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=X-RAY 63=

PROGRAM SYSTEM FOR X-RAY CRYSTALLOGRAPHY

FOR THE

IBM 709-7090-7094

THE DEPARTMENTS OF CHEMISTRY AT
THE UNIVERSITY OF WASHINGTON, SEATTLE
AND
THE UNIVERSITY OF MARYLAND, COLLEGE PARK

EDITION OF
APRIL 1964

=X-RAY 63=

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=X-RAY 63=

THE MAJOR RESPONSIBILITY FOR THE =X-RAY 63= PROGRAM SYSTEM LIES WITH JAMES M. STEWART AND DARRELL HIGH. THE WRITE-UP HAS BEEN COMPILED AND EDITED BY BRUCE W. BROWN.

THE PROGRAMMING, AS A WHOLE, HAS BEEN THE RESULT OF THE GROUP EFFORT BY MANY PEOPLE, INCLUDING ESPECIALLY JAMES R. HOLDEN, BRUNO MOROSIN, ROGER CHASTAIN, HIROSHI TAKEDA AND CHARLES DICKINSON. THE CONTRIBUTORS TO EACH PROGRAM ARE LISTED IN PART I, AND TO EACH SUBROUTINE IN APPENDIX X.

MANY THANKS ARE DUE TO PROFESSORS EDWARD C. LINGAFELTER, LYLE H. JENSEN, AND JOSEPH KRAUT, AND DR. JAMES R. BRATHOVDE FOR ADVICE, SUPPORT, AND ENCOURAGEMENT.

THE GROUP ACKNOWLEDGES THE FINANCIAL AID FROM THE NATIONAL INSTITUTES OF HEALTH, THE NAVAL RESEARCH LABORATORIES, THE SANDIA CORPORATION, THE ARMY RESEARCH OFFICE (DURHAM), AND NON-SUPPORTED RESEARCH GRANTS FROM THE RESEARCH COMPUTER LABORATORY AT THE UNIVERSITY OF WASHINGTON, AND THE COMPUTER SCIENCE CENTER AT THE UNIVERSITY OF MARYLAND.

=X-RAY 63=

PROGRAM SYSTEM FOR X-RAY CRYSTALLOGRAPHY

FOR THE IBM 709-7090-7094

PART I - METHOD OF CALCULATION

A. PROGRAM SYSTEM DESCRIPTION.

THE =X-RAY 63= PROGRAM SYSTEM IS DESIGNED TO RUN WITH THE SYSTEM CONTAINED ON A MASTER =PROGRAM TAPE= MADE UP OF LINKS, EACH OF WHICH IS A COMPLETE PROGRAM OR PROGRAM SEGMENT. THE CALCULATION IS STARTED BY A SMALL CALLING PROGRAM WHICH PERFORMS CERTAIN INITIALIZATIONS AND THEN TRANSFERS CONTROL TO THE PROGRAM TAPE. THE SYSTEM HAS BEEN DESIGNED TO RUN WITH ANY 709-7090-7094 MONITOR, OR WITH NO MONITOR, WITHOUT ANY MODIFICATION OF THE PROGRAM TAPE- THE NECESSARY CHANGES ARE MADE IN THE CALLING PROGRAM. A DISCUSSION OF THE SYSTEM FROM THE POINT OF VIEW OF A PERSON WISHING TO USE IT AT ANOTHER INSTALLATION IS GIVEN IN APPENDIX IX. THE DESCRIPTION THAT FOLLOWS IS ORIENTED TO A USER OF THE 709 FORTRAN MONITOR AT THE UNIVERSITY OF WASHINGTON RESEARCH COMPUTER LABORATORY (RCL). SAMPLES OF JOB SUBMISSION AT RCL ARE GIVEN IN APPENDIX VI.

THE =X-RAY 63= SYSTEM AS DESCRIBED HERE IS AVAILABLE ONLY FOR IBM 709-7090-7094. CONSIDERABLE WORK HAS BEEN DONE WITH A PRELIMINA VERSION OF THE SYSTEM AT THE CDC 1604 INSTALLATIONS AT SANDIA (MOROS AND THE UNIVERSITY OF CALIFORNIA AT SAN DIEGO (HIGH). PROVISION HAS BEEN MADE FOR THE PREPARATION OF A BUSING-LEVY ORFLX-TYPE REFLECTION TAPE FOR THE IBM 704 OR SIMULATOR, HOWEVER THE FORTRAN VERSION OF THIS PROGRAM HAS BEEN MODIFIED AND INCLUDED IN THE =X-RAY 63= SYSTEM. IT IS

ALSO POSSIBLE TO PUNCH AN IBM 650 REFLECTION DECK FOR SYSTEM COMPATIBILITY WITH IBM 650 PROGRAMS WRITTEN AT THE UNIVERSITY OF WASHINGTON. THE IBM 650 REFLECTION DECK CAN BE USED ON AN IBM 1620 WITH 20K STORAGE (PORTLAND STATE COLLEGE) OR 60K STORAGE (MONTANA STATE COLLEGE) USING THE UNIVERSITY OF WASHINGTON PROGRAMS CONVERTED TO IBM 1620 (BY PROF. CHARLES CAUGHLIN AND MR. GEORGE SVETICH, MONTANA STATE COLLEGE).

THE COURSE OF THE CALCULATION, WHICH MAY INVOLVE ANY NUMBER OF THE LINKS IN THE SYSTEM, IS CONTROLLED BY THE SEQUENCE OF CARDS IN THE INPUT DATA. THESE CONTROL FUNCTIONS ARE EXERCISED BY A SUBROUTINE CALLED =CALLER= THROUGH WHICH ALL INPUT PASSES. INPUT DATA CARDS ARE IDENTIFIED BY PUNCHING IN THE FIRST SIX CARD COLUMNS, USUALLY A MNEMONIC OF THE CARD FUNCTION. A DATA DECK CONSISTS OF THE FOLLOWING KINDS OF CARDS.

(A) OPERATIONAL CARDS (WHICH ARE ACCEPTABLE AT ANY TIME) PERFORM IMMEDIATE OPERATIONS SUCH AS ASSIGNING TAPES, PRINTING REMARKS AND INSTRUCTIONS, AND SUPPLYING A TITLE.

(B) A CALLING CARD SERVES TO CALL THE SPECIFIC PROGRAM LINK AND INITIATE THE PROGRAM.

(C) OTHER DATA CARDS ARE READ UNDER THE CONTROL OF THE PROGRAM TO SUPPLY, FOR EXAMPLE, PARAMETERS, INTENSITY DATA, AND CONTROL INFORMATION.

(D) THE LAST CARD OF THE DATA DECK MUST BE AN =END= CARD.

A SEQUENCE OF INTERDEPENDENT CALCULATIONS MAY BE PERFORMED BY STACKING UP AN APPROPRIATE SET OF DATA DECKS (FOR EXAMPLE- FC FOLLOWED BY A FOURIER SYNTHESIS, OR, SEVERAL CYCLES OF AUTOMATIC REFINEMENT). THIS SET OF DATA DECKS MUST BE PRECEDED BY A =*DATA= CARD. ANOTHER INDEPENDENT SEQUENCE OF CALCULATIONS MAY BE INITIATED BY FOLLOWING THE FIRST SEQUENCE BY A =*DATA= CARD AND ONE OR MORE DATA DECKS - ET CONTINUUM. EXECUTION TERMINATES AND CONTROL IS RETURNED TO THE CALLING MONITOR WHEN A =FINISH= CARD OR AN END-OF-FILE IS READ ON THE MONITOR INPUT TAPE.

THE SEQUENCE OF EVENTS DURING THE COURSE OF A CALCULATION IS AS FOLLOWS=

A =*DATA= CARD CAUSES IMMEDIATE INITIALIZATION OF TAPE ASSIGNMENTS, PAGE NUMBERS, TITLES, ETC. A CALLING CARD CAUSES THE INDICATED PROGRAM TO BE LOADED IF IT IS NOT ALREADY IN CORE AND CONTROL IS TRANSFERRED TO

THE PROGRAM. DATA CARDS ARE READ BY =CALLER= AT THE REQUEST OF THE PROGRAM. THE TYPES OF CARDS AND THEIR FORMATS ARE DISCUSSED IN DETAIL IN PART II OF THE WRITE-UP. NORMALLY, THE PROGRAM READS AND PROCESSES DATA CARDS UNTIL THE =END= CARD IS REACHED, WHEREUPON THE PROGRAM FINISHES THE CALCULATION, WRITES SUMMARY DATA, AND RETURNS CONTROL TO =CALLER=. ANOTHER CALLING CARD CAN THEN INITIATE A NEW CALCULATION WITH THIS OR ANY OTHER PROGRAM ON THE SYSTEM TAPE.

IF FOR ANY REASON THERE IS A CALCULATION FAILURE, CONTROL IS RETURNED TO =CALLER= WHICH SKIPS ALL SUBSEQUENT CARDS UNTIL ANOTHER =*DATA= CARD IS READ WHEREUPON THE CALCULATION IS RESUMED. BECAUSE OF THIS PROCEDURE THE CALCULATIONS THAT RUN INDEPENDENTLY SHOULD BE SEPARATED BY =*DATA= CARDS. A DEPENDENT SEQUENCE OF CALCULATIONS ARE NOT SEPARATED BY =*DATA= CARDS SO THAT FAILURE OF ONE LINK WILL DELETE REMAINING PARTS. THE END OF ALL CALCULATIONS IS INDICATED BY A =FINISH= CARD.

WARNING....WARNING....WARNING....WARNING....WARNING....WARNING...WARNING

DURING EXECUTION THE CALLING MONITOR IS EFFECTIVELY DISABLED. IT IS THEREFORE AN IMPERATIVE NECESSITY THAT USERS AT OTHER INSTALLATIONS STUDY CAREFULLY THE =LOGICAL= TAPE DESIGNATIONS OF THE X-RAY SYSTEM IN ORDER TO PREVENT INTERFERING WITH THE INSTALLATIONS NORMAL SEQUENCE OF EVENTS. REFERENCE TO THE MONITOR SPECIFIC PROGRAMS =B5FORT=, =B5BELL=, AND =B5IBSY= (SEE APPENDIX IX) WILL BE HELPFUL. THE SYSTEM MAY BE RUN INDEPENDENTLY OF ANY MONITOR BY USE OF THE =B5CARD= STARTING CARD.

(DISCLAIMER BASED ON THE IBM-SHARE DISCLAIMER.)

=ALTHOUGH EACH PROGRAM HAS BEEN TESTED BY ITS CONTRIBUTOR, NO WARRANTY, EXPRESS OR IMPLIED, IS MADE BY THE CONTRIBUTOR AS TO THE ACCURACY AND FUNCTIONING OF THE PROGRAM AND RELATED PROGRAM MATERIAL AND NO RESPONSIBILITY IS ASSUMED BY THE CONTRIBUTOR OR ANY MEMBER OF THE X-RAY SYSTEM GROUP IN CONNECTION THEREWITH.=

LIST OF OPERATION CARDS

REMARK INSERTS REMARKS ON THE BCD OUTPUT TAPE FOR OFF-LINE LISTING.

