISSICH CLAUDIC
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., MIN. INST. UNIV., FRANKFURT, SENCKENBERG ANLAGE 30, GERMANY
HAMILTON, W. C., BROOKHAVEN NATIONAL LABORATORY, BROOKHAVEN, NY
HARDING, MRS. M. M., CHEM. CRYST. LAB., SOUTH PARKS ROAD, OXFORD, ENGLAND
HARRIS,DAVID R., CHEMISTRY DEPT., UNIVERSITY OF COLORADO, BOULDER,COLO.
HELLNER, E., MIN.-PETRO. INST., KIEL, GERMANY

HENDE, SEE VAN DEN HENDE, J. H.
HIGH, UNIVERSITY OF WASHINGTON, SEATTLE, WASH.
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 LABORATORY, SILVER SPRING, MD.
HOP., SEE HOPPE
HOPPE,W., MPI. EIWEISSFORSCHUNG, MUENCHEN, LUISENSTR. 39, GERMANY
HOUSTON, B. J.,
HUBER,R., MPI. EIWEISSFORSCHUNG, MUENCHEN, LUISENSTR. 39, GERMANY
IBERS, J.A. DEPT. CHEM., BROOKHAVEN NATL. LAB., UPTON, L.I., N.Y.
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, FACULTE DES SCIENCES D*ORSAY, PHYSIQUE DU SOLIDE, ORSAY, S ET O, FRANCE
JEFFREY, G. A., CRYSTALLOGRAPHIC LAB., UNIVERSITY OF PITTSBURGH, PITTSBURGH, PA.
JENSEN, L. H., UNIV. OF WASHINGTON, SEATTLE, WASH.
JOHNSON, C.K. INST. FOR CANCER RES., 7701 BURHOLME AVE., PHILA. 11, PA.
JOHNSON, Q., UNIV. OF CALIFORNIA, BERKELEY, CALIF.
JONES, UNIV. OF CALIFORNIA, BERKELEY, CALIF.
KAPLOW, R., METALLURGY DEPT., MIT, CAMBRIDGE, MASS.
KAY, M.I. NASA, LEWIS RES. CTR., 21000 BROOKPARK RD., CLEVELAND 35, OHIO
KEILHAU, H., NORWEGIAN DEFENCE RESEARCH ESTABLISHMENT, KJELLER, NORWAY
KEMPTER,C.P.,LOS ALAMOS SCIENTIFIC LABORATORY,LOS ALAMOS,NM
KEUL, SEE KEULEMANS, E. W. M.
KEULEMANS, E. W. M., LAB. VOOR KRISTALLOGRAFIE, UNIV. OF AMSTERDAM, NETHERLANDS
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., BIOPHYSICS DEPT., JOHNS HOPKINS UNIV., BALTIMORE, MD.
KRAUSE, CH., DAW-STRUKTURFORSCHUNG, BERLIN, GDR
KRAUT, J., UNIVERSITY OF WASHINGTON, SEATTLE, WASH.
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
LARSON, A.C. LOS ALAMOS NATL. LAB., LOS ALAMOS, N.M.
LARSEN, F., DANISH INST. FOR COMPUTING MACHINERY, GL CARLSBERGV 2, VALBY,DENMARK
LEFKER, R., USASRDL-XE, FORT MONMOUTH, NJ
LENHERT, P. GALEN, BIOPHYSICS DEPT., JOHNS HOPKINS UNIV., BALTIMORE, MD.
LEVY,H. A., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
LIMINGA, R., DEPT. OF CHEMISTRY, UNIV. OF UPPSALA, UPPSALA, SWEDEN
LIND,M., CHEM. DEPT., CORNELL UNIV., ITHACA, N.Y.
LINEK, A., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
LINGAFELTER, E. C., UNIV. OF WASHINGTON, SEATTLE, WASH.
LINGFLTR, 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
LOVE, W. E., BIOPHYSICS DEPT., JOHNS HOPKINS UNIV., BALTIMORE, MD.
LUNDBERG, B., DEPT. OF CHEMISTRY, UNIV. OF UPPSALA, UPPSALA, SWEDEN
LUNDBRG, SEE LUNDBERG, B.
LOV, SEE LOVELL, F.M.
LOVELL, F.M. SCHOOL OF CHEM., UNIV. OF SYDNEY, N.S.W., AUSTRALIA
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., NATIONAL RESEARCH COUNCIL, OTTAWA, CANADA
MALLETT, G. R., DOW CHEMICAL CO., BOX 2131, DENVER, COLO.
MAR, SEE MARTIN,K. O.
MARTIN,K. O., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE

MARSH, R. E., CALIF. INST. OF TECH., PASADENA, CALIF
MASAKI, N., DEPT. PHYSICS, OSAKA UNIV., NAKANOSHIMA, OSAKA, JAPAN
MARIANI C., INSTITUTO DO CHIMICA FISICA, UNIVERSITA DI MILANO, MILANO, ITALY
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.
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
MILLER, D. P., TEXAS INSTITUTE, DALLAS, TEXAS
MOHN, G. J., WESTINGHOUSE ELECTRIC CO., BETTIS PLANT, PITTSBURGH, PA.
MONDRUP, P.,DANISH INST. FOR COMPUTING MACHINERY, GL CARLSBERGV 2,VALBY,DENMARK
MORGAN, C. H., CHEM. DEPT., QUEENS COLLEGE, DUNDEE, SCOTLAND
MORINO, Y., DEPT. OF CHEM., UNIV. OF TOKYO, BUNKYO-KU, TOKYO, JAPAN
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
MUSIL, F. J., GOODYEAR ATOMIC, BOX 628, PORTSMOUTH, OHIO
NADR, SEE NADRCHAL, J.
NADRCHAL, J., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
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,
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.
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
OSAKI, K., DEPT. PHYSICS, OSAKA UNIV., NAKANOSHIMA, OSAKA, JAPAN
PALENIK,G.J.,CODE 5058, USNOTS ,CHINA LAKE,CALIFORNIA
PALM, J. H., LAB. TECHN. PHYSICA, TECHNISCHE HOGESCHOOL, DELFT, NETHERLANDS
PALMER,R.A.,BIRKBECK COLLEGE RES.LAB., 21 TORRINGTON SQ., LONDON W.C.1, ENGLAND
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.
PIL, SEE PILLING, D.E.
PILLING, D.E., C.E.I.R., 84 KINGSWAY, LONDON W.C.2., ENGLAND
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
PTRSON, SEE PETERSON, D. P.
PREWITT, C. T., DEPT. OF GEOLOGY, MASS. INST. OF TECH., CAMBRIDGE, MASS.
PROUT, C. K., CHEM. CRYST. LAB., SOUTH PARKS RD., OXFORD, ENGLAND
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
ROSSMAN, M. G., DEPT. OF CHEM., UNIV. OF MINN., MINNEAPOLIS, MINN.
ROWE,J.M., I.C.I.LTD.,HEAVY ORG. CHEMICALS DIV., THE FRYTHE,WELWYN,HERTS,ENGLAND
RUDOLPH, G. J., N.R.I.MATH.SC., C.S.I.R., BOX 395, PRETORIA, SOUTH AFRICA
SAMET P., CO H.P. STADLER, KINGS COLLEGE, NEWCASTLE UPON TYNE, ENGLAND
SANDS, D. E., LAWRENCE LABORATORY, LIVERMORE, CALIF.
SASADA, Y., INSTITUTE FOR PROTEIN RESEARCH, OSAKA UNIV., KITAKU OSAKA JAPAN

SASS, R., RICE INSTITUTE, HOUSTON, TEXAS
SASVARI, K., M.T.A.KOZP.KEM.KUT.INT., BUDAPEST, HUNGARY
SAYRE, D., IBM CO., 590 MADISON AVE., NYC
SCHAPIRO, P.J. CRYST. LAB., U. OF PITT., PITTSBURGH 13, PA.
SCHMID,E., RECHENINSTITUT DER TECHN. HOCHSCHULE, STUTTGART, HERDWEG 51 GERMANY
SCHOONE, J. C., LAB. VOOR KRISTALCHEMIE, UNIVERSITY OF UTRECHT, NETHERLANDS
SCHWARTZ,L.H.,MAT. SCI. DEPT., NORTHWESTERN U. EVANSTON,ILL.
SENKO, M. E., IBM COMPANY, POUGHKEEPSIE, N Y
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, S. G., CHEM. DEPT., THE UNIVERSITY, GLASGOW W.2, SCOTLAND
SIMPSON, S. M., DEPT OF GEOL., MIT, CAMBRIDGE 39, MASS.
SLITER, J. A., 2162 14TH ST., TROY, N Y
SMITH, A. E., SHELL DEVELOPMENT CO., EMERYVILLE, CALIF.
SMITH, J., SEE SMITH, J.G.F.
SMITH, J. E. W. L., SCH. OF CHEM., UNIVERSITY OF SYDNEY, SYDNEY, AUSTRALIA
SMITH, J.G.F., SCHOOL OF CHEM., UNIVERSITY, LEEDS 2, ENGLAND
SMITS, D. W., MATHEMATISCH INSTITUUT, UNIVERSITY OF GRONINGEN, 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.
STADLER, H.P., KINGS COLLEGE, NEWCASTLE UPON TYNE, ENGLAND
STEMMLER, R. S., ILLINOIS GEOLOGICAL SURVEY, URBANA, ILL.
STEWART, J. M., UNIV. OF WASHINGTON, SEATTLE, WASH.
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., DEPT, OF CHEM., BOZEMANN, MONT.
TAKEUCHI, Y., DEPT. OF MINERALOGY, UNIV. OF TOKYO, HONGO, TOKYO, JAPAN
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
TOEPFER, RECHENINSTITUT PROF HAACK, TU BERLIN
TOMAN, K., INST. OF SOLID STATE PHYS., CSAV, PRAGUE, CZECHOSLOVAKIA
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.
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
VAN DEN HENDE, J.H., ESSO RES.AND ENGIN.CO., CBRL, PO BOX 45, LINDEN, NJ.
VAN DER HELM, D. INST. FOR CANCER RES., 7701 BURHOLME AVE., PHILA. 11, PA.
VAN DER SLUIS, , 51 CATHARIJNESINGEL, UTRECHT, NETHERLANDS
VAND, V., GROTH INST., PENN. STATE UNIV., UNIVERSITY PARK, PA.
VDHELM SEE VAN DER HELM, D.
VOGEL,R.E., KAMAN CORP COLO SPRINGS,COLO
VONK, C. G., CENTRAAL LAB. STAATSMIJNEN, GELEEN, NETHERLANDS
WEH, SEE WEHE,D. J.
WEHE,D. J., OAK RIDGE NATIONAL LABORATORY, OAK RIDGE, TENNESSEE
WEISS, H. G., DAW-STRUKTURFORSCHUNG, BERLIN, GDR
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. AND PHYS. CHEM., UNIV. OF STHLM., STOCKHOLM VA, SWEDEN
WHITTIER, V. E., DOW CHEMICAL COMPANY, MIDLAND, MICH.
WILL,G., MPI. EIWEISSFORSCHUNG,MUENCHEN,LUISENSTR. 39, GERMANY
WILLIAMS, D. E., IOWA STATE UNIVERSITY, AMES, IOWA
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.
WUNDERLICH, J., CENTRAL SCI. INDUSTR. RES. ORG., MELBOURNE, AUSTRALIA
WUENSCH, B.J., DEPT OF GEOL AND GEOPHYS, MIT, CAMBRIDGE 39, MASS
ZALKIN, A., LAWRENCE RADIATION LAB., P O BOX 808, LIVERMORE, CALIF.
ZANO, SEE ZANOVELLO RENATO
ZANOVELLO RENATO, C.E.C.S., V. PAOLOTTI 9, PADOVA, ITALY
ZILAHI-SEBESS, L., M.T.A.KOZP.KEM.KUT.INT., BUDAPEST, HUNGARY

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 SUPPRES ED.

PROGRAMS LISTED UNDER PSEUDO-MACHINES

```
 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        DS  /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.
 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
5013 ALGOL    FR 3       HOPPE/HUBER       3 DIM                               NNN
 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).

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.

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.

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.

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.

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.

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.

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

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.

4019 AUTOCODE LP PALMER PREC, LP ANY LEVEL NOT TRICLINIC LWA

362 FORTRAN2 ABS 3 BUSING*LEVY,WEH 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 AND 7090.

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.
 344 FORTRAN  FR2       KAY                IT A,3(CAL),FOBS.OT FR/DIF.        NPA
      CALCULATES  EL. DENSITY OR DIFFERENCE MAP USING SIN. TABLE
      CHECKED ON 8000 WORD 704
 345 FORTRAN  N,DP,2    KAY               NPD AND SPECTR.IT FOR 100PART TABLL  NPA
      CHECKED ON 8000 WORD 704
 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.

PROGRAMS LISTED UNDER ACTUAL MACHINE DESIGNATIONS

6012 ALWAC-3E FR 1      TUVLIND          10-28/                                LWA
6011 ALWAC-3E FR 2      TUVLIND          05-28/                                LWA
6010 ALWAC-3E SF        LAGERWALL        02-28/                                LWA
6013 ALWAC-3E SF 3 H    APPEL            KGK-1/                                LPA
      GENERATES ONE OR TWO TERM STRUCTURE FACTORS FOR POSITIVE HKL,
      USING 2 OR 3 TERM EXPONENTIAL APPROXIMATIONS OF LF.
7018 BULL GET LP        BASSI              L AND LP CALC,SIN SQUARE THETA      LWA
      CALC. L AND LP FACTORS AND SINUS SQUARE THETA
8001 BULL GET FR 3 AC   KEUNING,VONK*    TRICL, 1500 REFL                      NNN
      USES TRICL. EL.DENS. FORMULAE BUT ONE SIGN RELATION MAY BE INTRUDUCED
      SPEED 3 SEC/POINT (1500 REFL.).
8002 BULL GET LP        KEUNING,VONK*    D, LF, INT. OVER LP                   LWA
      INPUT REC. CELL CONST., TABLES OF LITTLE F (MAX. 5) AND H K L.
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 INCLUDE HKL, 2THETA OBS AND CAL TABLE IS PRINTED.

5020 BULLGAET LC TRANS ITAKA 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 C LINDRICAL SPECIMEN

5015 BULLGAET LS 3 IITAKA TRI,MONO,ORTH,.,DM,ISOTF.EACH ATOM LWA
REFINES FOR F SQ.ALL DATA ARE STORED IN THE M CHINE.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,TRI LINIC,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 CORRESPONDING 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.

4027 DEUCE FR 3 DF SIME P086/DIFFERENTIAL SYNTH SF IT ON DRUM MWA
STRUCTURE FACTOR DATA NORMALLY ON DRUM AS AT END OF S.F. PROGRAM.
REFINES ATOMIC COORDINATES AND INDIVIDUAL ISOTROPIC TEMPERATURE FACTORS.

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 O 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.

4026 DEUCE SF SIME P081-3/SF USING PAPER TAPE IT OT MWA
COMPUTES STRUCTURE FACTORS WITHOUT PUNCHING THEREBY ALLOWING THE R FACTOR
TO BE DETERMINED FIRST. THE DATA ARE STORED IN DEUCE IN THE FORM
REQUIRED BY THE DIFFERENTIAL SYNTHESIS PROGRAM.

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).

5007 ER 56 FR 2 THURN GENL, VARIABLE GRID, H, K UP TO 19 LWA
IT ABS(F)COS(ALPHA),ABS(F)SIN(ALPHA)

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.
6021 FACIT    FPK 2 3  LUNDBRG,OLOVSON LOKE/FR PK MAX, GAUSS ELLIPS APPROX    LWA
6022 FACIT 1K FR 2     EDSTRAND/ASB*   S1/C FAST                              LWA
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 LWA
6017 FACIT    LP       WERNER           PREC, LP FOR ANY LEVEL, H             LWA
6024 FACIT 2K LP       WESTMAN,ASBRINK LOPPA/LP OF INTENSITIES FROM WEIS      LWA
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.
6018 FACIT 1K P        WERNER           IQ81/INDEX APPR KNOWN PTRN,REFINES LC LWA
6025 FACIT    SF       ASB,WESTM,BLOMK PROSIT/P1 OR P-1,LF-CONSTS. FROM AFFE LWA
6015 FACIT    SF H     LIMINGA,OLOVSON STRIX/CALC SF+H FOR FR IT.ANY SYMM.    LWA
 108 G-15D    LC       MALLETT          CUBIC, COHN LS METHOD, DBL PREC
 109 G-15D    LC       MALLETT          MONO, ORTH, COHN LS METHOD, DBL PREC
 110 G-15D    P PK     MALLETT          POWD LINE PROFILE ANAL, STOKES
   6 G-15     SF AT S  SMITH A S        P-BCM ONLY, LONG CHAIN MOL
   7 G-15     SF S     SMITH A E        P-BNM FROM FT OF LONG CHAIN
 125 ILLIAC   S        STEMMLER/GRAF*   HENDRICKS AND TELLER MIXED LAYER EQN
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
  76 LGP30    DP       CARPENTER       M13-C3/REPROCESS DATA, PERMUTE HKL
  74 LGP30    DP LP    MEDRUD          M13-M1/CONVERTS INT TO F**2
   3 LGP30    FR 2 A   KOENIG          M-13 102/BL 1/64 ACENTR
   2 LGP30    FR 2 C   KOENIG          M-13 101/BL 1/64 CENTRO
  58 LGP30    FR 2 C   LEFKER           FR OR PATT 512 COEFS
  56 LGP30    FR 2 DF  LEFKER           DIFFERENTIAL SYNTH 512 COEFS
  73 LGP30    FR 2 3 C BAENZIGER       M13-B1/GRID 1/64
  57 LGP30    FR 3 S   NORMENT          FOR R3M + RELATED SP GRPS, 400 COEFS
  54 LGP30    H LP     NORMENT          HKL, LP
6512 LGP30    ID       LINEK*NKB        GENERAL FORMULA                       LWA
```

```
  75 LGP30    LP          CARPENTER       M13-C1/LP CORR FOR WEISS DATA
  72 LGP30    LS A AT     BAENZIGER       M13-B2/UP TO 26 UNIQUE ATOMS
  71 LGP30    LS C AT     BAENZIGER       M13-B3/UP TO 26 UNIQUE ATOMS
   5 LGP30    PATSUP 2    LOVE             PATT SHIFT MAP MAKER
  55 LGP30    PI          LEFKER           INDEX TETRAG AND HEX POWD PATTERNS
  53 LGP30    SF LP       LEFKER           GEN SF, LP, SP GR EXT 96 AT, 6 KIND
  52 LGP30    SF S        NORMENT          SF FOR R3M + RELATED GRPS, TO 64 AT
   4 LGP30    SF 2        LENHERT          PREP F OR DF FOR PGMS 2 OR 3
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.
4034 MERCURY  DP          PROUT           DR/04                                LWA
    TRANSFORMS I FROM WEIS OR OSCILLATION PHOTOGRAPHS TO F-SQUARED, F,
    AND MODIFIED F-SQUARED, APPLYING LORENTZ, POLARISATION AND
    INCLINATION FACTORS.
4032 MERCURY  DP          ROLLETT          SORT HKL DATA                       MPA
    GIVEN HKL DATA IN RANDON ORDER, PROVIDES DATA SORTED INTO ANY DESIRED
    ORDER OF INDICES.
4015 MERCURY  DP          NORTH           RIM46/TAPE-EDITING/CORRECTING        LWA
    TAPE IS READ IN AND COPIED BY COMPUTER.  WHENEVER A PRE-SELECTED
    CHARACTER IS ENCOUNTERED, IT MAY BE (1) COPIED AS IT STANDS,
    (2) OMITTED ENTIRELY, (3) REPLACED BY A DIFFERENT PRE-SELECTED
    CHARACTER, ACCORDING TO HANDSWITCH SETTINGS.
4017 MERCURY  DP          NORTH           RIM60/AUTOMATIC DIFFRACTOMETER DP    LWA
    (1) DIFFRACTOMETER OUTPUT CHECKED FOR PUNCHING ERRORS
    (2) DATA CHECKED FOR EVIDENCE OF CRYSTAL MIS-SETTING
    (3) BACKGROUND-CORRECTED INTENSITIES DERIVED
    (4) STANDARD ERRORS IN ABOVE CALCULATED
    (5) CORRECTIONS APPLIED FOR LP FACTOR, ABSORPTION, AND RADIATION DAMAGE
    (6) FINAL OUTPUT IN FORM SUITABLE FOR INPUT TO FOURIER OR LEAST SQUARES
           PROGRAM
4003 MERCURY  DP LP       BLAND, ROWE*    439/DATA REDUCTION                   LPA
    DATA TAPE REQUESTS OPTIONAL FACILITIES INCLUDING LP FACTOR, UPPER LAYER
    WEIS SPOT SHAPE CORRECTION, INTERPOLATION FOR ABSORPTION CORRECTION,
    WILSON PLOT, UNITARY SF.  INPUT PLANES TAPE CARRIES HKL INTENSITY.
    OUTPUT IS ANY OR ALL OF F SQD, F, U, SIN/LAMBDA SQD, SCALING AND TEMP.
    FACTORS FROM WILSON PLOT.
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.
4037 MERCURY  FPK         HARDING          PEAK SHAPES                         MPA
    CALCULATES 3-D FOURIER TRANSFORM OF GIVEN LF CURVE.
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.
6007 MERCURY ID DIDRIKSEN NDRE-R2286/ATOMIC DIST. AND ANGLES LWA
COMPUTES THE DISTANCES BETWEEN ANY TWO ATOMS SPECIFIED IN A GIVEN STRUCTURE AND ANY ANGLES IN ANY TRIANGLE FORMED BY ANY THREE ATOMS SPECIFIED. INPUT PGM NDRE DIP.
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.
4010 MERCURYA LF INTPL PAULING,DOLLIMORE/INTERPOLATES IN LF LPA
GIVEN LF TABULATED AT WIDE INTERVALS IN S, DOES POLYNOMIAL INTERPOLATION AT PRESET INTERVALS IN LAMBDA S OR LAMBDA S SQUARED. USED WITH ROLLETT SFLS.
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.
4004 MERCURY PK EHRLICH 868/RHO MAX AND CURVATURE LWA
FOR GIVEN F CURVE (FORSYTH WELLS), TEMPERATURE FACTORS AND WAVELENGTH OF RADIATION PREDICTS CURVATURE AND MAX VALUE OF ELECTRON DENSITY
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.
4005 MERCURY PLANE ROWE 353/BEST WEIGHTED PLANE LWA
EQUATION FOR WEIGHTED PLANE THROUGH GIVEN POINTS IS CALCULATED USING LEAST SQUARES METHOD, AND OUTPUT IN ORTHOGONAL AND CRYSTALLOGRAPHIC COORDINATES, DISTANCES OF THESE POINTS, THEN OF ANY OTHER GIVEN POINTS, FROM THE PLANE ARE ALSO OUTPUT.
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.
4016 MERCURY S NORTH RIM50/FOURIER INTERPOLATION LWA
GIVEN AN ELECTRON-DENSITY DISTRIBUTION EVALUATED AT THE POINTS OF A 3-DIMENSIONAL GRID, THE PROGRAMME USES LINEAR INTERPOLATION TO

CALCULATE THE ELECTRON DENSITIES AT THE POINTS OF A SECOND GRID, RELATED TO THE FIRST IN A DEFINED WAY.

4006 MERCURY SCL ROWE 347/LAYER SCALING LWA
PLANES TAPE OF INDICES AND F OR F SQD ASSEMBLED FROM SUCCESSIVE LAYERS UP THE AI AXIS IS MODIFIED BY APPLICATION OF SCALING FACTORS WHICH CAN BE DIFFERENT FOR EACH HI, USEFUL AFTER FOBS/FCALC CORRELATION IN INDIVIDUAL LAYERS DURING REFINEMENT.

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.

4018 MERCURY SPC FENN AUTOMATIC 3-CIRCLE DIFF. SETTINGS NPN
(1) INDICES GENERATED IN SPECIFIED ORDER OMITTING SPACEGROUP ABSENCES
(2) THREE ANGLES CALCULATED FOR EACH REFLEXION FOR ANY RECIPROCAL AXIS MOUNTED PARALLEL TO GONIOMETER AXIS
(3) ANGLE INCREMENTS OUTPUT IN FORM SUITABLE FOR INPUT TO DIFFRACTOMETER

4009 MERCURYP SF DOLLIMORE PROTEIN SF/SIMPLE,FAST LPA
CALCULATES INDIVIDUAL AND TOTAL SF FOR 2 GROUPS OF ATOMS IN P21. TOTAL ISOTROPIC B ONLY, UNLIMITED NUMBER OF ATOMS IN EITHER GROUP. FAST FOR BIG STRUCTURES. OTHER SPACEGROUPS EASILY AVAILABLE.

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.

4014 MERCURY 2SFRFRDF BALLARD,MAIN,DARLOW*/ LPA
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.

4013 MERCURY 3ABSLP WOOLFSON EQUI-INCLINATION WEIS
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 INTENSI-