TITLE FILLS IN PAGE TITLE. NEW =TITLE= CARD CHANGES STORED TITLE. =*DATA= CARD INITIALIZES STORED TITLE TO BLANKS.

PRINTR INSTRUCTIONS TO OFF-LINE PRINTER OPERATOR. ANY NUMBER MAY BE USED IN A GROUP FOR LONG INSTRUCTIONS.

OPRATR INSTRUCTIONS TO COMPUTER OPERATOR. ANY NUMBER MAY BE USED IN A GROUP FOR LONG INSTRUCTIONS.

PAUSE STOPS COMPUTER. USED ESPECIALLY AFTER A GROUP OF =OPRATR= CARDS. CAUSES REMARK =PRESS START TO CONTINUE= TO BE PRINTED ON THE ON-LINE PRINTER.

TAPES ASSIGNS TAPE UNIT DESIGNATIONS.

ENDFIL WRITES END-OF-FILE ON BCD OUTPUT TAPE (NTOUT).

ENDTAP WRITES REMARK =END OF OUTPUT TAPE= AND WRITES TWENTY END-OF-FILE MARKS. REWINDS TAPE =NTOUT= AND REDEFINES =NTOUT= TO =NTOUTM=. NOTE- IF (NTOUT)=(NTOUTM) THE =ENDTAP= CARD IS IGNORED. (THESE TAPE DESIGNATIONS ARE DEFINED IN 1.0-B.)

IGNORE CAUSES THE FOLLOWING CARD TO BE SKIPPED UNCONDITIONALLY AND SUBSEQUENT CARDS TO BE SKIPPED UNTIL A =*DATA= CARD IS REACHED. AN EXAMPLE OF THE USE OF THIS CARD IS TO PRECEDE A =*DATA= CARD WHOSE DATA DECK (SUCH AS A SET OF =OPRATR= CARDS DEFINING ERROR PROCEDURE) IS TO BE SKIPPED IF PRIOR OPERATION WAS SUCCESSFUL. ORDINARILY THE =IGNORE= CARD WILL CAUSE THE FOLLOWING =*DATA= CARD AND DATA CARDS TO BE SKIPPED. IF THE CALCULATION FAILS THE =IGNORE= CARD WILL BE SKIPPED BY =CALLER= AND THE =*DATA= CARD AND DATA CARDS WILL BE PROCESSED.

FINISH CAUSES IMMEDIATE RETURN TO LABORATORY SYSTEM (IF ANY). MUST BE USED WITH ANY LABORATORY MONITOR WHICH DOES NOT USE END-OF-FILE MARKS BETWEEN JOBS (E.G.- BELL).

SAVE ON THE 7090 AND 7094 CAUSES UNLOADING OF THE SPECIFIED LOGICAL TAPES THESE SHOULD NOT BE INCLUDED UNTIL THE END OF THE RUN. (THIS CARD SHOULD USUALLY BE PRECEEDED BY A *DATA CARD).

B. NOTES ON THE USE OF TAPE.

APART FROM OCCASIONAL REMARKS ON THE ON-LINE PRINTER, ALL INPUT AND OUTPUT IN THE SYSTEM IS ON MAGNETIC TAPE. A TYPICAL PROGRAM (E.G.- FC, CALCULATION OF STRUCTURE FACTORS) USES FOUR INPUT/OUTPUT TAPES- A BCD INPUT TAPE (FROM THE CARD READER), A BCD OUTPUT TAPE (FOR THE PRINTER), AND BINARY INPUT AND OUTPUT TAPES. IN ADDITION, ONE TAPE IS USED FOR THE PROGRAMS. THE FORTRAN LOGICAL TAPE NUMBER CORRESPONDING TO THE ACTUAL TAPE UNIT TO BE USED FOR EACH PURPOSE IS CONTAINED IN A BLOCK OF TAPE-ASSIGNMENT LOCATIONS WHICH ARE REFERRED TO BY ALL PROGRAMS. THESE TAPE NUMBERS ARE INITIALIZED BY THE PROGRAM WHEN A =*DATA= CARD IS ENCOUNTERED, AND MAY BE CHANGED BY THE USER WITH A =TAPES= CARD. SINCE ALL THE PROGRAMS REFER TO THE SAME ASSIGNMENT CELLS, IT IS POSSIBLE TO USE ONE =TAPES= CARD TO SET THE TAPES TO BE USED FOR AN ENTIRE CALCULATION INVOLVING SEVERAL PROGRAMS. IN PRACTICE, IT IS BETTER TO SET TAPES BETWEEN MOST CALCULATIONS - IF FOR NO OTHER REASON THAN IT FORCES ONE TO CONTEMPLATE THE SEQUENCE OF TAPE OPERATIONS.

THE NAMES OF THE TAPE-ASSIGNMENT CELLS, THE NAME AND USUAL CONTENTS OF THE CELLS FROM WHICH THEY ARE INITIALIZED, AND THE FUNCTIONS TO WHICH THEY CORRESPOND ARE INDICATED IN TABLE 1.0-I FOR THE FORTRAN (II) MONITOR SPECIFIC AT THE UNIVERSITY OF WASHINGTON. THE TAPE ASSIGNMENT FOR THE BELL AND IBSYS MONITORS ARE GIVEN IN TABLES 1.0-II AND 1.0-III, RESPECTIVELY.

THE ACTUAL 709-7090-7094 TAPE ADDRESSES CORRESPONDING TO THE FORTRAN LOGICAL TAPE NUMBERS ARE DETERMINED BY A SUBROUTINE CALLED =IOU=, THE INPUT-OUTPUT UNIT TABLE. THE =IOU= IN THE X-RAY SYSTEM THAT IS USED AT THE UNIVERSITY OF WASHINGTON IS GIVEN IN TABLE 1.0-IV. THE =IOU= TABLE FOR THE BELL AND IBSYS MONITORS ARE GIVEN IN TABLES 1.0-V AND 1.0-VI, RESPECTIVELY. BOTH THE =IOU= TABLE AND/OR THE DEFINITION OF =NTINM=, =NTOUTM=, ETC., MAY BE DEFINED BY THE MONITOR SPECIFIC CALLING PROGRAM LIKE =BSIBSY= (SEE APPENDIX 3.9).

FOR MOST EFFICIENT OPERATION, THE TAPE ASSIGNMENTS USED SHOULD BE COMPATIBLE WITH THIS SCHEME. AT THE UNIVERSITY OF WASHINGTON, CARD INPUT, PRINTER OUTPUT, AND PUNCHED CARD OUTPUT SHOULD BE ON TAPES 5, 6, AND 7 WHENEVER POSSIBLE. TAPES TO BE SAVED OR TAPES CONTAINING SPECIAL INPUT SHOULD BE ASSIGNED TO 9-12, SINCE THESE MAY BE CHANGED WITHOUT INTERFERING WITH STANDARD MONITOR OPERATION.

ALL THOSE TAPES WHICH ARE NOT TO BE SAVED AND FOR WHICH NO INITIAL INPUT IS REQUIRED ARE CALLED =SCRATCH= TAPES- ANY TAPE TO BE USED IN THIS WAY MAY MOST CONVENIENTLY BE ASSIGNED TO 2, 3, OR 4, SINCE THESE TAPES ARE AVAILABLE AT ALL TIMES WITHOUT SPECIAL OPERATOR ACTION. IT IS NECESSARY TO GIVE INSTRUCTIONS TO THE OPERATOR (IN THE FORM OF =*TAPE= OR =*SAVE= CARDS AT RCL) FOR ANY USE OF TAPES 9 TO 12. IT IS CONVENTIONAL TO MOUNT THE X-RAY PROGRAM SYSTEM TAPE ON 10 (B5), SINCE ALL CALLING PROGRAMS WRITTEN SO FAR (E.G.- =B5CARD=, =B5FORT=, ETC.) HAVE BEEN FOR UNIT B5.

TABLE 1.0-I

TAPE ASSIGNMENTS

FORTRAN (II) MONITOR SPECIFIC FOR THE UNIVERSITY OF WASHINGTON

TAPE ASSIGNMENT LOCATION	=LOGICAL= NUMBER	FUNCTION
NTPROG	10	PROGRAM TAPE FOR X-RAY SYSTEM. (NOTE 1)
NTIN	5	BCD INPUT TAPE FROM OFF-LINE CARD READER (NOTE 2).
NTOUT	6	BCD OUTPUT TAPE FOR OFF-LINE PRINTER.
NTAPEA	11	BINARY REFLECTION TAPE (NOTE 3). OUTPUT OF DATA REDUCTION. INPUT TO STRUCTURE FACTORS.
NTAPEB	12	BINARY FC TAPE (NOTE 3). OUTPUT OF STRUCTURE FACTORS. INPUT TO FOURIER.
NTAPEC	7	BCD USUAL LABORATORY PUNCH TAPE.
NTAPED	6	BCD FOURIER OUTPUT TAPE.
NTAPEE	2	SPECIAL UTILITY OUTPUT.
NTAPEF	4	SPECIAL UTILITY INPUT.
NTAPEG	0	UNASSIGNED (NOTE 4).
....	...	.....
NTAPEJ	0	UNASSIGNED.

NOTE 1- THE ASSIGNMENT OF =NTPROG= IS NOT UNDER =TAPES= CARD CONTROL. IT IS NORMALLY SET TO 10 BY =SYSCOM=, BUT IF THE PROGRAM TAPE IS GENERATED BY MONITOR =CHAIN= AND EXECUTED DIRECTLY, IT WILL BE SET TO 3 BY =BEGIN=.

NOTE 2- =NTIN= IS INITIALIZED TO =NTINM= WHEN THE SYSTEM IS FIRST STARTED, BUT IS NOT RESET WHEN A =*DATA= CARD IS ENCOUNTERED. IT IS RESET WHEN AN END-OF-FILE IS SENSED ON =NTIN= WHEN =NTIN= IS NOT EQUAL TO =NTINM=.

NOTE 3- THE TERMS =BINARY REFLECTION TAPE= AND =BINARY FC TAPE= REFER TO FUNCTION AND NOT TO THE TAPE FORMAT ITSELF. A PREVIOUS OUTPUT OF =FC= MAY BE USED AS THE REFLECTION TAPE IN A LATER RUN, AND THE OUTPUT OF DATA REDUCTION MAY BE USED AS =NTAPEB= FOR CALCULATING A PATTERSON, FOR EXAMPLE.