```
     TIES.
6514 NE803    ID       LINEK              GENERAL FORMULA                        LWA
8511 PC1      BL 1D    MORINO             MOLECULAR INTENSITY - 1 GAS EL         LWA
     MOL INT AT EACH Q IN REGION INSTRUCTED. SCATTERING AMP, ID AND VIB MA FOR
     EACH KIND OF ATOM PAIR ARE INSTRUCTED. CAL UP TO 65 KINDS OF ATOM PAIRS.
8509 PC1      BL 1D    MORINO             MOLECULAR INTENSITY - 2 GAS EL         LWA
     MOL INT WITH CORRECTION FOR NON-NUCLEAR SCATTERING. CORRECTION FACTORS
     ARE INSTRUCTED AS TABLE ON TAPE. THEY ARE READ ONE BY ONE DURING CAL.
     OTHERWISE SIMILAR TO PGM MOL INT-1.  CAL UP TO 30 KIND OF ATOM PAIRS.
8510 PC1      BL 1D    MORINO             MOLECULAR INTENSITY - 3 GAS EL         LWA
     MOL INT WITH PHASE SHIFTS. OTHERWISE SIMILAR TO PGM MOL INT-1. CAL UP TO
     41 DIFFERENT KINDS OF ATOM PAIRS.
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.
8512 PC1      FT 1D    MORINO             INVERSE TRANSFORMATION OF RD GAS EL  LWA
     USES OUTPUT TAPE OF PGM RD AS INPUT WITHOUT FURTHER PROCESSING. REMOVES
     ARTIFICIAL TF. NUMBER OF TERMS IS RESTRICTED TO 88 OR LESS.
8508 PC1      FT 1D    MORINO             RADIAL DISTRIBUTION GAS EL             LWA
     RD CURVE BY FT MOL INT WITH OR WITHOUT MODIFICATION BY ARTIFICIAL TF.
     TF, REGION AND INTERVAL OF R ARE INSTRUCTED. NUMBER OF TERMS IS RESTRICT-
     ED TO 145 OR LESS.
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.
8519 PC1      ID       TAKEUCHI,IITAKA  ID, ANGLE INVOLVED                       LWA
     FEED COORDINATES OF THREE ATOMS AND CALCULATE THREE DISTANCES AND AN
     ANGLE.
8513 PC1      LS       MORINO             LS ANALYSIS OF MOL INT CURVE GAS EL  LWA
     LS FIT OF OBSD MOL INT CURVE BY CALD ONE. PARAMETERS TO BE ADJUSTED ARE
     INDEX OF RESOLN, VIB MA AND ID. APPLICATION TO MOLECULES WITH 4 OR LESS
     DIFFERENT KINDS OF ATOM PAIRS IS PRACTICAL. CONSISTS OF A SERIES OF PGMS
     OPERATED SERIALLY. NUMBER OF OBSD POINTS IS RESTRICTED TO 99 OR LESS.
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.
3507 PEG 7K   DIR3     HINE                                                      MPA
     PROGRAM FOR APPLICATION OF GRANT, HOWELLS, ROGERS SIGN RELATION METHOD
     (ACTA. CRYST. 10,489) TO 3 DIMENSIONAL DATA.
3505 PEG 4K   DP       SMITH,J/TRUTER*  LP+PHILLIPS+ABS FOR WEIS AND LIN DIF MPA
     INPUT VISUAL EST. WEIS OR OUTPUT OF ARNDT-PHILLIPS LINEAR DIFFRACTOMETER.
     LP ANY AXIS. ABS SPHERES OR CYLINDERS FOR MR LESS THAN 5. PHILLIPS CORR.
3510 PEG 4K   FR 2     SAMET/STADLER    COFS/SINGL CHARACTR OUTPUT.VAR MESH    LWA
     OUTPUT FOR DIRECT CONTOURING PATCH OR FULL SYNTHESIS. SUMS BY REGRESSION.
     FACILITIES FOR FR 3 SECTIONS BY PRELIM SUMMATION FOR UNLIMITED L
     H UP TO 40, K UP TO 45. 500 TERMS 30X60 POINTS 15 MIN FOR P2/M
     35 MIN FOR P21/C INCL PRINT-OUT
3508 PEG 4K   FR 2 C   GREEN              RI4B/BL,GRID 1/64, 10 MIN,SEE RI4A     LPM
```

```
3503 PEG 7K   FR 2 3   PIL,LOV,BUJ/TRUTER*/VAR. GRID. ALL SG                 MPA
    ANY GRID TO 1/400. BL TABLE GENERATED. OUTPUT VARIABLE ACROSS PAGE.
    ALL OR BLK. USES UNIQUE PLANES THRU ORTHORHOMBIC,
    REQUIRES EQUIV. PLANES FOR HIGHER SYM. USES 7K AND 2 MAG TAPES.
    FOR DESCRIP OF SLIGHTLY EARLIER VERSION SEE BOOK (PERGAMON PRESS)
    ON GLASGOW CRYST COMPUTER CONFERENCE OF 1960, P. 56.
3506 PEG 7K   H3       HINE                                                  MPA
    USED IN CONJUNCTION WITH PROGRAM FOR APPLICATION OF
    GRANT, HOWELLS, ROGERS SIGN RELATION METHOD
3504 PEG 4K   ID       TRUTER            DIST,ANGLES,ANY SYM                 MPA
    DIST. (ANGLES OPT) LESS THAN L1 BETWEEN GIVEN ATOMS. DIST (ANG)LESSTHANL2
    BETWEEN PROGRAM-GENERATED SYM-AND TRANS-RELATED ATOMS AND GIVEN SET.
    FOR DESCRIP SEE BOOK (PERGAMON PRESS) ON GLASGOW CRYST
    COMPUTER CONFERENCE OF 1960, P. 69.
3511 PEG 4K   LP       CORFIELD          PREC,WEIS OTLP OR CORRECTED SF      NPA
3509 PEG 4K   PREC DP  GREEN            RI4A/LP,SCL,H,USED WITH RI4B         MPA
3502 PEG 4K   SFLS AT  CRUICK,PILLING    GEN LS,ALL SG,R,E,PARTIAL DIAG      MPA
    FOR FULL DESCRIP SEE BOOK (PERGAMON PRESS) ON GLASGOW
    CRYST COMPUTER CONFERENCE OF 1960, P. 41
3501 PEG 4K   VIB ANAL BUJOSA/CRUICK*    FROM AT,TRANS+ROT VIBS,COORD CORRNS NPA
    GIVEN ATOMIC UIJ FINDS PRINCIP AXES, RIGID BODY TRANS
    + ROT VIB TENSORS, UIJ CALC, COORD CORRNS FOR ROT ERROR.
    FOR DESCRIP SEE BOOK (PERGAMON PRESS) ON GLASGOW
    CRYST COMPUTER CONFERENCE OF 1960, P. 73.
3007 SILLIAC  ABS      LOVELL            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            BOND ANGLES ONLY                    LWX
    COMPUTES ALL ANGLES SUBTENDED AT A CENTRAL ATOM BY PAIRS OF ATOMS FROM A
    SPECIFIED GROUP.
3001 SILLIAC  DP LP    SMITH J,FREEMAN V15/CORRECTS INT.,GIVES SIN THETA     LWX
3002 SILLIAC  FR 2     FREEMAN          V7/GRID N/128, UP TO 1280 TERMS
3008 SILLIAC  ID       LOVELL            BOND DISTANCES ONLY                 NPX
    COMPUTES ALL DISTANCES LESS THAN A SPECIFIED LIMIT WITHIN BASIC CELL AND
    26 SURROUNDING CELLS. ALL SPACE GROUPS CAN BE HANDLED.
3004 SILLIAC  LF       FREEMAN          V14/POLYNOM REP. OF SCAT CURVES
3003 SILLIAC  LS       FREEMAN           AUTOMATIC LS, MONOCLINIC ONLY
3005 SILLIAC  SF MONO  FREEMAN          V8/SF MONOCLINIC ONLY
3006 SILLIAC  SF ORTH  FREEMAN          V10/SF ORTHORHOMBIC ONLY
3010 SILLIAC  SF 3ATN  LOVELL            ALL SYMM N/XDIFF  DOES 2X2 FOR SCLTF NPX
    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
6504 URAL 1   FR 2 C   BAEHR*WEISS       UP TO 1600 WORDS(OCTAL)IN 2GROUPS,BL LWA
6508 URAL 1   FT       TOMAN             FOR AMORPHE MATERIALS.OT RAD.DISTR. NPX
    RADIAL DISTRIBUTION FUNCTION OF SCATTERING MATTER FROM 0 TO 16 ANGSTROMS.
6505 URAL 1   SF       LINEK,NVK,NADR   E82/GENERAL FORMULA.ICA              LPA
6503 URAL 1   SF C     BAEHR*KRAUSE      IT=LC,COORD,DEBYE,LF,F(OB),OT ALSO R LWA
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.
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.
8005 X 1      FR 3     KEULEMANS        THREE ORTH                           MWA
8006 X 1      SF 3     KEUL,MACGILL     TRICL,INDIV ISOTROPIC TF             MWA
3034 ZEBRA    D AND PI DELF             ZK50/D AND SINTHETA FROM CELLDATA    LWS
    LISTS ALL HKL SINTHETA AND D FOR D LESS THAN SPECIFIABLE LIMIT.
    ALL CLASSES EXCEPT CUBIC.
3038 ZEBRA    D SORT   DELF             ZK57/SORT D OT OF ZK50               MNA
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
3032 ZEBRA    LP WEIS    GRANT             ZK40/LP EAUI-INCL WEIS                MNA
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          BO5/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          BO3/SHIFT TELEPRINTER MARGIN 10 SF    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
3024 ZEBRA    PK LOCN    GRANT             ZK11/LS PEAK POSN                     MNA
     27-POINT 3D DATA. SPHERICAL LS TREATMENT.
3025 ZEBRA    PK LOCN    GRANT             ZK12/LS PEAK LOCN                     MNA
     64-POINT 3D DATA SPHERICAL LS TREATMENT.
3026 ZEBRA    PK LOCN    GRANT             ZK13/LS PEAK LOCN                     MNA
     64 POINT 3D DATA. ELLIPSOIDAL LS TREATMENT.
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    BO4/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          BO2/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
3020 ZEBRA    TABLE      DELF,ROGERS       ZK71/TABLE 4SINSQTHETA                MNA
     THETA 1 DEG/PAGE, 0(0.01)90 DEG.  4SINSQTHETA TO 5 DEC PL, FIRST DIFF
     TABULATED.  COPIES TABLE AVAILABLE.
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 ASYMMETPIC 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.
 3030 ZEBRA    3D-GEOM  RICHARDS        ZK33/3D COORDS FROM 2D AND PLANE       MNA
        PRODUCES 3D COORDS FROM  D COORDS IN A SPECIFIED PLANE
 6502 ZRA1     FR 2     BAEHR*WEISS      UP TO 3000 SF IN MAX.4GROUPS.TF,SCL  LPA
 6501 ZRA 1    SF C     BAEHR*KRAUSE     IT=LC,COORD,LF,DEBYE,F(OB),OT ALSO R LPA
 5034 Z22 R    ER2      BRUHN
 5035 Z22 R    SF       TOEPFER-BRUHN