NOTE 4- IN THE =X-RAY 63= SYSTEM, =NTAPEG= TO =NTAPEJ= ARE NOT USED AND ARE NOT INITIALIZED.

NOTE 5- ALL =LOGICAL= NUMBER VALUES REFER TO THE UNIVERSITY OF WASHINGTON =ICU= TABLE.

TABLE 1.0-II

TAPE ASSIGNMENTS

BELL MONITOR AS USED AT NAVAL ORDNANCE LABORATORY AND BUREAU OF STANDARDS

TAPE ASSIGNMENT LOCATION	=LOGICAL= NUMBER	FUNCTION
NTPROG	15	PROGRAM TAPE FOR X-RAY SYSTEM. (NOTE 1)
NTIN	2	BCD INPUT TAPE FROM OFF-LINE CARD READER (NOTE 2).
NTOUT	3	BCD OUTPUT TAPE FOR OFF-LINE PRINTER.
NTAPEA	6	BINARY REFLECTION TAPE (NOTE 3).
NTAPEB	16	BINARY FC TAPE (NOTE 3).
NTAPEC	14	BCD USUAL LABORATORY PUNCH TAPE.
NTAPED	3	BCD FOURIER OUTPUT TAPE.
NTAPEE	12	SPECIAL UTILITY OUTPUT.
NTAPEF	4	SPECIAL UTILITY INPUT.
NTAPEG	0	UNASSIGNED (NOTE 4).
....	...	.....
NTAPEJ	0	UNASSIGNED.

NOTE 1- THE ASSIGNMENT OF =NTPROG= IS NOT UNDER =TAPES= CARD CONTROL. IT IS SET TO 15 BY =SYSBCL=.

NOTE 2- =NTIN= IS INITIALIZED TO =NTINM= WHEN THE SYSTEM IS FIRST STARTED, BUT IS NOT RESET WHEN A =*DATA= CARD IS ENCOUNTERED. IT IS RESET WHEN AN END-OF-FILE IS SENSED ON =NTIN= WHEN =NTIN= IS NOT EQUAL TO =NTINM=. SINCE THE BELL SYSTEM IS SOMETIMES RUN WITH BCD INPUT FROM THE ON-LINE CARD READER, THE BELL INITIATING ROUTINE THROUGH SUBROUTINE =FOOLBE= MOVES THE STACKED CARDS FROM THE CARD READER TO LOGICAL UNIT 2. GREAT CARE MUST BE EXERCISED BECAUSE OF THIS IDIOSYNCRASY.

NOTE 3- THE TERMS =BINARY REFLECTION TAPE= AND =BINARY FC TAPE= REFER TO FUNCTION AND NOT TO THE TAPE FORMAT ITSELF. A PREVIOUS OUTPUT OF =FC= MAY BE USED AS THE REFLECTION TAPE IN A LATER RUN, AND THE OUTPUT OF DATA REDUCTION MAY BE USED AS =NTAPEB= FOR CALCULATING A PATTERSON, FOR EXAMPLE.

NOTE 4- IN THE =X-RAY 63= SYSTEM, =NTAPEG= TO =NTAPEJ= ARE NOT USED AND ARE NOT INITIALIZED.

NOTE 5- ALL =LOGICAL= NUMBER VALUES REFERRED TO BELL =IOU= TABLE.

TABLE 1.0-III

TAPE ASSIGNMENTS

IOSYS MONITOR AS USED AT THE UNIVERSITY OF MARYLAND

TAPE ASSIGNMENT LOCATION	=LOGICAL= NUMBER	FUNCTION
NTPROG	10	PROGRAM TAPE FOR X-RAY SYSTEM. (NOTE 1)
NTIN	5	BCD INPUT TAPE FROM OFF-LINE CARD READER (NOTE 2).
NTOUT	8	BCD OUTPUT TAPE FOR OFF-LINE PRINTER.
NTAPEA	11	BINARY REFLECTION TAPE (NOTE 3). OUTPUT OF DATA REDUCTION. INPUT TO STRUCTURE FACTORS.
NTAPEB	12	BINARY FC TAPE (NOTE 3). OUTPUT OF STRUCTURE FACTORS. INPUT TO FOURIER.
NTAPEC	2	BCD USUAL LABORATORY PUNCH TAPE.
NTAPED	8	BCD FOURIER OUTPUT TAPE.
NTAPEE	6	SPECIAL UTILITY OUTPUT.
NTAPEF	4	SPECIAL UTILITY INPUT.
NTAPEG	0	UNASSIGNED (NOTE 4).
....	...	.....
NTAPEJ	0	UNASSIGNED.

NOTE 1- THE ASSIGNMENT OF =NTPROG= IS NOT UNDER =TAPES= CARD CONTROL. IT IS NORMALLY SET TO 10 BY =SYSCOM=, BUT IF THE PROGRAM TAPE IS GENERATED BY MONITOR =CHAIN= AND EXECUTED DIRECTLY, IT WILL BE SET TO 3 BY =BEGIN=.

NOTE 2- =NTIN= IS INITIALIZED TO =NTINM= WHEN THE SYSTEM IS FIRST STARTED, BUT IS NOT RESET WHEN A =*DATA= CARD IS ENCOUNTERED. IT IS RESET WHEN AN END-OF-FILE IS SENSED ON =NTIN= WHEN =NTIN= IS NOT EQUAL TO =NTINM=.

NOTE 3- THE TERMS =BINARY REFLECTION TAPE= AND =BINARY FC TAPE= REFER TO FUNCTION AND NOT TO THE TAPE FORMAT ITSELF. A PREVIOUS OUTPUT OF =FC= MAY BE USED AS THE REFLECTION TAPE IN A LATER RUN, AND THE OUTPUT OF DATA REDUCTION MAY BE USED AS =NTAPEB= FOR CALCULATING A PATTERSON, FOR EXAMPLE.

NOTE 4- IN THE =X-RAY 63= SYSTEM, =NTAPEG= TO =NTAPEJ= ARE NOT USED AND ARE NOT INITIALIZED.

NOTE 5- ALL =LOGICAL= NUMBER VALUES REFER TO THE UNIVERSITY OF WASHINGTON =IOU= TABLE.

TABLE 1.0-IV

INPUT-OUTPUT UNIT TABLE

FORTRAN (II) MONITOR

FORTRAN NUMBER	709 TAPE ADDRESS	FUNCTION
1	A1	SYSTEM MASTER.
2	B2	MONITOR SCRATCH (ALSO USED BY =PDUMP= AND =DUMP=).
3	B3	MONITOR SCRATCH.
4	A4	MONITOR SCRATCH.
5	A2	MONITOR INPUT.
6	A3	MONITOR OUTPUT.
7	B4	MONITOR PUNCHED-CARD OUTPUT.
8	B1	USED BY MONITOR CHAIN TO STACK BINARY INPUT CARDS, OTHERWISE NOT ORDINARILY USED.
9	A5	NOT USED BY MONITOR. AVAILABLE FOR PROGRAM INPUT/OUTPUT.
10	B5	DITTO.
11	A6	DITTO.
12	B6	DITTO.

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TABLE 1.0-V

INPUT-OUTPUT UNIT TABLE

BELL MONITOR

FORTRAN NUMBER	BELL NUMBER	FUNCTION
1	1	SYSTEM MASTER.
2	12	MONITOR SCRATCH (ALSO USED BY =PDUMP= AND =DUMP=).
3	13	MONITOR SCRATCH.
4	4	MONITOR SCRATCH.
5	2	MONITOR INPUT.
6	3	MONITOR OUTPUT.
7	14	MONITOR PUNCHED-CARD OUTPUT.
8	11	USED BY MONITOR CHAIN TO STACK BINARY INPUT CARDS, OTHERWISE NOT ORDINARILY USED.
9	9	NOT USED BY MONITOR. AVAILABLE FOR PROGRAM INPUT/OUTPUT.
10	20	DITTO.
11	6	DITTO.
12	16	DITTO.

TABLE 1.0-VI

INPUT-OUTPUT UNIT TABLE

IBSYS MONITOR

FORTRAN NUMBER	IBSYS NUMBER	FUNCTION
1	A1	SYSTEM MASTER.
2	B2	MONITOR PUNCHED-CARD OUTPUT.
3	B3	MONITOR SCRATCH.
4	A4	MONITOR SCRATCH.
5	A2	MONITOR INPUT.
6	A3	USED BY MONITOR CHAIN TO STACK BINARY INPUT CARDS, OTHERWISE NOT ORDINARILY USED.
7	B4	MONITOR SCRATCH.
8	B1	MONITOR OUTPUT.
9	A5	NOT USED BY MONITOR. AVAILABLE FOR PROGRAM INPUT/OUTPUT.
10	B5	DITTO.
11	A6	DITTO.
12	B6	DITTO.

NOTE - UNDER =IBSYS= THERE IS THE DANGER THAT THE OPERATOR MAY ON WHIM CHANGE THE SHOP =IOU= TABLE OR TAPE FUNCTION. THEREFORE LET IT BE KNOWN TO THE OPERATORS IN THE SHOP, IN ADVANCE, THAT =X-RAY63= PROGRAM SYSTEM SUPERCEDES =IBSYS= DURING EXECUTION.

C. GENERAL DESCRIPTION OF THE METHOD.

THE PROGRAMS DESCRIBED HERE ARE DESIGNED TO CONSTITUTE A =SYSTEM= FOR X-RAY CRYSTALLOGRAPHY WHICH WILL RUN INDEPENDENTLY OF, OR IN CONJUNCTION WITH, EXISTING IBM 709-7090-7094 MONITORS. THE MAJOR SUBROUTINES OF THE =SYSTEM= DO THE CALCULATIONS NECESSARY TO INTERPRET X-RAY DIFFRACTION PATTERNS AND TO ESTABLISH ACCURATE ATOMIC PARAMETERS IN CRYSTALS. CONTROL IS INSTITUTED BY CALLING CARDS WHOSE FUNCTION IS TO CALL THE VARIOUS SEGMENTS OF THE SYSTEM AS THEY ARE NEEDED. TO THIS END CRYSTALLOGRAPHIC DATA ARE TRANSFORMED FROM THE RAW STATE ON CARDS AND STORED ON TAPE AT THE TIME OF DATA REDUCTION IN A FORM USEFUL TO THE PROGRAMS WHICH FOLLOW.

FOR CONVENIENCE IN USE, THIS MANUAL IS DIVIDED INTO THREE PARTS. THE FIRST PART IS A =USERS GUIDE= GIVING THE METHOD AND PLAN OF CALCULATION. THE SECOND PART GIVES DIRECTIONS FOR USE OF THE PROGRAMS IN TERMS OF CARD FORMATS AND CARD ORDER. THE THIRD PART IS A SERIES OF APPENDICES TO AID IN ADAPTING THE SYSTEM TO VARIOUS MONITORS AND INSTALLATIONS. ALL PROGRAMS, SUBPROGRAMS, AND SUBROUTINES IN THE X-RAY CRYSTALLOGRAPHY PROGRAM SYSTEM DEPEND UPON THE FORTRAN(II)-FAP PROGRAMMING SYSTEM. THEREFORE IT IS HELPFUL TO BE AWARE OF THE CARD FORMATS AND LIMITATIONS OF THESE SYSTEMS. THE DIRECTIONS ATTEMPT TO BE EXPLICIT WHEREVER CONFUSION MIGHT ARISE, BUT LET THE USER BEWARE OF COMPUTER LABORATORY SPECIFIC PROCEDURES.

THROUGHOUT THE PROGRAMS CHECKS ARE MADE ON THE NUMBERS SUPPLIED BY THE USER. IF THESE DO NOT FALL WITHIN CERTAIN ARBITRARY LIMITS SET IN ANY GIVEN PROGRAM A REMARK WILL BE PRINTED AND THE CALCULATION MAY BE REJECTED. THE REMARKS WHICH THE PROGRAMS WRITE IN THESE EVENTS MUST TAKE INTO ACCOUNT THE SENSIBILITIES OF A 709-7090-7094.

NOTE THAT EACH CARD TYPE HAS A CERTAIN INVIOLABLE NAME (E.G.- =CELL=) WHICH MUST BE PUNCHED IN ITS FIRST SIX COLUMNS. THE WHOLE PROCESS OF CONTROL IS BASED UPON THESE CARDS AND UPON THEIR ORDER. EXERCISE CARE

IN THE PUNCHING AND ORDERING OF CARDS SO THAT THE PROGRAMS WILL RUN. A GENERAL PRINCIPLE APPLIES TO LEAVING COLUMNS BLANK, OR OMITTING NUMBERS IN ALL THE VARIOUS KINDS OF CARD FORMS= IF THE NUMBERS WHICH THE PROGRAM REQUIRES HAVE ALREADY BEEN SUPPLIED IN PRECEEDING CARDS THEN THOSE NUMBERS WILL BE USED UNCHANGED= IF THEY HAVE NOT BEEN SUPPLIED, EITHER AN ERROR WILL BE RECORDED OR A VALID =BEST= VALUE WILL BE SUBSTITUTED (E.G.- 1.00 FOR A MULTIPLICATIVE SCALE FACTOR). THE CONVENIENCE OF THIS FEATURE SHOULD BECOME APPARENT AS THE INDIVIDUAL CARD APPLICATIONS ARE STUDIED. AN ALPHABETICAL LIST OF ALL CARD FORMATS IN THE SYSTEM IS GIVEN IN APPENDIX II (SECTION 3.2).

AN ATTEMPT HAS BEEN MADE TO SAVE AS MUCH DATA AS POSSIBLE ON THE BINARY =REFLECTION= TAPES. THE FORMAT OF THESE TAPES ARE DESCRIBED IN APPENDIX IV (SECTION 3.4). IN THIS WAY CARD PUNCHING CAN BE KEPT TO A MINIMUM AND THE NUMBER OF CARDS NECESSARY TO ACCOMPLISH A GIVEN CALCULATION KEPT AT A FAIRLY LOW FIGURE (E.G.- A FOURIER OFTEN REQUIRES ONLY THREE CARDS- =FOURR=, =LAYOUT=, AND =END=.)

USUALLY, ONCE A NUMBER IS SUPPLIED TO ANY PROGRAM, THIS NUMBER IS CARRIED UNCHANGED ON THE BINARY TAPE UNTIL A NEW VALUE IS EITHER CALCULATED OR SUPPLIED. WHENEVER POSSIBLE INPUT DATA FROM CARDS ARE NOT STORED IF THE CARD COLUMNS ARE BLANK. IF THE DATA MUST BE STORED THE WRITE-UP INDICATES THIS FACT.

THE STRUCTURE OF THE SYSTEM TAPE ITSELF MIMICS THAT OF A FORTRAN(II)-CHAIN TAPE IN THAT IT CONSISTS OF A SET OF DOUBLE RECORDS, THE FIRST OF WHICH TELLS THE LENGTH OF THE PROGRAM IN THE SECOND RECORD AND THE ENTRY POINT OF THAT PROGRAM. THE SECOND RECORD OF THE PAIR IS THE ABSOLUTE RELOCATED PROGRAM READY FOR EXECUTION. BECAUSE OF THE STRUCTURE OF THE SYSTEM TAPE, IF IT IS DESIRED TO =PATCH= THE VARIOUS PROGRAMS THE SYSTEM TAPE MUST BE GENERATED ANEW THROUGH THE =LOADER= PROVISION (SECTION 1.1 AND 2.1).

THE SYSTEM ITSELF IS DESIGNED TO BE RUN INDEPENDENTLY OF ANY MONITOR, BUT SINCE IT IS A =CHILD= OF THE UNIVERSITY OF WASHINGTON RESEARCH COMPUTER LABORATORY MONITOR IT MAY SHOW CERTAIN GENETIC TRAITS OF THAT

SYSTEM. THE CONSIDERATIONS WHICH HAVE GONE INTO THE DESIGN HAVE TRIED TO BE MADE GENERAL WHENEVER POSSIBLE. THERE IS ONE AREA, HOWEVER, WHICH ANY POTENTIAL USER IN ANY SHOP MUST CONSIDER CAREFULLY, AND THAT IS THE USE OF MAGNETIC TAPE. IT IS ALWAYS WISE TO MAKE A CAREFUL STUDY OF TAPE HANDLING PROCEDURES IN ORDER TO SAVE THE EMBARRASSMENT THAT MAY ATTEND INJUDICIOUS TAPE ASSIGNMENTS (E.G.- REWINDING THE LABORATORY BCD OUTPUT TAPE AND USING IT FOR SCRATCH, OR TRYING TO WRITE ON THE SHOP MONITOR).. TO AID IN TAPE HANDLING, SECTION 1.0 DESCRIBES VARIOUS TAPE ASSIGNMENTS SCHEMES THAT ARE IN USE. CONSIDERATION FOR USE IN OTHER SHOPS MAY REQUIRE CONSULTATION WITH THE SYSTEM PROGRAMMERS IN THOSE SHOPS. IN THESE CASES, STUDY OF APPENDIX IX (SECTION 3.9) SHOULD REVEAL THE STEPS NECESSARY TO ACHIEVE MONITOR COMPATIBILITY.

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LOADER PROGRAM TO INITIATE X-RAY SYSTEM

THE FIRST LINK ON THE =X-RAY 63= SYSTEM TAPE IS CALLED =LOADER=. THIS LINK SERVES TWO PURPOSES- FIRST IT IS UTILIZED BY =B5CARD=, =B5PUNT=, =B5BELL=, =B5IBSY=, OR ANY OTHER MONITOR SPECIFIC X-RAY SYSTEM CALLING PROGRAM THAT MAY BE WRITTEN TO INITIATE EXECUTION OF THE X-RAY SYSTEM. WHEN THE X-RAY SYSTEM TAPE IS MOUNTED ON B5, REWOUND, AND THEN THE FIRST TWO RECORDS READ, CONTROL IS SENT TO THE ENTRY POINT OF =LOADER=. =NTIN= THE BCD INPUT TAPE IS THEN READ FOR THE FIRST CONTROL CARD. EXECUTION THEN PROCEEDS FROM THIS POINT.

THE SECOND, AND PERHAPS MORE INTERESTING FEATURE OF =LOADER= IS ITS ABILITY TO RECOGNIZE A =LOADER= CARD AND THEN GENERATE A NEW SYSTEM TAPE ON ANOTHER UNIT. IF THE GENERATION IS SUCCESSFUL, =LOADER= TURNS CONTROL OVER TO THE =NEW= SYSTEM. THIS FEATURE PROVIDES A WAY OF ADDING REPLACING OR PATCHING ANY OR ALL OF THE LINKS IN THE =CALLER= DICTIONARY (SEE APPENDIX V). THUS THIS FEATURE IS USED FOR SPECIAL WORK OR FOR SYSTEM UPDATING.

A PROGRAM OF THE SYSTEM MUST MEET SEVERAL FUNDAMENTAL REQUIREMENTS-

(1) THE FIRST 112 LOCATIONS OF HIGH COMMON STORAGE MUST BE RESERVED AND PROTECTED FOR THE EXCLUSIVE USE OF THE SYSTEM. THIS MEANS THE INCLUSIVE OCTAL LIMITS 77461 THROUGH 77302. TO INCLUDE A PROGRAM IN THE SYSTEM ONE MUST BE AWARE OF THE QUANTITIES STORED IN THIS REGION (SEE APPENDIX VIII).

(2) THE FIRST EXECUTABLE STATEMENT OF THE MAIN PROGRAM MUST BE-

```
1   CALL CALLER (6HXXXXXX)
WHERE =XXXXXX= IS A VALID LINK LABEL OF THE
=CALLER= DICTIONARY (SEE APPENDIX V).
```

IF THERE IS ANY INFORMATION TO BE PICKED UP FROM THE CALLING CARD THE STATEMENT =CALL CALLER (6HXXXXXX)= MUST BE FOLLOWED BEFORE ANY OTHER CARDS ARE READ BY MEANS OF A CALL CALLER(...) STATEMENT. THIS IS DONE BY-

```
READ 1, . . . .
WHERE =1= IS THE FORMAT OF THE CALLING CARD.
```

(3) ALL INPUT/OUTPUT MUST BE DONE BY STATEMENTS WHICH USE AN APPROPRIATE TAPE DESIGNATION IN THE LIST OF TAPES (REFER TO 1.0-B2 FOR DETAILS). FURTHERMORE ANY TIME ONE WRITES ON THE BCD OUTPUT TAPE =NTOUT=, THE SUBROUTINE =LINES= (AN ENTRY OF =CALLER=) SHOULD BE CALLED IN ORDER TO KEEP PAGINATION NEAT. THIS SUBROUTINE HAS SEVERAL VERY PLEASANT FEATURES-

CALL LINES(2) FOR ANY =HO= FORMATS.

CALL LINES (N) FOR A CALCULATED REPETITIVE FORMAT.

LINCT = 0 TO OBTAIN NEW RESTORED PAGE TO START LIST

WRITE OUTPUT TAPE NTOUT,2 IF NO NEW PAGE WANTED (PRECEEDED BY =CALL LINES (2)= OR =CALL LINES (N)=).