  161 1103     DP       ROSSMAN/LIPSC*   PATT SHARPENING, ART TEMP FAC.
  163 1103     DP       ROSSMAN,JACOBSON/LIPSC*/ADJUNCTS TO 158,159,161
  164 1103     DP       ROSSMAN/LIPSC*   BAD PLANE STATISTICS
  157 1103     DP LP    MATHEWS/LIPSC*   LP + PHILLIPS CORR FOR WEISSENBERG
  160 1103     FR 2 SC  HIRSHFELD/LIPSC*FLEXRAC/FAST 2D FR, CONSOLE SGN CHG
  158 1103     FR 2 3   JACOBSON/LIPSC*  FOURIER, BL, GRID N/60
  165 1103     ID       HIRSHFELD/LIPSC* USED WITH PGM 159
  159 1103     LS DM AT ROSSMAN/LIPSC*   GENL LS
  162 1103     PATT     JACOBSON/LIPSC*  PREDICTS PATT PKS FROM COORDS
 7525 1103 2K  PAT2     MARIANI          FIAT INTP LANG PAT2 COS COS          LWA
 7524 1103 2K  SF       MARIANI          FIAT INTP LANG SPACEGROUP 14 0 LEVEL LWA
  166 1103     UTILITY  JACOBSON,ROSSMAN,LIPSC*/P CHEM LIB, BOOTSTRAP
  341 1105     FR2      MORROW          5/                                     LWA
  342 1105     SFC      MORROW          6/                                     LWA
  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               NPA
        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    VAILABLE
  277 1620 40K D P      HAENDLER        2/ORTHORHOMBIC D SPACINGS              LPA
        CALCULATES Q(HKL)  SQUARE OF SIN THETA, D(HKL) FROM UNIT CEL  DATA
        FOR HKL VALUES FROM 000 TO NNN.
  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.
  284 1620 40K D P      HAENDLER        11/HEXAGONAL D SPACINGS                LPA
        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                LPA
        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.
  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       LPA
        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.
  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.
```

```
 280 1620 40K H        HAENDLER,COONEY 5/INDICES TRANSFORMATION              LPA
       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      LPA
       CONVERTS ANY SET (B) OF HKL VALUES TO SECOND SET (A) IF MATRIX OF
       TRANSFORMATION FOR SET A TO SET B IS GIVEN.
8003 1620     H D      KING            ERA119/HKL + SIN THETA/LAMBDA         LPA
       INPUT REC. CELL CONST. + MAX SIN THETA/LAMBDA. GENERATES HKL, CALCULATES
       2/D OR 4/DSQ OMITTING LATTICE ABSENCES ALL SYSTEMS. SPS FOR 20K TAPE 1620
 278 1620 40K LC       HAENDLER,COONEY 3/DIRECT LATTICE FROM RECIPROCAL      LPA
       CALCULATES DIRECT LATTICE PARAMETERS FROM RECIPROCAL LATTICE PARAMETERS
       INCLUDES ANGLE FUNCTIONS AND VOLUMES.
 288 1620 40K LC       HAENDLER,COONEY 16/RECIPROCAL LATTICE FROM DIRECT     LPA
       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.
 286 1620 40K LF       HAENDLER        13/FORM FACTORS                       LPA
       CALCULATES FORM FACTORS USING DATA FROM ACTA CRYST.,12,412(1959).
 293 1620 SPS SCL      MACINTYRE        ABSOLUTE SCALE.
 282 1620 40K SF       HAENDLER        7/STRUCTURE FACTORS FOR P2-1/C        NPA
       CALCULATES STRUCTURE FACTOR FOR ANY SELECTED VALUE OF HKL.
8004 1620     SF       KING            ERA164/TRICL                          LPA
       INDIV ISOTR TF, MAX 750 ATOMS, 9 TYPES. SPS FOR 20K. TAPE 1620.
 296 1620 SPS SF       MAC/HARRIS       INDIV. TF
 372 1620T20K SFLS     VDHELM/PATT*     TRICL,MONOCL,ORTH.INDIV TF AT,BLOCDM LWA
       THE PROGRAM COMPUTES AND TAPES OUT LEAST SQUARES SUMS FOR A BLOCK-
       DIAGONAL MATRIX.  TYPES AND TAPES STRUCTURE FACTORS.
 369 1620     SF R SCL AHMED            SF+R+SCL ALL SPACE GRPS. VERY FAST   LPA
       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.
 295 1620 FTN WEIS     MAC/WERKEMA      EQUI. INC. WEISS. COORD.
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)
5009 2002     FR 3     WILL                 /HAHN PROGR. WITH CHANGED OUTPUT LWA
       SEE PGM NO. 5027.
5008 2002     SF 3     WILL             3DIM MAXIMUM INDIC MUST BE FED IN    LWA
5010 2002     S        WILL             DIFFUSE SCATTERING                   LXA
8505 2203B    FR 2     OSAKI           N3FR1B/BL,GRID N/100                  LPA
       BEEVERS-LIPSON PRINCIPLE. SIN, COS VALUES FROM TABLE. TYPES OF TERMS
       TREATED, COSCOS, SINCOS, COSSIN AND SINSIN. LOWER AND UPPER LIMITS AND
       INTERVALS OF THE GRID POINTS CAN BE SET AT ANY MULTIPLE OF 1/100.
8501 2203B    FR 2     SASADA,OGAWA    PR3FR1/PGG POINT BY POINT GRID N/100  LPA
       OT TAPE FROM THE CALC OF SF OR A NEW DATA IS USED AS THE IT. APPLICABLE
       TO ANY SPACE GROUP THRU CENTRIC ORTHORHOMBIC BY CORRECTION OF JUDGEMENT
       OF H,K. STRAIGHT AND DIFFERENCE FR POSSIBLE. THE OT SHEET PERMITS DIRECT
       CONTOURING. LIMIT 1500 REFLECTIONS. REFER ALSO PR3SF1.
8506 2203B    LS       OSAKI           N3LSIMC/LS MONOCL C                   LWA
       STRUCTURE FACTORS AND LEAST SQUARES PGM. ISOTROPIC INDIVIDUAL THERMAL
       PARAMETERS. MONOCLINIC CENTRIC. BLOCK DIAGONAL, CROSS TERMS BETWEEN
       SCALE AND OVERALL TEMPERATURE FACTORS, BETW. X AND Z FOR EACH ATOM, ONLY.
       F(OBS) FED BY PLANE TAPE. UP TO 35 ATOMS OF 6 KIND. ATOMIC F-VALUES FROM
       TABLE. WEIGHTS CAN BE GIVEN EITHER BY A SUBROUTINE OR FROM PLANE TAPE.
```

8507 2203B LS AT 2 MASAKI N3LSAMC2/LS AT MONOCL C LPA
2 DIM SF AND LS PGM. APPLICABLE TO PLANE GROUP P2, PMG OR PGG BY SELECTION OF SYMMETRY TAPE. 2 BY 2 MATRIX AND 3 BY 3 MATRIX FOR POSITIONAL AND THERMAL PARAMETERS FOR EACH ATOM, 2 BY 2 FOR SCALE AND OVERALL TEMP FACTORS. WEIGHTS EITHER FROM HUGHES METHOD OR AS IT DATA. UP TO 20 ANISOTROPIC ATOMS OF 2 KINDS.

8503 2203B SF 2 SASADA,OGAWA PR3SF2/PGG LPA
REFER TO PR3SF1. CONNECT TO PR3FR1.

8504 2203B SF 2 SASADA,OGAWA PR3SF3/P2 LPA
ANISOTROPIC TF AVAILABLE. TRIGONOMETRIC FUNCTION IS IN SUBROUTINE OF TAYLOR EXPANSION. UP TO 100 ATOMS.

8502 2203B SF 2 3 SASADA,OGAWA PR3SF1/P212121 LPA
PRINT OUT FO, FC, AND PHASE ANGLE. OUTPUT TAPE CAN BE USED AS THE INPUT OF FR PROGRAM. UP TO 100 ATOMS. TRIGONOMETRIC FUNCTION BY INTERPOLATION FROM THE TABLE IN 100 PARTS.

191 204(5) DP WHITTIER,PETERSON/718,719,720/DATA REDUCTION

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

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

193 204(5) FR 2 WHITTIER,PETERSON/730/

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.

194 204(5) FR 3 WHITTIER,PETERSON/731/

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.

190 204(5) H D WHITTIER,PETERSON/717/GEN HKL, SIN THETA, SPACINGS

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.

343 205 ID S IBERS SECOND MOMENT ETC FOR NMR LPX
FROM UNIT CELL AND PARAMETER DATA PROGRAM CAUSES PRINT OUT OF R SQUARE /LESS THAN DESIGNATED MAX/, R, R MINUS SIX, AND SELECTED SUMS OF R MINUS SIX TOGETHER WITH THREE INDICES WHICH DESIGNATE DISTANCE CALCULATED.

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.

192 204(5) SF 2 3 WHITTIER,PETERSON/721A/SF CALCULATION

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.
 299 220       SF        LIND              X-11/SF + ASSIGN SIGNS, CENTRIC MONOC LPA
        SIGN ASSIGNMENT FOR FR ON BASIS OF VARIABLE AGREEMENT CRITERIA
 297 220       SPC       SILVERTON         X-1/GONIOSTAT SETTINGS                LPA
7506 6001 1K   DP        PANATT/LOMBARD*    RESCALING FOR SF                     LWM
7510 6001 3K   DP PREC   PANATT NI,ZANO*    LP LF THETA                          NWN
7509 6001 1K   DP PREC   PANATTONI,ZANO*    LP LF THETA                          LWA
7512 6001 3K   DP SCLTF  PANATTONI,ZANO*    WILSON PLOT RESCALING                LWA
7508 6001 3K   DP WEIS   PANATTONI,ZANO*    LP LF THETA                          NWN
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
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
6511 628       LP 1/D    SASVARI*ZILAHI     MONOCLINIC                           LPA
        NECESSARY 10 STORAGES FOR DATA, 11 FOR WORK AND 7 FOR RESULT. ALL
        POSSIBLE VALUES OF (HKL) WILL BE COLLECTED AUTOMATICALLY. DATA OF
        1000 REFLEXIONS ARE COMPUTED AND PUNCHED IN EMPTY CARDS IN ABOUT
        15 MINUTES. FOR OTHER SYMMETRY ONLY A LITTLE CHANGE OF THE
        PROGRAM IS NECESSARY.
6510 628       LS 2      SASVARI*ZILAHI     RHOMBIC P NAM                        LPA
        IN ONE CYCLE THREE COORDINATE-REFINEMENT CAN BE MADE. ONE HEAD-CARD
        FOR COORDINATES OF THREE ATOMS AND ONE CARD FOR EVERY REFLEXION
        CONTAINING THE VARIABLE DATA OF THE REFLEXION IS NECESSARY.
        COMPUTATION TIME OF ONE SYCLE BY 150 REFLEXIONS LASTS 5 MINUTES.
6509 628       SF        SASVARI*ZILAHI     RHOMBIC P NAM                        LPA
        FROM A HEAD CARD THE DIFFERENT ATOMIC COORDINATES AND THE NECESSARY
        CONSTANTS ARE STORAGED INTO THE COMPUTER. FOR EVERY REFLECTION A
        DISIINCT CARD GIVES THE HKL VALUES AND THE SCATTERING FACTORS AND IN
        THESE CARDS WILL BE PUNCHED THE RESULTS. COMPUTATION IS POSSIBLE IN ONE
        CYCLE IF THE NUMBER OF DIFFERENT COORDINATES IS SMALLER THA  15.
        COMPUTATION TIME OF 800 SF IS ABOUT 50 MINUTES.
  34 650       ABS       SANDS             ABCOR/PLOTS ABS COR TEMPLATE FOR WEIS
  33 650       D         MATHER             RECIP CELL CONST + INTERPLANR SPAC
 199 650       D         HOUSTON,CLOSS     WES-LMVD PGM 1031/INTERPLANAR SPAC
 107 650       D H       AHMED             (HKL) + D(HKL) IN SPECIFIC SPHERE     LNA
        INDICES AND SPACINGS FOR BASIC 650, GENERATES THE INDICES AND CALCULATES
        THE SPACINGS FOR ALL REFLECTIONS WITHIN A SPECIFIED SPHERE OR PART OF
        SPHERF IN RECIPROCAL SPACE. TO BE USED FOR INDEXING OF POWDER LINES.
  48 650       DEBYF     MILLER            008001/DEBYE TEMP FROM X-RAY DATA
 105 650       DF 3      AHMED              GENL E.D. + CURVATURES + ATOM SHIFTS LWA
        GENL 3-D DIFFERENTIAL FOURIER FOR BASIC 650. CALCULATES THE ELECTRON
        DENSITY, 3 FIRST DERIVATIVES AND 6 SECOND DERIVATIVES AT ASSUMED ATOMIC
        POSITIONS, AND THE ATOMIC SHIFTS FOR OBS OR CALC DATA IN ANY SPACE GROUP.
```

```
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).
 180 650      DP        BROWN,STEWART      5303,4,5/DATA REDUCT, WEISS, PREC
 218 650      DP        BROWN,STEWART      440X/FO DATA RESCALING
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
 210 650      DP         HAHN*             INT CORR FOR EQUIINCL WEISSENBERG
 212 650      DP        /HAHN*             N(Z) TEST
 213 650      DP        /HAHN*             VARIANCE TEST
 155 650      DP        MCGANDY           PITTSBURGH DATALOADER/
 156 650      DP        MCGANDY           INPUT TDF-2/PREP INPUT FOR PGM 37
 223 650      DP        SVETICH            INTENSITY SCALING
 224 650      DP        SVETICH            CONV U OF WASH DECK TO PITTSBURGH
 222 650      DP        SVETICH,PTRSON     INTEG INT FROM DENSITMTR TRAC
 181 650      DP ABS    STEWART           5308/CORR FOR ABSORPTION, WEISSENBERG
 151 650      DP LP     MCGANDY           INCOR-P/MOD OF PGM 146 FOR PREC
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
  44 650      DP LP     WILLIAMS          INCOR-IM/CONVEN. MOD OF INCOR-I (146)
 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
```

```
         DP R SCL AHMED            SCALE DIFFERENT LEVELS AGAINST FCALC LNA
    SCALING OF LEVELS. BASIC 650. CALCULATES THE SCL AND R FOR EACH LEVEL
    SEPARATELY BY COMPARISON OF OBS AND CALC DATA, THEN REEVALUATES R FOR
    EACH LEVEL AND FOR ALL DATA USING THE EVALUATED SCALES FOR THE LEVELS.
    THE LEVELS MAY BE FOR CONSTANT H, K, OR L.
 211 650     DP SCL   /HAHN*           WILSON TEST
  23 650     DP STAT  KRAUT            AVG EQUIV REFL, CALC R, GET STATIST
 185 650     DP TF    BROWN            WILSON PLOT, SCL AND TEMP FACTOR
 100 650     E        AHMED            SUMS REQUIRED FOR S.D. OF COORDS    LNA
    E.S.D. BASIC 650. CALCULATES SUMS REQUIRED FOR S.D. OF ELECTRON DENSITY
    AND OF COORDS + R + SCL. NORMALLY USED AFTER REFINEMENT IS COMPLETED.
 325 650     E        SHIONO           STAND.DEV OF ELECTRON DENSITY ETC   LWA
    BASIC 650
  46 650     FPK      WILLIAMS        BLOCK PEAK/LS FIT TO 2  POINTS
 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.
  39 650     FR BLK   FITZW,KEYES     TDF-80B/4X4X4 BLK IN 1/80
 356 650     FR PCH   JENSEN           CC SS SC CS TABLE EXPAN  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
 168 650     FR 2     BOOTH            GENL PROJ CC SS CS SC
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)
 169 650     FR 2     HELLNER,WOLFEL   PROJ,CC AND SS, N/500
 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
 173 650     FR 2     TULINSKY         GENL PROJ CC SS CS SC N/1000 X N/100
 208 650     FR 2     /HAHN*           GENL 2 DIM FOURIER ALL SYMMETRIES
 104 650     FR 2 1   AHMED            FR 2 ALL PLANE GROUPS GRID N/120    LNA
    GENL 2-D FOURIER FOR BASIC 650. CALCULATES PROJECTIONS IN ANY PLANE GROUP
    AT INTERVALS N1, N2/120. THE INTERVALS AND NO. OF POINTS MAY BE DIFFERENT
    IN THE TWO DIRECTIONS.
 337 650     FR 2 (2) AHMED            FAST, GENL FR 2 GRID N/120          LNA
    2-D FOURIERS ON AUGMENTED 650 (4000 WORD DRUM, 3 INDEXING ACC.) FAST,
    GENL. GRID INTERVALS N1, N2/120.
  37 650     FR 2 3   FITZW,WILLIAMS  TDF-2/FAST, 1/40 OR 1/80
 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
 334 650     FR 3     AHMED            FR 3 ALL SPACE GROUPS GRID N/120    LNA
    GENL 3-D FOURIER FOR AUGMENTED 650 (4000 WORD DRUM AND 3 INDEXING
    ACCUMULATORS). GRID INTERVALS N1, N2, N3/120. ANY SPACE GROUP. COMPUTES
    FOR MESH THROUGHOUT ASYMMETRIC UNIT OR FOR BLOCKS OF POINTS.
 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
7019 650     H THETA  JAMARD           H AND THETA TRICLINIC               MPA
    H AND THETA VALUES, TRICLINIC, UP TO GIVEN MAXIMUM VALUES OF
    H,K,L.  375 HKL MAXIMUM. EXTINCTION RULES MAY BE TAKEN IN ACCOUNT
```

183 650 HYDROGEN STWRT,LINGFTR 5105/GEN H COORDS, BOND LGTHS, ANGLES
5033 650 ID HILDEB,HAHN* ID FOR GIVEN ATOMS ANY SYM LWA
CALCULATES ID BETWEEN GIVEN CENTRAL ATOMS AND ANY NUMBER OF
SPECIFIED NEIGHBOURS FOR TRICLINIC LATTICE.
184 650 ID SHIONO DIST,ANGLES,S.D. OF ANGLE, ANY SYM LWA
BASIC 650
220 650 ID STWRT,LINGFLTR,BRWN/5102/BOND LENGTHS ANGLES
221 650 ID LINGFLTR,BROWN 5112/INTERMOLECULAR DISTANCES
106 650 ID 1 AHMED BOND LENGTHS AND ANGLES LNA
INTERATOMIC BOND LENGTHS AND BOND ANGLES FOR BASIC 650. CALCULATES THE
DISTANCES OR DISTANCES AND ANGLES BET. SPECIFIED ATOMS WHOSE FRACTIONAL
COORDS ARE ALREADY AVAILABLE TO THE MACHINE IN THE STORED LIST OF COORDS.
335 650 ID 2 AHMED INTER + INTRA MOLECULAR DISTANCES LNA
INTERMOLECULAR DISTANCES FOR BASIC 650. GIVEN THE FRACTIONAL ATOMIC
COORDS OF ATOMS IN THE ASYMMETRIC UNIT AND EXPRESSIONS FOR THE EQUIVALENT
POSITIONS, IT CALCULATES ALL INTRAMOLECULAR AND INTERMOLECULAR DISTANCES
WHICH ARE LESS THAN A SPECIFIED MAX. LIMIT FOR EACH.
152 650 LC MCGANDY CELL TRANSFORMATION
153 650 LF MCGANDY LTL F CURVES FROM 3-TERM GAUSSIAN
327 650 LF SHIONO 4 POINT INTERPLTN PGM 176
650 WITH IXA. ON-LINE 407(OPTIONAL)
21 650 LP KRAUT PREC, LP FOR ANY LEVEL
43 650 LS DM FITZW,WILLIAMS LS-IIM/MOD LS-II (147) FOR ALL SP GRP
179 650 LS DM FITZWATER LS IIM/MOD OF (147) FOR OTHER SYMM
141 650 P PK BOYKO,MOHN FOURIER SYNTH OF LINE SHAPE
197 650 P PK SUMNER CONVO I/PEAK PROFILE CONVOLUTION
321 650 P PK SCHWARTZ/COHEN POWD LINE PROFILE ANAL, STOKES LWA
DETERMINES COSINE AND SINE COEFFICIENTS, STOKES CORRECTED, FOR WARREN
ANALYSIS OF PARTICLE SIZE, STRAIN, TWIN FAULT PROBABILITY.
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 20, LINEAR ABSORPTION
COEFFICIENT OF SAMPLE. PROGRAM OUTPUT IS RELATIVE INTENSITY VS. 20,
REFERENCED TO TRUE 20 POSITION.
24 650 PATSUP KRAUT 3-D PATT SUPERPOS USED W PGM 198
182 650 PLANE STEWART LS PLANE THRU UP TO 98 ATOMS, ETC
22 650 SCL KRAUT SCALES ONE SET OF INT TO ISOMRPH SET
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
8 650 SIGN TRAUB SIGN PERMUT, USED WITH 173
101 650 SF AHMED CORRECT SF FOR HEAVY ATOM DISPERSION LNA
SF CORR 1. BASIC 650. CORRECTS PREVIOUSLY COMPUTED (A,B,F) CALC FOR HEAVY
ATOM DISPERSION, THEN EVALUATES (A,B)OBS, SCL AND R.
102 650 SF AHMED ADD TO SF CONTRIBUTION OF NEW ATOMS LWA
SF CORR 2. BASIC 650. CALCULATES CONTRIBUTION OF A FEW NEW ATOMS, ADDS
THEM TO THOSE OF THE OTHER ATOMS. ALL SPACE GROUPS. MAY BE USED FOR
EXAMPLE IN ADDING CONTRIBUTIONS OF THE HYDROGEN ATOMS.
175 650 SF BOOTH P1, NO TF, NEED LTL F, 200 ATOMS
209 650 SF /HAHN* ISOTROPIC TF, ALL SYMMETRIES
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)
154 650 SF AT MCGANDY 5 ANISO, 20 ISOTR UNIQ AT, R, SCL
273 650 SF AT DIETRICH X5/CALCULATES ALSO SCL LPA
IT COORDINATES OF ATOMS (MAXIMUM 200/CELL), CONSTANTS FOR UP TO 58 AT

```
         AND FOR UP TO 42 ISOTROPIC TF, SYMMETRY (P1 OR P-1), OT OF (272)
     OT  INDICES, WEIGHTS, FO, FC. FOR SYMMETRY P1 ALSO  AC, BC, AC/FC, BC/FC
         EXTRA CARD  SCALING FACTOR ( CALCULATED BY LS OF WEIGHTED FO-FC)
 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.
  77 650       SF AT 3   BROWN,JENSEN,LINGAFELTER,STEWART/400X,410X,4010/
  99 650       SF R SCL  AHMED             SF + R + SCL ALL SPACE + PLANE GRPS  LWA
     SF R SCL. BASIC 650, 2000 WORD  RUM, NO INDEXING REGISTERS. ALL SPACE AND
     PLANE GROUPS. TAKES ADVANTAGE OF THE SYMMETRIES. ALSO CALCULATES SCL + R
     BEFORE AND AFTER ADJUSTMENT OF ASSUMED SCL. MAX. OF 50 ATOMS IN ASYM-
     METRIC UNIT AND 11 SCATTERING FACTOR CURVES. ISOTROPIC TF ONLY.
 215 650       SF UNIT   /HAHN*            UNITARY STRUCTURE FACTORS
5032 650       SF 3      HILDEB/HAHN*      SF FOR ANY SYM IND ISOTR TF          LWA
     COMPUTES 3 DIM SF FOR ANY SYM WITH INDIV. ISOTR. TF FOR EACH ATOM.
     PROGRAM USES TRICLINIC SF FORMULA
  25 650       SPC       HIGH              GONIOSTAT SETTINGS
  38 650       SPC       WILLIAMS         SCO-2/GONIOSTAT, XTLS IN GEN ORIENT
 195 650       SPC H     TULINSKY          GONIOSTAT SETTINGS
 333 650       SPC H LP  AHMED             (HKL) + GONIOSTAT SETTINGS + 1/LP    LNA
     GONIOSTAT SETTINGS FOR BASIC 650. GENERATES THE INDICES AND CALCULATES
     THE GONIOSTAT SETTINGS AND 1/LP FOR ALL REFLECTIONS WITHIN ANY PART OF
     A SPECIFIED SPHERE IN RECIPROCAL SPACE.
 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          4500/ISO T F CORR BY LST SQ
 326 650       TF        SHIONO            ANISOTROPIC TF FROM PGM 174,176      LWA
     BASIC 650. USE OUTPUT OF PGM 174
 336 650       TF SCL    AHMED             OVERALL CORRECTION TO SCL AND TF     LNA
     OVERALL CORRECTIONS TO SCALE AND TEMP. FACTOR ON BASIC 650. CALCULATES
     LOG(SUM FCALC)/LOG(SUM FOBS) AND (SIN SQ THETA) MEAN FOR THE REFLECTIONS
     WITHIN SPECIFIED RANGES OF SIN SQ THETA, THEN CALCULATES THE OVERALL
     CORRECTIONS TO THE ASSUMED SCALE AND TEMPERATURE FACTORS.
 328 650       TF UNIF   SHIONO            WILSON PLOT, UNITARY SF              LPA
     650 WITH IXA,IAS, ON-LINE 407.
5045 650       THETA     DIETRICH         X14/                                  MWA
     IT  WAVE LENGTH, OT OF (5039), (5040) OR OTHER
     OT  SIN**2 THETA, SIN THETA, THETA IN DEGREES
 225 704       ABS EXT   HAMILTON          ESAF/ABS SEC EXT POLYHEDRAL XTLS     LWA
     CALCULATES ABS AND SECONDARY EXT. CORRECTIONS FOR ARBITRARILY
     SHAPED CRYSTALS. SHAPE APPROXIMATED BY POLYHEDRON.METHOD USED IS
     MODIFICATION OF THAT DESCRIBED IN ACTA CRYST. 10, 629 (1957)
     TIME REQUIRED IS A FEW SECONDS PER REFLECTION, DEPENDS ON VARIABLE
     GRID SIZE. SUPPLIED AS FORTRAN 2 SUBROUTINES FOR VERSATILITY IN USE
 132 704       D P       BRYDEN           4214/CALC TABLE OF D FOR POWD
 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.
 207 704       DP LS FR  PENFOLD/LIPSC*    CONV OUTPT ORXLS (12) TO MIFR1 (118)
 203 704       DP PAT    PENFOLD/LIPSC*    SCL + SHRPN FOR PAT WITH MIFR1 (118)
  80 704 8K    DP PHASE  HOLDEN            TAKES OT FROM 79 MAKES IT FOR 78     LWA
 206 704       DP R      /LIPSC*           R FACTOR FOR ORXLS OUTPUT (12)
 205 704       DP W      /LIPSC*           WEIGHTS FOR ORXLS (12)
  11 704       FPK       SLITER            LOCATES FR PK CNTRS, SEE PGM 10
 131 704 4K    FPK       BRYDEN           4208/FIND MAX ON 2 OR 3D FOURIER
 196 704       FPK       SLITER            ELLIPSOIDAL PK ANALYZER, SEE PGM 10
  10 704       FR 2      SLITER            VARIABLE INCLINED PLANE FOURIER SEC
  27 704 32K   FR 2      TREUTNG,ABRAHMS   GENL PLANE ELECTRON DENSITY
  29 704       FR 2      SASS             2DF/FAST 2-DIM
 216 704       FR 2      SIMPSON           REQ DUMP ROUTINE FOR OUTPUT
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).
127 704 4K   FR 2 3    BRYDEN          4201,2,4,6/
 78 704 8K   FR 3      BLOCK,HOLDEN*    GRID N/60, USE EQUIV REFLNS, ANY SG  LWA
 84 704 32K  FR 3      BLOCK,HOLDEN*    GRID N/60, USE EQUIV REFLNS, ANY SG  LWA
201 704      FR 3      BORN,HELLNER*   RHOPAT/ORTHORHOMBIC PATTERSON
202 704      FR 3      BORN,HELLNER*   MONOPAT/MONOCLINIC PATTERSON
234 704      FR 3      HILDEBRAND,HAHN  ANY SYMMETRY
204 704      ID        WUNDERLICH/LIPSC*/
 13 704      ID E      BUSING,LEVY     ORXFE/FUNCTION AND ERROR,DISTANCE ETC LWA
      USED INDEPENDENTLY OR WITH ORXLS. CALCULATES 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 DISPLACE-
      MENT, DISTANCE CORRECTED FOR THERMAL MOTION.
 47 704 32K  LC        KEMPTER*VOGEL   HER/PREC REFINMT OF LATTICE CONSTS    LWA
      A CONVERGENT ITERATIVE TECHNIQUE (R.E.VOGEL AND C.P.KEMPTER,CHEM.ABSTR.
      54,16087F),WITH EXACT STATISTICAL WEIGHTS ASSIGNED TO THE OBSERVED POINTS
      IS USED TO DETERMINE LATTICE PARAMETERS AND THEIR STANDARD DEVIATIONS FOR
      THE CUBIC,HEXAGONAL,TETRAGONAL,AND ORTHORHOMBIC SYSTEMS FROM DEBYE-
      SCHERRER,SYMMETRICAL BACK REFLECTION,OR DIFFRACTOMETER DATA.
226 704      LC        MUELLER,HEATON  MET 124/ CUBIC THROUGH ORTHORHOMBIC   LWA
      PROGRAM PERMITS THE DETERMINATION OF LATTICE CONSTANTS FOR ORTHORHOMBIC
      THROUGH CUBIC 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.
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.
129 704 4K   LP        BRYDEN          4203/CORRECTS INT FROM EQUIINCL WEIS
 82 704 32K  LP WEIS   HOLDEN           MAKES IT FOR 83,12 AND IT FOR 84-PAT NWA
 12 704      LS AT FM  BUSING,LEVY     ORXLS/GENL LS, FULL MATRIX, AT        LWA
      STRUCTURE FACTOR LEAST SQUARES. ANY SPACE GROUP. VARIABLES ARE SCALE
      FACTORS, NEUTRON SCATTERING FACTORS, COORDINATES, ISOTROPIC OR ANISO-
      TROPIC TEMPERATURE FACTOR COEFFICIENTS. FULL MATRIX LEAST SQUARES.
      CAPACITY- 120 VARIABLES WITH 8K, 251 WITH 32K MEMORY. GENERAL WEIGHTS.
      FEATURES- REFINEMENT BASED ON F OR F SQUARED, ARBITRARY SELECTION OF
      PARAMETERS TO BE VARIED.
144 704      LS DM     SAYRE,VAND*      VAND MOD OF NYXR1 (143), SEE 145
145 704      LS DM DF  VAND,PEPINSKY   PSXR3/CONVERG AIDS + OTHER FEATURES
313 704      LS P FM   HAMILTON        POWLS/GENL 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 FOR
      HANDLING PARTIALLY OVERLAPPING PEAKS. USER MUST SUPPLY SUBROUTINE FOR
      DEFINITION OF INTENSITY FUNCTIONS. LIMITED TO 50 OBSERVATIONS AND 20
      REFINED PARAMETERS. CAN BE CHANGED BY RECOMPILATION OF FORTRAN DECKS.
      CAN BE USED FOR SF AND/OR SINTHETA CALCULATION SEPARATELY.
121 704      LS P N    SHOEMAKER,C+D    REF NEUT SCAT FAC, SITE OCCUPANCY    LNX
 28 704      LS 2 FM   HAMILTON        2DLS/FULL MATRIX LS, AT, 2DIM         LWA
      FULL MATRIX, ANISOTROPIC TEMPERATURE FACTOR LEAST SQUARES AND SF
      PROGRAM FOR CENTROSYMMETRIC SPACE GROUPS. SYMMETRY UP TO ORTHOROMBIC
      TWO-DIMENSIONAL DATA. 14 ATOM MAXIMUM. USES ANALYTIC APPROXIMATION
```

```
     TO SCATTERING FACTORS. TIME COMPARABLE TO ORXLS. MORE CONVENIENT
     IN OPERATION FOR LIMITED TYPE OF PROBLEM IT CAN HANDLE.