IF (LINES(N)) HEAD, LIST, HEAD MAKES IT POSSIBLE TO HEAD A LISTING AT THE TOP OF EACH PAGE. IF N LINES WILL NOT FIT ON A PAGE THE PAGE IS RESTORED, THE LINE COUNT RESTORED TO =LINMX= AND THEN DECREMENTED BY =N= AND NON-ZERO RETURNED IN THE =IF= STATEMENT. IF THERE IS ROOM ON THE PAGE FOR THE LINE, THE LINE COUNT IS DECREMENTED AND ZERO IS RETURNED. AT =HEAD= OF COURSE A =CALL LINES(M)= KEEPS THE COUNT CORRECT. EXAMPLE-

```
      DO 5 J = 1,NM
      IF (LINES(1)) 1, 3, 1
1     CALL LINES(2)
      WRITE OUTPUT TAPE NTOUT,2
2     FORMAT (3HO A )
3     WRITE OUTPUT TAPE NTOUT,4,A(J)
4     FORMAT (1XF3.0)
5     CONTINUE
```

(4) ALL CARD INPUT FROM =NTIN= MUST BE DONE THROUGH THE =IFFI= ENTRY IN =CALLER=. THIS GIVES =CALLER= THE OPPORTUNITY TO FIND SYSTEM INSTRUCTION CARDS (SEE 1.0-A4). THE FOLLOWING IS AN EXAMPLE OF ONE WAY IN WHICH =IFFI= (MNEMONIC FOR =IF FRIEND OR FOE INPUT=) MAY BE USED. IT MUST BE STRESSED THAT THIS SUBROUTINE HAS MANY VARIED APPLICATIONS.

EXAMPLE 1- =ATCN= CARDS ARE TO BE LOADED AND EXECUTION STARTED UPON ENCOUNTERING AN =END= CARD. ANY OTHER CARDS MUST BE TREATED AS REASON TO CALL =EXIT=.

```
    1   CALL IFFI (KZZ, 4HATOM, 3HEND)
        GO TO (11, 101, 9975), KZZ
   11   READ 12, ATOMID, X, Y, Z, B, MULT
   12   FORMAT (7XA6, 3F8.4, F6.3, F5.2, 3F8.5)
        .
        .
        .
        GO TO 1
  101   CONTINUE
        .
        .
        .
        GO TO 1
 9975   CALL EXIT
```

EXAMPLE 2- ONLY A SINGLE =CELL= CARD IS PERMITTED AT THIS POINT

```
    1   CALL IFFI(KZZ, 4HCELL)
        GO TO (11, 9975), KZZ
   11   READ
   11   READ 12, ....
   12   FORMAT (7XA6, 3F8.3, 3F9.5, F7.0)
        .
        .
        .
  101   CONTINUE
        GO TO ....
 9975   CALL EXIT
```

NOTE THAT =CALLER= WRITES THE CARD ORDER DIAGNOSTIC SO THAT A SALUTORY OR INSULTING GOOD-BYE IS OPTIONAL BEFORE CALLING =EXIT=. IT IS HOWEVER USUALLY APPROPRIATE TO PRINT AS MUCH SUMMARY INFORMATION AS POSSIBLE FOR DIAGNOSTIC PURPOSES ON THE WAY OUT.

(5) AN IRRECONCILABLE ERROR SHOULD AFTER AN APPROPRIATE COMMENT, CALL =EXIT=. WHENEVER A SUCCESSFUL CALCULATION IS CARRIED OUT THE PROGRAM SHOULD TRANSFER BACK TO STEP 1 =CALL CALLER(6HXXXXXX)=.

TO SUMMARIZE-

(1) ALL MAIN PROGRAMS OF LINKS MUST CALL =CALLER=.
(2) HIGH COMMON MUST BE PROTECTED AND USED.
(3) READ ALL CARDS THROUGH =IFFI=.
(4) TAPE DESIGNATIONS MUST BE CAREFULLY OBSERVED.
(5) FOR CORRECT PAGINATION =LINES= SHOULD BE USED.
(6) CALL =EXIT= FOR BAD END, CALL =CALLER= FOR HAPPY END.

ONCE A BINARY DECK HAS BEEN ASSEMBLED WITH ALL THE ROUTINES IT CALLS, SAVE THOSE IN THE SYSTEM UTILITY SUBROUTINE PACKAGE (DESIGNATED BY THE =BEGIN= CARD IN AN INITIAL SYSTEM LOAD), THIS DECK MAY BE PLACED ON THE SYSTEM TAPE BY MEANS OF =LOADER= IN ONE OF TWO WAYS-

(1) IT MAY BE INSERTED BY UTILIZING THE FOLLOWING CARD ORDER (SEE 2.1-81 FOR CARD FORMATS)-

```
LOADER
LINK
  (BINARY DECK WHICH MAKES UP THE SPECIFIED LINK)
END
```

IF THE LOADING IS SUCCESSFUL THE PROGRAM MAY THEN BE EXECUTED FROM THE NEW SYSTEM TAPE.

(2) IT MAY BE LOADED ALONG WITH THE WHOLE SYSTEM FROM CARDS WHICH INCLUDE THE =BEGIN= DECK OF THE UTILITY SUBROUTINE PACKAGE-

```
LOADER
BEGIN
  (BINARY DECK OF UTILITY SUBROUTINE PACKAGE)
LINK
  (BINARY DECK WHICH MAKES UP THE SPECIFIED LINK)
LINK
  (BINARY DECK WHICH MAKES UP THE SPECIFIED LINK)
LINK
.
.
.
END
```

AT THE TIME =LOADER= IS EXECUTED A STORAGE MAP IS PREPARED GIVING THE RELOCATED ENTRY POINT OF ALL SUBROUTINES AS WELL AS THEIR RELOCATION INCREMENT, AND, IF NECESSARY, ANY DIAGNOSTIC REMARKS. THE GENERATED PROGRAM TAPE WILL BE USED FOR EXECUTION ONLY IF GENERATION IS SUCCESSFUL IF IT FAILS, EXECUTION WILL CONTINUE FROM THE OLD PROGRAM TAPE (N.B.- USE ==DATA= CARD WITH CARE).

PROGRAM FOR THE CALCULATION OF STRUCTURE FACTORS (LINK 1000)

THE BASIC PROGRAMMING OF THE STRUCTURE FACTOR PROGRAM WAS DONE BY JAMES M. STEWART AT THE OHIO STATE UNIVERSITY DURING 1958-1960 FOR THE IBM 704. THIS PROGRAM WAS WRITTEN FOR THE IBM 709 BY JAMES M. STEWART AND DARRELL HIGH AT THE UNIVERSITY OF WASHINGTON DURING 1960-1962.

THE STRUCTURE FACTOR CALCULATION IS ACCOMPLISHED BY TWO PROGRAMS AND THEIR SUBROUTINES- A PARAMETER LOADING PROGRAM =FCONE= (OR, FC ONE), AND A TAPE WRITING AND STATISTICS CALCULATING PROGRAM =FCTWO= (OR, FC TWO).

THE PARAMETER LOADING, CHECKING, AND STORING PROGRAM, =FCONE=, READS ATOM PARAMETER DATA, USUALLY FROM CARDS ALTHOUGH RESULTS FROM A CYCLIC REFINEMENT SEQUENCE ON TAPE WILL ALSO BE ACCEPTED. THE POSITIONAL PARAMETERS MAY BE IN FRACTIONAL CELL COORDINATES (IN AN =ATOM= CARD) OR IN FOURIER GRID COORDINATES (IN AN =ATOMG= CARD). AN OVERALL ISOTROPIC TEMPERATURE FACTOR, WHEN USED, IS PUNCHED IN A =B= CARD. INDIVIDUAL ATOM ISOTROPIC TEMPERATURE FACTOR COEFFICIENTS MAY BE PUNCHED IN THE =ATOM= OR =ATOMG= CARDS, OR IN =B= CARDS. THE PROGRAM WILL RECOGNIZE VARIOUS INDIVIDUAL ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS BY THE CARD NAMES-

=BETA= WHERE BETA(I,J) = 2*(PI**2)*(A(I)STAR)*(A(J)STAR)*U(I,J)
AND T = EXP**-(BETA(1,1)*H**2+....+2*BETA(1,3)*H*L)

=BIJ= WHERE B(I,J) = 8*(PI**2)*U(I,J)

=BNORM= WHERE THE FACTOR IS EXPRESSED IN TERMS OF B(I) USING THREE PRINCIPAL AXES OF THE ELLIPSOID OF VIBRATION, AND E(I,J) VECTORS EXPRESSING THE AXIAL DIRECTIONS OF THE VIBRATION ELLIPSOID.

=BNORMG= SIMILAR TO =BNORM= WITH COEFFICIENTS BASED ON GRID POINTS.

=UIJ= RMS AMPLITUDE OF VIBRATION IN THE CRUICKSHANK FORMAT (REF. 1).

ANISOTROPIC TEMPERATURE FACTORS ARE CONVERTED INTERNALLY TO THE FORM CORRESPONDING TO =BETA= FOR COMPUTATIONS, AND TO =BIJ= FOR OFF-LINE LISTING.

THE PROGRAM WILL ACCEPT MIXED ISOTROPIC-ANISOTROPIC DATA- ISOTROPIC COEFFICIENTS ARE PUNCHED IN THE =ATOM= CARD OR IN =B= CARDS, AND THE ANISOTROPIC COEFFICENTS ARE PUNCHED IN A TEMPERATURE FACTOR CARD JUST FOLLOWING THE =ATOM= CARD TO WHICH IT APPLIES.

A NUMBER OF RULES APPLY TO THE SELECTION OF TEMPERATURE FACTOR DATA BY THE PROGRAM-

(1) IF A TEMPERATURE FACTOR CARD IS READ BEFORE ANY =ATOM= OR =ATOMG= CARDS, THE PROGRAM IS AUTOMATICALLY PLACED IN THE OVERALL TEMPERATURE FACTOR MODE AND ANY OTHER TEMPERATURE FACTOR DATA SUPPLIED ARE IGNORED.

(2) IF AN =ATOM= OR =ATOMG= CARD IS READ FIRST, THE PROGRAM IS AUTOMATICALLY PUT INTO INDIVIDUAL ATOM TEMPERATURE FACTOR MODE AND VALID TEMPERATURE FACTOR COEFFICIENTS MUST BE SUPPLIED FOR EACH ATOM.

(3) A FOLLOWING TEMPERATURE FACTOR CARD SUPERCEDES THE VALUE OF =B= (IF ANY) PUNCHED IN THE PRECEDING =ATOM= OR =ATOMG= CARD.

(4) IN THE INDIVIDUAL ATOM TEMPERATURE FACTOR MODE WITH SEPARATE CARDS, THE ATOM IDENTIFICATION PUNCHED IN THE TEMPERATURE FACTOR CARD MUST BE IDENTICAL WITH THE IDENTIFICATION CODE PUNCHED IN THE =ATOM= OR =ATOMG= CARD PRECEEDING TO WHICH THE TEMPERATURE FACTOR APPLIES. MOREOVER, THE TEMPERATURE FACTOR CARD MUST FOLLOW DIRECTLY AFTER ITS =ATOM= OR =ATOMG= CARD.