5026 704 8K   LS 3     HILDEB,HAHN*       GEN LS AT BLOCK MATRIX                 NPA
     FOR ANY SPACEGROUP,SF AND LS WITH ISOTR. OR ANISOTR. TF. REFINES
     F. USES WEIGHTS PROVIDED BY USER 4.4 OR 3.3 AND 6.6 MATRICES FOR
     EACH ATOM. DAMPING FACTORS MAY BE APPLIED.
  36 704 32K  P PK     ALLEN              POWDER PEAK SHAPE ANALYSIS
 126 704      P PK     SENKO              DIFFRACTION PROFILE CORRECTION
  35 704 32K  P S      KAPLOW             BINARY ALLOY DIFFUSE X-RAY DATA
3011 704FTN   P        PISTORIUS, M.C. WP02/P BASED ON LC IT                     NPN
     AID TO PI. IT LC, OT OF P LISTED ACCORDING TO H OR SIN(THETA)
 167 704      PATSUP 3 PENFOLD/LIPSC*     PAT SUP, USE WITH MIFR1 (118)
   9 704      SF       SLITER             3 PGMS USED TOGETHER FOR SF
  79 704 8K   SF ICA   BLOCK,HOLDEN*      USES SG FORTRAN SUBRTN, IT FOR 80,12 LWA
  83 704 32K  SF ICA   HOLDEN             USES SG FORTRAN SUBRTN, IT FOR 84    LWA
  31 704      SPC      HAMILTON          SINT/ZONAL SPECTROM SETTINGS
 119 704 4K   SPC LP   SHOEMAKER         GONIOSTAT I/GEN HKL GONIO STGS LP ABS LWA
     GENERATES MILLER INDICES ASYMMETRIC UNIT ANY LATTICE ANY LAUE GROUP.
     CALCULATES SETTINGS PHI CHI PSI FOR GE XRD5 SINGLE CRYSTAL ORIENTER
     (GONIOSTAT). ALSO CALC RECIPROCAL LP FACTOR AND ABS FACTOR FOR
     SPHERICAL CRYSTAL OR ZONE FOR CYLINDRICAL CRYSTAL.
 122 704      SPC N    SHOEMAKER,C+D     PRPLOT/SMOOTH AND PLOT SPECROM DATA   LPA
     HEART OF PGM IS SUBROUTINE PRPLOT WHICH MAKES OUTPUT PRINTER BEHAVE
     LIKE A STRIP-CHART RECORDER. ABSCISSA AND ORDINATE PRINTED AT LEFT OF
     SHEET, ORDINATE PLOTTED AS A PERIOD IN ONE OF 101 POSITIONS ACROSS SHEET.
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 INTER-
     VENTION AT SOME POUNTS. USES PRINCIPLES DESCRIBED IN ACTA CRYST 10,116/
     11,277/11,393.
 348 7070 10K ABS      SCHAPIRO           POLYHED,XTALS,OSC WEIS.XRD-5           MPA
 383 7070 AUC COORD    SCHAPIRO/SHIONO    GENERATES ADDTL AT COORDS
     GIVEN SET OF ATOMIC COORDINATES, DISTANCES, STEREOCHEMICAL RELATIONS,
     GENERATES ADDITIONAL ATOMIC COORDINATES.
 323 7070 10K DF3 AT E SHIONO             COORD AND TF SHIFTS I/O ON-LINE        LPA
     AUTOCODER 10K,7400,7500,7550,TP21. USE OT OF SF. TRI.,MONOCL.,ORTHO..
 373 7070 AUC DISPERSN SHIONO             DAUBEN-TEMPLETON DISPERSION CORR
     REF. ACTA CRYST 8, 841 (1955)
 350 7070  5K DP       SCHAPIRO,SMITH     XRD-5 DATA TO SHIONO SF PROGRAM        MPA
 375 7070 AUC DP SCL   MCMULLAN/SHIONO    INTERLAYER SCALING USING CALC SF
 374 7070 FTN DP WEIS  CRAVEN/SHIONO      MONOCL, ORTHO
     (1) CALCN OF MULTIFILM SCALING FACTORS, (2) CALCN OF INTENSITIES AS
     OBSERVED IN EACH LAYER, (3) LP CORRECTION, (4) CALCN OF INTERLAYER
     SCALING FACTORS BY LEAST SQUARES, (5) GENL PGM FOR CALCULATING EIGEN-
     VALUES AND EIGENVECTORS OF SYMMETRIC MATRIX UP TO ORDER 30, (6) CALCN OF
     SCALED INTENSITIES, (7) AVERAGING OF INTENSITIES FOR REFLECTIONS OBSERVED
     ON MORE THAN ONE LAYER.
 376 7070 AUC DF       SHIONO             TRICL, MONOCL, ORTHO, AT
 380 7070 AUC FR 2     MCMULLAN/SHIONO    CENTROSYMM MONOCL, A OR C PROJ
 377 7070 AUC FR 3 A   CHU,MCMULLAN/SHIONO/ACENTRIC, MONOCL
 379 7070 AUC FR 3     MCMULLAN/SHIONO    PM3M,CMC21,I43D,P4232,P42/MNM
 378 7070 AUC FR 3 C   MCMULLAN/SHIONO    CENTROSYMM, MONOCL
 381 7070 AUC FT CLAY  SHIONO             MCEWEN FT FOR LAYER STRUCTURE (CLAY)
     FOR CLAY MINERALS. REF. KOLLOID Z., 149, 96 (1956).
 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/SHIONO         ANY SYM, 50 ATOMS MAX
 347 7070 10K SF AT    SCHAPIRO           300 SETS EQUIV AT ANY S G              MPA
     CAN BE USED IN CONJ. WITH SHIONO 7070, SF,DS PROGRAMS
 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
 351 7070 5K  SPC      SCHAPIRO           PICKER OSC SPECTR                      MPA
```

```
352 7070 5K  SPC      SCHAPIRO         XRD-5                                     MPA
349 7070 10K SPEC     SCHAPIRO         PARALLEL OR PERSP PROJ OF PTS             NPA
    CAN SEARCH AUTOMAT., MATCH PATTERN
353 7070 10K SPEC     SCHAPIRO         GENERATES ATOM COORD FROM STEREOCHEM MPA
338 709 32K  ABS      BURNHAM         GNABS/CORR FOR XLS OF ARBITRARY SHAPE LWA
    WRITTEN AS SUBROUTINES FOR EQUI-INCLINATION WEIS GEOMETRY.
    REQUIRES A MAIN PROGRAM WITH CALLING SEQUENCE GIVING RECIPROCAL LATTICE
    LEVEL INDEX, UPSILON, AND PHI FOR EACH REFLECTION.  CHOICE OF 64, 216,
    OR 512 NUMERICAL INTEGRATION POINTS.  LIMITS - 25 XTL FACES (NO REENTRANT
    ANGLES), 25 RECIPROCAL LATTICE LEVELS.  COLUMN BINARY AND/OR SYMBOLIC
    (FORTRAN AND FAP) DECKS AVAILABLE.
367 7090      ABS      WUENSCH,PREWITT ACAC/ABS CORR FOR ARBITRARY CRYSTAL   NNN
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.
 51 709,7090 D        WOLTEN           TABLE D VS Q                              LWA
 49 709,7090 D P PI   WOLTEN           CALC D,Q,INDIC FROM LAT PARAM         LWA
303 709       DP       PALENIK         14701/ PREP BIN DATA TAPE                 LNA
    PREP BINARY DATA TAPE FOR INPUT INTO ALL PROGRAMS THREE POINT INTERPOLA-
    TION FOR SCATTERING FACTOR CAN ALSO BE USED TO CORRECT WEISSENBERG DATA
    ANY AXIS OR LEVEL
339 709 32K  DP       BURNHAM         DTRDA-B/CORR INT,COMPUTE FOBS             LPX
    DTRDA COMPUTES INTEGRATED INTENSITIES FROM EQUI-INCLINATION WEIS
    COUNTER DATA.  DTRDB CORRECTS DTRDA OUTPUT FOR LP AND ABS (USING GNABS),
    COMPUTES FOBS AND SIGMA(FOBS).  PUNCHED OUTPUT IN ARBITRARY FORMAT.
    COLUMN BINARY AND/OR SYMBOLIC (FORTRAN) DECKS AVAILABLE.
318 709       DP FR    GANTZEL/TRBD*   UCLAPAT1/ PATTERSON, SHARPEN OPTIONS  MNN
    UCLAPAT1/  USES PARTS OF UCLANC1.  VARIOUS SHARPENING AND APPROX ORIGIN-
    PEAK REMOVAL OPTIONS.
322 7090/709 FPK      IBERS            27 PT. LS 10 PARAMETER GAUSSIAN FIT  LWA
    PROGRAM TAKES 27 POINT INPUT FROM MAP AND FITS THESE DATA WITH A 10 PARA/
    METER 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.
128 709       FR 2 3   BRYDEN           4201,2,4,6/
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.
363 7090 FT2 ID E     BUSING*LEVY,MAR ORFFE/FORTRAN FUNCTION AND ERROR      LWA
    SAME AS ORXFE BUT FOR USE 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 DISPLACE-
    MENT, DISTANCE CORRECTED FOR THERMAL MOTION. WRITTEN IN FORTRAN 2.
340 709       LC       BURNHAM         LCLSQ/PRECISION LC BY LEAST-SQUARES   MPA
    USES PRECISION BACK-REFLECTION WEIS SINGLE XTL DATA TO COMPUTE LC BY
    LEAST-SQUARES FOR ANY XTL SYMM.  INCLUDES CORR FOR FILM SHRINKAGE,
    ABSORPTION, AND ECCENTRICITY.  PROVISION FOR OPTIONAL WEIGHTING
    SUBROUTINE.  COLUMN BINARY DECK FOR FORTRAN MONITOR SYSTEM AVAILABLE.
130 709       LP       BRYDEN           4203/CORRECTS INT FROM EQUIINCL WEIS
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.
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. FORTRAN 2 EXCEPT FOR MATRIX INVERTER WHICH IS FAP SUITABLE FOR 704, 709, OR 7090.

360 7090 FT2 LS AT FM BUSING*LEVY,MAR 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. WRITTEN IN FORTRAN 2 EXCEPT FOR MATRIX INVERTER WHICH IS FAP SUITABLE FOR 704, 709, OR 7090.

364 7090 LS AT FM PREWITT SFLSQ2/LEAST SQUARES REFINEMENT MPA
STRUCTURE FACTOR, LEAST SQUARES. VERY FLEXIBLE WITH SEPARATE SPACE GROUP, WEIGHTING,IT/OT SUBROUTINES. PROVISION FOR ANOM DISPERSION CORR, CORRELATION MATRIX, INPUT TAPE TO FR PROGRAMS, ID AFTER END OF CYCLE, REFINEMENT OF ATOM SCL. WRITTEN IN FORTRAN AND FAP.

319 7090 32K LS DM DF VAN DEN HENDE ERBR1/ LEAST SQUARES REFINEMENT PM LWA
ERBR1 ALLOWS LEAST-SQUARES AND DIFFERENTIAL SYNTHESIS REGRESSION FOR ALL 230 SPACEGROUPS. IT CAN BE USED FOR STRUCTURE FACTOR CALCULATION AND HAS SIMPLE CONTROLS. ADDITIONAL OUTPUT IN FORMAT FOR USE WITH SLY-SHOEMAKER FOURIER PROGRAM IS INCLUDED. UP TO MORE THAN 100 ATOMS/ASYM. UNIT. FAST. ALSO GOOD FOR NEUTRON DATA.
SPECIAL FEATURES FOR MINERALOGICAL PROBLEMS.

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

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

366 7090 FTN S ID PEACOR,PREWITT DRILL/COORD FOR XL STRUCT MODELS NPA
COMPUTES DRILLING COORDINATES PHI AND RHO PLUS INTERATOMIC DISTANCES FOR CONSTRUCTION OF CRYSTAL STRUCTURE MODELS.

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
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).
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
346 7090     SPC LP   LARSON/DODGE*   CRYSTAL 8/GONIOSTATSETNGS, LP         LPA
    THIS PROGRAM IS WRITTEN IN FORTRAN
365 7090     SPC LP   PREWITT         DFSET2/EQUI-INCL WEISS SPC            MPA
    COMPUTES UPSILON AND PHI FOR EQUI-INCLINATION WEISSENBERG DIFFRACTOMETER.
    ALSO COMPUTES 1/LP AND SIN THETA.  PRINTED AND/OR PUNCHED OUTPUT.
    PUNCHED OUTPUT IN FORMAT FOR BURNHAM DTRDA-B. WRITTEN IN FORTRAN AND FAP.
315 709      SPC N    SHOEMAKER,C+D   PRPLOT/SMOOTH AND PLOT SPECROM DATA   LPA
    709 VERSION OF PGM 122
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)
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)
7520 9002 1K  DP WEIS  PANATTONI/FRASS 045/039/LP LF THETA                  LWM
7518 9002 1K  FR 2 A   PANATTONI/FRASS 114/ BL                              LWM
7519 9002 1K  FR 2 C   PANATTONI/FRASS 011/012/102/IT OT  FR BLK            LWM
7514 9002 1K  FR 3     PANATT/BENOFFI* 109 MONOCLINIC/GENERAL/FR/BL/107/OT  LWM
7516 9002 1K  FR 3     PANATT/BENOFFI* 112 ORTHORHOMBIC/GENERAL/FR/BL/107OT LWM
7515 9002 1K  FR 3 A   PANATT/BENOFFI* 089 TRICLINIC/BL/107/OT              LWM
7513 9002 1K  FR 3 C   PANATT/BENOFFI* 091 TRICLINIC BL 107 OT              LWM
7521 9002 1K  ID       PANATTONI/FRASS 017/TRICLINIC SYM  PAC LANGUAGE      LWM
7517 9002 1K  PLANE    FRASSON GRUBISS  LS PLANE ETC.     PAC LANGUAGE      LWM
7523 9002 1K  SF3AAT   PANATTONI/FRASS 003/004/042/043/FOUR PROGRAM ACENTRIC LWM
7522 9002 1K  SF3CAT   PANATTONI/FRASS 001/002/040/041/FOUR PROGRAM CENTRIC  LWM
```

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.

104	650	FR	191	204(5	DP	262	220	LF	333	650	SP	3016	ZEBRA	MA
105	650	DF	192	204(5	SF	263	220	LP	334	650	FR	3017	ZEBRA	SF
106	650	ID	193	204(5	FR	264	220	H	335	650	ID	3018	ZEBRA	LS
107	650	D	194	204(5	FR	265	220	FR	336	650	TF	3019	ZEBRA	1F
108	G-15D	LC	195	650	SP	266	205	FR	337	650	FR	3020	ZEBRA	TA
109	G-15D	LC	196	704	FP	267	205	EL	338	709 3	AB	3021	ZEBRA	DP
110	G-15D	P	197	650	P	268	220	LS	339	709 3	DP	3022	ZEBRA	DP
111	205	H	198	650	FR	269	205	EL	340	709	LC	3023	ZEBRA	FR
112	205	ID	199	650	D	273	650	SF	341	1105	FR	3024	ZEBRA	PK
113	205	LP	201	704	FR	277	1620	D	342	1105	SF	3025	ZEBRA	PK
114	205	FR	202	704	FR	278	1620	LC	343	205	ID	3026	ZEBRA	PK
115	205	LP	203	704	DP	279	1620	D	344	FORTR	FR	3027	ZEBRA	3
116	220	LF	204	704	ID	280	1620	H	345	FORTR	N,	3028	ZEBRA	3
118	704 8	FR	205	704	DP	281	1620	H	346	7090	SP	3029	ZEBRA	3
119	704 4	SP	206	704	DP	282	1620	SF	347	7070	SF	3030	ZEBRA	3D
120	FORTR	DP	207	704	DP	283	1620	D	348	7070	AB	3031	ZEBRA	EN
121	704	LS	208	650	FR	284	1620	D	349	7070	SP	3032	ZEBRA	LP
122	704	SP	209	650	SF	285	1620	D	350	7070	DP	3033	ZEBRA	SP
125	ILLIA	S	210	650	DP	286	1620	LF	351	7070	SP	3034	ZEBRA	D
126	704	P	211	650	DP	287	1620	D	352	7070	SP	3035	ZEBRA	PI
127	704 4	FR	212	650	DP	288	1620	LC	353	7070	SP	3036	ZEBRA	PR
128	709	FR	213	650	DP	289	1620	LC	354	1620T	FR	3037	ZEBRA	DP
129	704 4	LP	215	650	SF	290	650	H	355	1620T	SP	3038	ZEBRA	D
130	709	LP	216	704	FR	291	709 F	SF	356	650	FR	3501	PEG 4	VI
131	704 4	FP	218	650	DP	292	1620	AB	357	7090	FR	3502	PEG 4	SF
132	704	D	219	650	TF	293	1620	SC	360	7090	LS	3503	PEG 7	FR
133	650	PA	220	650	ID	294	1620	AT	361	7090	LS	3504	PEG 4	ID
141	650	P	221	650	ID	295	1620	WE	362	FORTR	AB	3505	PEG 4	DP
144	704	LS	222	650	DP	296	1620	SF	363	7090	ID	3506	PEG 7	H3
145	704	LS	223	650	DP	297	220	SP	364	7090	LS	3507	PEG 7	DI
151	650	DP	224	650	DP	298	220	DP	365	7090	SP	3508	PEG 4	FR
152	650	LC	225	704	AB	299	220	SF	366	7090	S	3509	PEG 4	PR
153	650	LF	226	704	LC	300	220	FR	367	7090	AB	3510	PEG 4	FR
154	650	SF	230	709	SP	301	704 4	LC	368	7090	CO	3511	PEG 4	LP
155	650	DP	231	709	SP	302	650	FP	369	1620	SF	4001	7090F	LS
156	650	DP	232	709	TF	303	709	DP	370	1620	FR	4002	704FT	2D
157	1103	DP	233	704	DI	304	709	PA	371	1620T	FR	4003	MERCU	DP
158	1103	FR	234	704	FR	305	709	PA	372	1620T	SF	4004	MERCU	PK
159	1103	LS	235	650	ST	306	709	SF	373	7070	DI	4005	MERCU	PL
160	1103	FR	236	ALGOL	D	307	709	SF	374	7070	DP	4006	MERCU	SC
161	1103	DP	237	ALGOL	SF	308	709	LS	375	7070	DP	4007	MERCU	LS
162	1103	PA	238	ALGOL	LP	309	709	LS	376	7070	DF	4008	MERCU	P
163	1103	DP	239	ALGOL	S	310	709	LP	377	7070	FR	4009	MERCU	SF
164	1103	DP	240	ALGOL	H	311	709	M	378	7070	FR	4010	MERCU	LF
165	1103	ID	241	ALGOL	LC	312	1620,	D	379	7070	FR	4011	MERCU	DI
166	1103	UT	242	ALGOL	TF	313	704	LS	380	7070	FR	4012	MERCU	LC
167	704	PA	243	ALGOL	LF	314	FORTR	SP	381	7070	FT	4013	MERCU	3A
168	650	FR	244	ALGOL	LP	315	709	SP	382	7070	PL	4014	MERCU	2S
169	650	FR	245	ALGOL	S	316	709	SF	383	7070	CO	4015	MERCU	DP
170	650	FR	246	ALGOL	PR	317	709	LS	384	7090	LS	4016	MERCU	S
171	650	FR	247	ALGOL	E	318	709	DP	3001	SILLI	DP	4017	MERCU	DP
172	650	FR	248	ALGOL	DF	319	7090	LS	3002	SILLI	FR	4018	MERCU	SP
173	650	FR	249	ALGOL	DF	320	7090	LP	3003	SILLI	LS	4019	AUTOC	LP
174	650	FR	250	ALGOL	DF	321	650	P	3004	SILLI	LF	4020	DEUCE	ID
175	650	SF	251	ALGOL	DF	322	7090/	FP	3005	SILLI	SF	4021	DEUCE	FR
176	650	SF	252	ALGOL	LS	323	7070	DF	3006	SILLI	SF	4022	DEUCE	R
177	650	SF	253	ALGOL	LS	324	650	DP	3007	SILLI	AB	4023	DEUCE	DP
179	650	LS	254	ALGOL	SF	325	650	E	3008	SILLI	ID	4024	DEUCE	T/
180	650	DP	255	ALGOL	SF	326	650	TF	3009	SILLI	AN	4025	DEUCE	PL
181	650	DP	256	ALGOL	FR	327	650	LF	3010	SILLI	SF	4026	DEUCE	SF
182	650	PL	257	ALGOL	SC	328	650	TF	3011	704FT	P	4027	DEUCE	FR
183	650	HY	258	ALGOL	SC	329	650	DP	3012	ZEBRA	LI	4028	DEUCE	FR
184	650	ID	259	ALGOL	SC	330	7070	SF	3013	ZEBRA	PL	4029	DEUCE	SF
185	650	DP	260	220	DF	331	7070	ID	3014	ZEBRA	P	4030	DEUCE	SF
190	204(5	H	261	220	ID	332	7070	ID	3015	ZEBRA	SF	4031	MERCU	DP