IN ORDER TO UTILIZE THE NUMBERS STORED BY DATA REDUCTION THE FIRST SEVEN RECORDS FROM THE =REFLECTION TAPE= ARE READ. THESE RECORDS CONTAIN THE FOLLOWING DATA (SEE APPENDIX IV, SECTION 3.4, FOR DETAILS)-

RECORD	NUMBER OF WORDS	CONTENTS
1	63	COMPOUND AND TAPE ID, CELL CONSTANTS.
2	3 TO 18	BCD EQUIVALENCE TABLE OF ATOM TYPE CODES.
3	33	TEMPLETON DISPERSION CORRECTIONS.
4	15 TO 578	SYMMETRY OPERATIONS FOR SPACE GROUP.
5	149	F-RELATIVE SCALE FACTORS.
6	19 MINIMUM	ATOM POSITIONAL AND TEMPERATURE FACTOR PARAMETERS.
7	10	FLAG TO INDICATE NEXT RECORD CONTAINS REFLECTION DATA AND MAXIMUM VALUES OF H, K, AND L.

AT THIS TIME, THE ATOM PARAMETERS FROM INPUT =ATOM= AND TEMPERATURE FACTOR CARDS ARE WRITTEN ON RECORD 6 OF THE BINARY OUTPUT TAPE, =ATOMG= CARD DATA ARE CONVERTED TO FRACTIONAL CELL COORDINATES BEFORE WRITING.

THE STATISTICS COMPUTING PROGRAM, =FCTWO=, CALLS THE SUBROUTINE =GENRAT= WHICH GENERATES THE SYMMETRIC ATOMS FROM THE SYMMETRY OPERATIONS WRITTEN ON THE =REFLECTION TAPE= AT DATA REDUCTION TIME.

DURING OPERATION, =FCTWO= CALLS =FCALC= WHICH CLEARS SUMS FOR R, K, ETC. IT THEN SETS THE INDEXING INSTRUCTIONS BASED ON THE TYPE OR TYPES OF TEMPERATURE FACTORS INVOLVED. A SET OF CODE WORDS IN MEMORY CALLED =CALCOS(J)= ARE QUERIED AND SWITCHES WHICH BY-PASS UNNECESSARY PARTS OF THE PROGRAM ARE SET. THE =CALCOS(J)= ARE GIVEN IN MORE DETAIL IN APPENDIX III, SECTION 3.3, AND HAVE THE FOLLOWING FUNCTIONS (I.E.- CONTROL THE FOLLOWING CALCULATION ROUTES), WHERE EACH =CALCOS= HAS A YES-NO USAGE-

(1) ACENTRIC, OR CENTRIC CELL.

(2) OVERALL, OR INDIVIDUAL TEMPERATURE FACTOR.

(3) PARTIAL ATOM CONTRIBUTION TO BE APPLIED, WHERE ANY DESIRED SET OF ATOMS MAY BE TREATED AS =FIXED= AND THEIR CONTRIBUTION TO FC IS STORED ON THE REFLECTION TAPE.

(4) CONSIDER VALUE OF FC FROM PREVIOUS CALCULATION AS A PARTIAL ATOM CONTRIBUTION.

(5) ISOTROPIC ONLY, OR MIXED ISOTROPIC-ANISOTROPIC TEMPERATURE FACTORS.

(6) =HI-FI= (5 DECIMAL PLACE), OR =LO-FI= (3 DECIMAL PLACE) TRIG AND EXPONENTIAL FUNCTIONS, WHERE THE LATTER HAS ADVANTAGE OF GREATER COMPUTING SPEED AND HAS ADEQUATE ACCURACY FOR MOST STAGES OF REFINEMENT.

(7) NORMAL (I.E.- 1,2,4,8), OR UNUSUAL SCALING OF FC TO ACCOUNT FOR CENTERING, SPECIAL POSITIONS, ETC.

(8) SOME ATOMS REQUIRE DISPERSION CORRECTION.

(9) SOME ATOMS REQUIRE INDIVIDUAL SCALE FACTOR.

(10) SOME REFLECTION DATA EDITING NEEDED.

(11) USE THE INCLUDED =USER PATCH= SUBROUTINE.

(12) APPLY LEVEL-BY-LEVEL F-RELATIVE RESCALING.

(13) AUTOMATIC SCALING OF ATOMS AT SYMMETRY CENTERS.

(14) OBTAIN LEAST SQUARES REFINEMENT OF OVERALL ISOTROPIC TEMPERATURE FACTOR.

AFTER THE =CALCOS(J)= CODES HAVE BEEN INTERPRETED, THE STRUCTURE FACTOR SUB-PROGRAM =FCALC= CARRIES OUT THE CALCULATIONS (EQUATIONS 1-5) NECESSARY TO OBTAIN THE STRUCTURE FACTOR. FOR EACH REFLECTION, IF (FOR EXAMPLE) NEITHER =H= NOR =K= INDICES HAVE CHANGED, ONLY =LZ= IS COMPUTED TO OBTAIN THE ARGUMENT (H*X(1) + K*Y(1) + L*Z(1)). FURTHER, THE ATOMIC SCATTERING FACTOR IS NOT MULTIPLIED UNTIL A DIFFERENT ATOM TYPE IS SENSED BY THE PROGRAM. FROM THE FOREGOING THERE EMERGE TWO POINTS WHERE SPEED IS OF PRIMARY CONCERN. NEITHER CONDITION, HOWEVER, IS MANDATORY TO THE CORRECT CALCULATION OF THE STRUCTURE FACTOR BUT COMPUTATION TIME WILL BE MEASURABLY SHORTENED IF THERE ARE MANY ATOMS IN THE CELL.

(1) THE =ATOM= (AND CORRESPONDING TEMPERATURE FACTOR) CARDS SHOULD BE ORDERED IN GROUPS OF ATOM TYPES (I.E.- ALL ATOMS WITH THE SAME SCATTERING FACTOR SHOULD BE LOADED TOGETHER).

(2) AT DATA REDUCTION TIME, THE REFLECTIONS SHOULD BE SORTED SO THAT INDICES CHANGE AS LITTLE AS POSSIBLE.

THERE IS NO PRACTICAL LIMIT TO THE NUMBER OF REFLECTIONS THAT MAY BE HANDLED SINCE PROVISIONS HAVE BEEN MADE FOR FILES OF REFLECTION TAPES

SHOULD THE VOLUME OF DATA AVAILABLE COMPLETELY FILL A TAPE. THERE IS A LIMIT OF 64 FACTORS FOR SCALING LEVELS AND HENCE A LIMIT OF 64 LEVELS OR GROUPS OF REFLECTIONS.

THERE IS A FURTHER RESTRICTION OF 16 DIFFERENT ATOM TYPES FOR THE ATOMIC SCATTERING FACTOR DATA. PROVISION HAS BEEN MADE FOR SCALING SCATTERING FACTOR DATA FOR EACH ATOM IN ORDER TO TAKE CARE OF ATOMS AT SYMMETRY CENTERS (WHICH CAN BE CODED TO BE DONE AUTOMATICALLY BY =CALCOS(13)=), OR ANY OTHER SCALING REQUIREMENT. EACH ATOMIC FORM FACTOR AS STORED ON THE REFLECTION TAPE HAS ONLY ONE SCALE. THEREFORE, IF ANY ATOM-TYPE IS LOCATED IN A GENERAL POSITION AND AT A SYMMETRY CENTER, DUPLICATE SCATTERING FACTOR DATA MUST BE STORED ON TAPE AT DATA REDUCTION TIME OR ELSE INDIVIDUAL ATOM SCALE FACTORS WILL BE ASSIGNED BY THE =FC= PROGRAM.

THE ALGORITHM USED IN THE FC PROGRAM IS ONE IN WHICH ATOMS ARE GENERATED SO THAT ATOMS IN SPECIAL POSITIONS ARE DETECTED AND THE SUPERFLUOUS ONES ARE DISCARDED. NOTE FURTHER THAT IN THE SYSTEM =ONFLS= LEAST SQUARES PROGRAM =REFLECTIONS= ARE GENERATED SO THAT ONE MAY HAVE TO TAKE PRECAUTIONS WITH RESPECT TO SCATTERING FACTOR SCALE WHEN USING THAT PROGRAM. IT MAY BE FOUND USEFUL AT DATA REDUCTION TIME TO PLACE ADDITIONAL SCALED SCATTERING FACTOR DECKS FOR USE WITH ATOMS AT SPECIAL POSITIONS. THESE EXTRA SCATTERING FACTORS WILL BE UNNECESSARY AND UNWANTED FOR THIS FC PROGRAM BUT MAY BE USEFUL AND NEEDED FOR THE LEAST-SQUARES PROGRAM.

THE ATOMIC FORM FACTOR SCALING FEATURE FACILITATES CALCULATIONS FOR STRUCTURES CONTAINING VARIATE ATOM EQUI-POINTS. IT IS MORE CONVENIENT, AND REDUCES COMPUTING TIME, IF A WEIGHTED SCATTERING FACTOR DECK IS PREPARED AT DATA REDUCTION TIME SINCE ONLY ONE =ATOM= WOULD THEN HAVE TO BE CALCULATED AT EACH EQUI-POINT.

EACH OF THE ATOM-TYPE SCATTERING FACTORS MAY HAVE THE TEMPLETON DISPERSION CORRECTION (2,3) APPLIED AS DESIRED IF THESE CORRECTION DATA HAD BEEN STORED ON THE REFLECTION TAPE DURING DATA REDUCTION. THE

SCATTERING FACTOR IS GIVEN BY EQUATION 6. FOR THIS CORRECTION, THE MAGNITUDE OF FC WHICH IS TO BE COMPARED WITH THE EXPERIMENTAL VALUE IS GIVEN BY EQUATION 7, THE CORRECT COEFFICIENT FOR ELECTRON-DENSITY MAPS IS GIVEN BY EQUATION 8, AND THE AMPLITUDE FOR DIFFERENCE SYNTHESES IS GIVEN BY EQUATION 9.

THE LIMIT TO THE NUMBER OF NON-EQUIVALENT ATOMS WHICH MAY BE CALCULATED DEPENDS UPON THE SUBROUTINES USED BY THE PROGRAM AND THE NUMBER AND COMPLEXITY OF THE USER-SUPPLIED ROUTINES. THERE ARE APPROX. 22,000-24,000 CELLS AVAILABLE IN MEMORY FOR THIS ATOM PARAMETER DATA- THE NUMBER OF ATOMS BEING DETERMINED BY THE TEMPERATURE FACTORS.