4032 MERCU DP	5023 BULLG ID	6016 FACIT ID	7016 BULL LS	8010 ZEBRA SF
4033 MERCU SC	5024 BULLG PE	6017 FACIT LP	7017 BULL SF	8011 ZEBRA LS
4034 MERCU DP	5025 704 8 FR	6018 FACIT P	7018 BULL LP	8012 ZEBRA IT
4035 MERCU SF	5026 704 8 LS	6019 FACIT AB	7019 650 H	8013 ZEBRA LP
4036 MERCU SF	5027 2002 FR	6020 FACIT AB	7501 6001 FR	8014 ZEBRA LP
4037 MERCU FP	5028 650 DP	6021 FACIT FP	7502 6001 FR	8015 ZEBRA LP
4038 MERCU DP	5029 650 DP	6022 FACIT FR	7503 6001 FR	8016 ZEBRA FI
4039 MERCU E	5030 650 ST	6023 FACIT LS	7504 6001 SF	8501 2203B FR
4040 MERCU PA	5031 650 ST	6024 FACIT LP	7505 6001 SF	8502 2203B SF
4041 MERCU R	5032 650 SF	6025 FACIT SF	7506 6001 DP	8503 2203B SF
4042 MERCU TF	5033 650 ID	6026 FACIT LF	7507 6001 DP	8504 2203B SF
4043 MERCU GE	5034 Z22 R ER	6501 ZRA 1 SF	7508 6001 DP	8505 2203B FR
4044 MERCU TF	5035 Z22 R SF	6502 ZRA1 FR	7509 6001 DP	8506 2203B LS
4045 MERCU ID	5036 650 DP	6503 URAL SF	7510 6001 DP	8507 2203B LS
4046 MERCU GE	5037 650 SF	6504 URAL FR	7511 6001 SC	8508 PC1 FT
4047 MERCU GE	5038 650 DP	6505 URAL SF	7512 6001 DP	8509 PC1 BL
4048 MERCU PK	5039 650 H	6506 URAL DP	7513 9002 FR	8510 PC1 BL
4049 DEUCE FR	5040 650 DP	6507 URAL ST	7514 9002 FR	8511 PC1 BL
5001 ER 56 TH	5041 650 DP	6508 URAL FT	7515 9002 FR	8512 PC1 FT
5002 ER 56 TH	5042 650 DP	6509 628 SF	7516 9002 FR	8513 PC1 LS
5003 ER 56 LC	5043 650 SC	6510 628 LS	7517 9002 PL	8514 M1B SF
5004 ER 56 FR	5044 650 DP	6511 628 LP	7518 9002 FR	8515 M1B ID
5005 ER 56 ID	5045 650 TH	6512 LGP30 ID	7519 9002 FR	8516 M1B A
5006 ER 56 LP	5046 650 DP	6513 LGP30 D	7520 9002 DP	8517 M1B SP
5007 ER 56 FR	5047 650 FR	6514 NE803 ID	7521 9002 ID	8518 M1B FR
5008 2002 SF	6001 WGMAT LP	7001 CAB 5 LS	7522 9002 SF	8519 PC1 ID
5009 2002 FR	6002 MERCU FR	7002 CAB 5 LS	7523 9002 SF	8520 PC1 DP
5010 2002 S	6003 MERCU FR	7003 CAB 5 SP	7524 1103 SF	8521 PC1 SF
5011 2002 DI	6004 MERCU FR	7004 CAB 5 LF	7525 1103 PA	8522 PC1 DP
5012 ALGOL FR	6005 MERCU FR	7005 CAB 5 SP	7526 CEP SF	8523 PC1 TA
5013 ALGOL FR	6006 MERCU FR	7006 CAB 5 SC	7527 CEP SF	8524 PC1 D
5014 ALGOL SF	6007 MERCU ID	7007 CAB 5 SF	8001 BULL FR	8525 PC1 ID
5015 BULLG LS	6008 DASK FR	7008 CAB 5 SF	8002 BULL LP	
5016 BULLG DP	6009 DASK SF	7009 CAB 5 SF	8003 1620 H	
5017 BULLG DP	6010 ALWAC SF	7010 CAB 5 SF	8004 1620 SF	
5018 BULLG LP	6011 ALWAC FR	7011 CAB 5 LP	8005 X 1 FR	
5019 BULLG H	6012 ALWAC FR	7012 CAB 5 ID	8006 X 1 SF	
5020 BULLG LC	6013 ALWAC SF	7013 BULLG FR	8007 ZEBRA FR	
5021 BULLG LC	6014 FACIT FR	7014 BULLG SF	8008 ZEBRA FR	
5022 BULLG SF	6015 FACIT SF	7015 BULLG D	8009 ZEBRA SF	

THE TOTAL NUMBER OF PROGRAMS LISTED HERE IS 577.

ADDITIONAL COPIES OF THIS DOCUMENT, SUBJECT TO LIMITED SUPPLY, MAY BE OBTAINED ON REQUEST FROM
D. P. SHOEMAKER (EDITOR), MASS. INST. OF TECH., CAMBRIDGE 39, MASS., USA
D. W. SMITS (SECRETARY-GENERAL, I U CR), MATH. INST., UNIV. OF GRONINGEN, REITDIEPSKADE 4, GRONINGEN, THE NETHERLANDS
G. A. JEFFREY (CHAIRMAN, I U CR COMMISSION ON CRYSTALLOGRAPHIC COMPUTING), CRYSTALLOGRAPHIC LABORATORY, UNIVERSITY OF PITTSBURGH, PITTSBURGH, PA., USA

WE WISH TO CALL TO THE ATTENTION OF AUTHORS OF CRYSTALLOGRAPHIC PAPERS (AND ALSO REFEREES AND EDITORS) THE FACT THAT DETAILED RECOMMENDATIONS HAVE BEEN FORMULATED BY THE I U CR COMMISSION ON CRYSTALLOGRAPHIC COMPUTING CONCERNING (1) THE REPORTING OF THE COMPUTING ASPECTS OF CRYSTAL STRUCTURE ANALYSIS IN PAPERS TO BE PUBLISHED, AND (2) THE PUBLICATION OF PAPERS ON COMPUTING METHODS AND PROGRAMS IN CRYSTALLOGRAPHIC JOURNALS. THESE RECOMMENDATIONS HAVE BEEN PUBLISHED IN ACTA CRYST., 15, 515 (1962).