TEMPERATURE FACTOR	STORAGE REQUIREMENTS	APPROX. NO. OF ATOMS
OVERALL ISOTROPIC	9 CELLS/ATOM	2444-2666
INDIVIDUAL ISOTROPIC	10 CELLS/ATOM	2200-2400
INDIVIDUAL ANISOTROPIC	22 CELLS/ATOM	1000-1090

THIS LIMITIATION ON THE NUMBER OF NON-EQUIVALENT ATOMS CAN BE READILY OVERCOME BY ANY MULTIPLE BY THE USE OF A =PARTIAL CONTRIBUTION= CALCULATION IN A MULTI-PASS METHOD. CALCOS(4) CAN BE CODED SO THAT THE FC OBTAINED FROM ONE PASS CAN BE CONSIDERED AS A PART OF THE TOTAL CONTRIBUTION TO THE FINAL FC. THIS PARTIAL CONTRIBUTION IS ADDED TO THE VALUE OBTAINED IN A SECOND PASS, AND THE TOTAL MAY, IF NECESSARY, THEN BE CONSIDERED A PARTIAL CONTRIBUTION TO A THIRD PASS, ETC., AD ABSURDUM.

THE USE OF THE =PARTIAL CONTRIBUTION= MODE IS MORE OFTEN USED IF A GROUP OF ATOMS ARE TO BE =FIXED= IN PLACE (WHETHER AS ATOMS AT SPECIAL POSITIONS, OR A GROUP OF ATOMS IN A TRIAL STRUCTURE WHOSE PARAMETERS ARE NOT VARIED). THE CONTRIBUTION OF THESE =FIXED= ATOMS TO THE STRUCTURE FACTOR IS CALCULATED ON ONE PASS, AND ONLY THOSE ATOMS WHOSE TRIAL PARAMETERS ARE TO BE VARIED NEED BE CALCULATED IN ALL SUBSEQUENT COMPUTATIONS. THIS MODE WILL BE OF INCREASING USE WHERE PORTIONS OF LARGE MOLECULES ARE FIXED WHILE VARIOUS TRIAL STRUCTURES FOR THE REMAINING ATOMS ARE CALCULATED.

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WHEN THE CALCULATION FOR A GIVEN REFLECTION IS COMPLETE THE RECORD IS WRITTEN OUT, THE STATISTICS COMPILED AND THE NEXT REFLECTION READ. WHEN THE PROGRAM ENCOUNTERS AN =END-OF-REFLECTION= RECORD ON THE TAPE THE CALCULATION OF STRUCTURE FACTORS IS TERMINATED.

=FCTWO= COMPLETES THE COMPUTATION BY WRITING OUT REFLECTION COUNTS AND NEW SCALE FACTORS FOR EACH LEVEL. IT IS POSSIBLE TO MAINTAIN THE RELATIVE GROUP-TO-GROUP SCALING, AND APPLY AN OVERALL MULTIPLICATIVE SCALE FACTOR CHANGE. THIS MEANS THAT THE GROUP-TO-GROUP RELATIVE SCALING DOES NOT CHANGE, ONLY THEIR MAGNITUDES. THE MULTIPLICATIVE SCALE FACTOR IS LOADED AFTER THESE GROUP-TO-GROUP FACTORS TO BE MODIFIED AND ANY SUBSEQUENTLY LOADED GROUP-TO-GROUP FACTORS WILL SUPERCEDE VALUES ALREADY STORED. THE FRONT OF THE BINARY TAPE IS REWRITTEN WITH THE NEW RESCALE FACTORS AND (IF OVERALL ISOTROPIC) THE LEAST SQUARES CHANGE IN OVERALL TEMPERATURE FACTOR. THE RELIABILITY INDEX, R, IS WRITTEN FOR EACH LEVEL AND FOR ALL DATA.

THE NEW SCALE FACTOR, K, IS OBTAINED FROM THE OLD SCALE FACTOR, K-PRIME, BY EQUATION 10, THE LEAST SQUARES CORRECTION TO THE OVERALL ISOTROPIC TEMPERATURE FACTOR IS COMPUTED BY MINIMIZING THE RESIDUAL IN EQUATION 11, AND THE RELIABILITY INDEX IS GIVEN BY EQUATION 12. FINALLY =FCTWO= PRINTS ON-LINE THE FINAL OVERALL VALUE OF =R= INDICATING THE COMPLETION OF THE CALCULATION.

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=ORFLS= BUSING-MARTIN-LEVY
FULL-MATRIX LEAST-SQUARES PROGRAM

THE FORTRAN CODING OF THE FULL-MATRIX LEAST-SQUARES PROGRAM BY W.R.BUSING, K.O.MARTIN, AND H.A.LEVY (ORNL-TM-305, OAK RIDGE NATIONAL LABORATORY) HAS BEEN MODIFIED TO CONFORM WITH THE =X-RAY 63= SYSTEM BY J.M.STEWART. REFERENCE TO THE OAK RIDGE REPORT WILL BE FOUND TO BE HELPFUL.

THE SYSTEM VERSION OF THIS PROGRAM RETAINS ONLY THOSE PARTS CONNECTED WITH FINDING DERIVATIVES, BUILDING THE MATRIX, AND DETERMINING THE SHIFTS IN ATOMIC PARAMETERS. NONE OF THE DATA CARDS OF THE ORIGINAL PROGRAM ARE USED BY THE SYSTEM VERSION. THE STRUCTURE FACTOR SECTION USES SEVERAL OF THE FEATURES OF THE =X-RAY 63= SYSTEM. THE NUMBER OF OBSERVATIONS IS LIMITED ONLY BY THE NUMBER OF REFLECTIONS THAT MAY BE STORED ON ONE REEL OF TAPE.

PATCHING FOR SPECIAL POSITIONS MAY BE CARRIED OUT IN THE SAME WAY AS DESCRIBED IN THE OAK RIDGE =ORFLS= WRITE-UP. THIS, HOWEVER, WILL NECESSITATE MAKING A SEPARATE SYSTEM TAPE FOR EACH COMPOUND THAT REQUIRES SPECIAL PATCHING (SEE =LOADER=, 1.0). AN IMPORTANT CHANGE WITH RESPECT TO PATCHING INVOLVES THE SUBROUTINES =ORPAC=, =ORRES=, AND =ORBET=, WHOSE CALLING SEQUENCES ARE NOW-

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CALL PATCH(IMSYM,I,TJ,HJ,HHJ,IREJKT,ATOM(1))
WHERE      IMSYM   IS THE NUMBER OF THE CURRENT SYMMETRY
                     OPERATION IN PROCESS

           IREJKT  IF RETURNED = 1 CAUSES CONTRIBUTIONS TO BE
                     MADE TO FC AND THE DERIVATIVES, WHILE IF = 2
                     CAUSES THE CONTRIBUTIONS FOR THE I,TH ATOM
                     GENERATED BY THE IMSYM,TH GENERATION TO BE
                     LEFT OUT.

           ATOM(I)   IS THE BCD DESIGNATION OF THE ATOM BEING
                     PROCESSED.

CALL RESETX(XYZ,ATOM,NA)
CALL RESTEB(BETA,ATOM,NA)
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THE SYSTEM VERSION OF =ORFLS= PERMITS 175 VARIABLES, 724 PARAMETERS, 60 ATOMS IN THE ASYMMETRIC UNIT, 64 SCALE FACTOR, AND 16 FORM FACTOR TYPES. FIXED ATOM CALCULATIONS ARE POSSIBLE SO THAT THESE RESTRICTIONS MAY BE MITIGATED BY LARGE BLOCK REFINEMENT.

THE LIST OF CONTROL CARDS REQUIRED HAS BEEN REDUCED SINCE THE MAIN CELL AND REFLECTION INFORMATION IS READ FROM THE SYSTEM BINARY TAPE =NTAPEA= AND AN UPDATED TAPE IS GENERATED AT THE END OF THE SPECIFIED NUMBER OF CYCLES ON =NTAPEB= FOR SUBSEQUENT USE (SIMILAR TO =ORXLS= AND EXACTLY LIKE =FOUREF=).

THE BINARY TAPE HAS STORED UPON IT ALL THE SCATTERING FACTOR, CELL, SYMMETRY, REFLECTION, AND PREVIOUS ATOM PARAMETER INFORMATION. =ORPRF= OF THE SYSTEM INITIALIZES THE PARAMETER REFINEMENT INDICATOR TO REFINE ON FC SCALE FACTORS, X, Y, Z, AND THE TEMPERATURE FACTORS OF ALL ATOMS IN THE ASYMMETRIC UNIT. =NOREF=, =REF=, =NOTEMP=, AND =NOSCALE= CARDS MAY BE USED TO CHANGE THESE INDICATORS AS DESIRED (E.G.- FOR REFINEMENT WHEN ATOM PARAMETERS ARE ALREADY ON TAPE AND THE SCALE FACTORS ARE TO BE HELD CONSTANT AN =ORFLS=, =NOSCAL=, AND =END= CARD ARE THE ESSENTIAL CARDS NEEDED BY =ORFLS=).

SUBROUTINES =ORFUN=, =ORIN=, OROUT=, =ORWT=, AND THE USUAL SYSTEM SUBROUTINES LIKE =CALLER=, =TIME=, ETC., HAVE BEEN ADDED TO THE ORIGINAL PROGRAM. =ORFUN= IS ANALOGOUS TO =FOFUN= OF THE FOURIER PROGRAM IN THAT IT UTILIZES THE SYMMETRY INFORMATION OF =GEN= OF DATA REDUCTION TO MAKE POSSIBLE THE GENERATION OF EQUIVALENT REFLECTIONS BY MEANS OF FOUR COMPUTED (GO TO),S PER REFLECTION. THUS THE FOURIER CODES SERVE FOR STRUCTURE FACTOR AND DERIVATIVE CALCULATIONS. =ORWT= CAUSES THE LATEST RESULTANT PARAMETERS TO BE WRITTEN ON THE FRONT OF THE OUTPUT TAPE =NTAPEB= TO SERVE AS INPUT TO SUBSEQUENT CYCLES (AS IN THE 704 ORXLS). IF ONE CHOOSES, =ATOM= AND =BIJ= CARDS MAY BE PUNCHED AT THE END OF EACH CYCLE AS INSURANCE AGAINST MATRIX SINGULARITIES OR NON-POSITIVE DEFINITE TEMPERATURE FACTORS.

THE FOLLOWING OPTIONS ARE NOW PROGRAMMED INTO =ORFLS=.

1. NUMBER OF CYCLES (MAXIMUM 9 PER =ORFLS= CARD). NOTE THAT AN R ((SUM DELTA F)/(SUM FC) FOR OBSERVED REFLECTION) GREATER THAN 0.60 WILL CAUSE ONLY ONE CYCLE TO BE CALCULATED. AN INCREASE IN R OF 0.04 WILL CAUSE CALCULATION TO TERMINATE AT THE END OF THE CYCLE IN WHICH THE INCREASE OCCURS. OF COURSE REFINEMENT CAN BE FORCED BY MORE =ORFLS= CARDS.

2. EITHER INDIVIDUAL ANISOTROPIC OR ISOTROPIC TEMPERATURE FACTORS MAY BE REFINED, BUT ONLY ONE MODE FOR ALL ATOMS IS PERMITTED. ALL REFERENCE TO AN OVERALL TEMPERATURE FACTOR HAS BEEN REMOVED. THE PROGRAM IS CODED TO CONVERT IN EITHER DIRECTION OR FROM MIXED MODE IF PREVIOUS CALCULATIONS WERE DONE ON THE SYSTEM FC PROGRAM. THE CONVERSION FROM ANISOTROPIC TO ISOTROPIC IS ACCOMPLISHED BY AVERAGING B11, B22, AND B33.

3. REFINEMENT MAY BE BASED ON F,F**2 OR F CORRECTED FOR DISPERSION. THE DISPERSION CORRECTION RATIOS ARE CALCULATED BY THE FC LINK AND UTILIZED BY ORFLS TO CORRECT F OBSERVED.

4. F RELATIVE SCALE FACTORS MAY BE LOADED FROM CARDS OR SPECIFIED TO BE TAKEN FROM THE SCALE OR RESCALE STORAGE OF THE BINARY TAPE (SEE FC WRITE-UP). SCALE FACTORS USED ARE SCALE FACTORS THAT APPLY TO F-RELATIVE SO THAT DURING EXECUTION OF THE LEAST-SQUARES REFINEMENT THE RECIPROCALS ARE COMPUTED. ALL OUTPUT HOWEVER NOW REFERS TO F-RELATIVE SCALE FACTORS.

SCALE FACTOR REFINEMENT IS HANDLED IN TERMS OF TWO SELECTION MECHANISMS. COLUMN 25 IN THE =ORFLS= CARD SPECIFIES WHETHER SCALE OR RESCALE FACTORS FROM THE BINARY INPUT TAPE ARE TO BE USED. =SCALE= CARDS MAY BE USED TO SUPERCEED OR ALTER THE BAND AS USUAL. =NOSCAL= CARDS SET THE REFINEMENT SWITCHES OF =ORFLS= ACCORDING TO THE FOLLOWING.....

A =NOSCAL= CARD BLANK OR ZERO IN COLS 17-20 SHUTS OFF ALL SCALE FACTOR REFINEMENT.

A = NOSCAL= CARD WITH -1 IN COLS 19-20 SETS REFINEMENT ON OVERALL LINEAR SCALE. ALL LEAST SQUARES GROUP BY GROUP SCALE REFINEMENT IS SHUT OFF.

A =NOSCAL= CARD WITH A SCALE GROUP NUMBER IN COLS 19-20 SHUTS OFF SC REFINEMENT FOR THE SPECIFIED GROUP.

WHEN NO =NOSCAL= CARD(S) IS INCLUDED.... SCALE FACTOR REFINEMENT WIL BE TURNED ON FOR ALL GROUPS ESTABLISHED AT DATA REDUCTION TIME.

AFTER REFINEMENT THE SCALE FACTOR BAND CONTAINS THE STARTING SCALE FACTORS SPECIFIED ON THE =ORFLS= CARD AND THE RESULTS OF THE FINAL CYCLE IN THE RESCALE BAND OF THE BINARY OUTPUT TAPE. IF THE CARD PUNCHING FUNCTION IS USED THE INTERMEDIATE RESULTS ARE PUNCHED.

5. TRIG FUNCTIONS MAY BE SPECIFIED TO BE EITHER THREE OR FIVE DECIMAL ACCURACY (LO-FI OR HI-FI).

6. EITHER THE WEIGHTS STORED ON =NTAPEA= OR UNIT WEIGHT MAY BE SPECIFIED.

7. THE PUNCHING OF =SCALE=, =ATOM=, AND =BIJ= (IF ANISOTROPIC) CARDS AT THE END OF EACH CYCLE MAY BE SPECIFIED. REMEMBER THAT IN THIS CASE THESE CARD IMAGES WILL APPEAR ON =NTAPEC=.
IN ADDITION TO PUNCHING INTERMEDIATE RESULTS THIS SWITCH MAKES POSSIBLE THE IGNORING OF NON POSITIVE DEFINITE TEMPERATURE PARAMETERS OR ELSE THE SETTING BACK TO POSITIVE DEFINITENESS ANY WHICH GO BAD.

8. ALL REFLECTION INFORMATION MAY BE LISTED DURING THE LAST CYCLE IF DESIRED. IF THIS SIGNAL IS =TURNED ON= THE CORRELATION MATRIX WILL BE LISTED AT THE END OF THE LAST CYCLE. THE CORRELATION MATRIX IS LISTED IN A =FOLDED= FORMAT IN WHICH EACH ROW IS NUMBERED WITH THE VARIABLE NUMBER AND STARTING FROM THE DIAGONAL ELEMENT AND GOING ACROSS THE COLUMNS TEN ON A LINE. CERTAIN OTHER LISTING FEATURES OF THE PROGRAM HAVE BEEN CHANGED TO CONFORM WITH THE SYSTEM (E.G.- TITLE HANDLING, PARAMETER LISTING, ETC.).

9. DURING EVERY CYCLE THOSE REFLECTIONS FOR WHICH THE WEIGHTED MAGNITUDE OF DELTA-F IS GREATER THAN RR MAY BE LISTED. THIS INDICATOR MAY ALSO BE USED TO CAUSE THE CORRELATION MATRIX TO BE LISTED AT THE END OF EACH CYCLE.

10. ONE MAY SPECIFY THAT A =FIXED ATOM= CALCULATION IS DESIRED. THE OPTIONS ARE THE SAME AS IN THE FC PROGRAM

(A) NO FIXED ATOM CONTRIBUTION.

(B) THE STORED VALUES FOR FIXED ATOMS AS ESTABLISHED BELOW IS TO BE USED AS THE FIXED ATOM CONTRIBUTION.

(C) THE PREVIOUS FC'S ON THE BINARY INPUT TAPE =NTAPEA= ARE TO BE USED AND THEIR VALUES ESTABLISHED AS THE FUTURE =FIXED ATOM= CONTRIBUTION FOR FUTUTRE FC'S.

11. THE OPTION OF TREATING NEUTRON DATA IS RETAINED.

12. IF A PARAMETER DAMPING OR ENHANCING FACTOR IS SPECIFIED AS A FLOAT. POINT NUMBER ALL PARAMETER SHIFTS WILL BE MULTIPLIED BY IT. THE FACTOR CAN NOT BE ZERO OR NEGATIVE.

13. A REJECTION RATIO (RR) MAY BE SPECIFIED TO ESTABLISH A CUT OFF FOR LISTIN REFLECTIONS WHOSE WEIGHTED DELTA-F IS LARGER THAN RR.

14. A LIMIT MAY BE SPECIFIED FOR THE WEIGHTED DELTA-F'S SUCH THAT ANY DELTA-F HIGHER THAN THIS LIMIT WILL BE REJECTED FROM CONSIDERATION DURING THE LEAST SQUARES CYCLE IN WHICH IT OCCURS.

15. THE NEED FOR PATCHING MAY BE SIGNALED.

THE PATCHING OF ORFLS FOR ATOMS IN SPECIAL POSITIONS REQUIRES CAREFUL CONSIDERATION. IN THE X-RAY 63 VERSION TWO WAYS MAY BE USED TO HANDLE THIS PESKY DETAIL. ONE IS TO FOLLOW THE BUSING-LEVY METHOD AS DESCRIBED IN THE OAK RIDGE REPORTS. THE OTHER IS TO USE THE ADDED TESTING FACILITIES OF THE =SYSTEM= TO THROW OUT REDUNDANT ATOMS. BOTH METHODS ARE ILLUSTRATED IN APPENDIX VII OF THIS MANUAL. IN EITHER CASE GREAT CARE MUST BE EXERCISED. THE ORDER OF THE SYMMETRY OPERATIONS, THE ATOMS, AND THEIR RELATIVE =SPECIAL= POSITION, THE POSSIBILITIES OF INDIVIDUAL ATOM SCALING, ALL NEED TO BE CONSIDERED. THE STRUCTURE FACTOR LINK (FC) WILL CALCULATE FOR ALL SPACE GROUPS AND IDENTIFY THE TYPE OF SPECIAL POSITION OF EACH ATOM. THIS MAY BE VERY HELPFUL IN PLANNING A PATCH FOR ORFLS.
BECAUSE FC AUTOMATICALLY THROWS OUT REDUNDANT ATOMS WHEN ONE CHOOSES TO PATCH ORFLS BY THE SETTING BACK OF H, K, AND L THE TWO PROGRAMS MAY NOT AGREE UNLESS TWO DIFFERENT SETS OF ATOM CARDS ARE USED. ONE FOR THE FC PROGRAM ANOTHER FOR ORFLS.

FOURIER SYNTHESIS PROGRAM (LINK 4000)

THE INITIAL PLAN FOR PROGRAMMING THE FOURIER SYNTHESIS PROGRAM WAS WORKED OUT BY LYLE H. JENSEN AND DARRELL F. HIGH. THE INITIAL PROGRAMMING WAS DONE BY DARRELL F. HIGH AND BROUGHT TO ITS PRESENT FORM BY JAMES R. HOLDEN AND JAMES M. STEWART.

THE REFINEMENT OF CRYSTAL STRUCTURES IS FACILITATED BY USE OF FOURIER TRANSFORMS. COCHRAN AND LIPSON (1), BUERGER (2), AND MANY OTHERS SUPPLY INFORMATION ON THE USE OF THIS VALUABLE TECHNIQUE. THIS FOURIER PROGRAM WAS DESIGNED TO HAVE A NUMBER OF FEATURES-

(A) AUTOMATIC OPERATION FOR ALL SPACE GROUPS.

(B) ANY CONVENIENT GRID (I.E.- 1/60, 1/13, 1/373 - SUB-DIVISIONS OF AXIS ARBITRARY WITHIN LIMITS 1 TO 1/2627 IN FIRST DIRECTION, 1/400 IN SECOND, AND 1/200 IN THIRD DIRECTION).

(C) PRINT OUT OF FOURIER MAP READY TO BE CONTOURED. WITH SUPPRESSION OF BACKGROUND TO FACILITATE THIS OPERATION OR PERHAPS ELIMINATE ITS NECESSITY.

(D) MANY EASILY SWITCHED OPTIONS FOR COEFFICIENTS.

(E) REASONABLE SPEED.

(F) NO RESTRICTIONS ON REFLECTION ORDER (EXCEPT FOR MAXIMUM SPEED).

(G) PREPARE A BINARY TAPE OF THE MAP TO SERVE AS INPUT TO OTHER ROUTINES.

A PAPER BY JURG WASER (3) AND A MONOGRAPH BY LIPSON AND TAYLOR (4) SERVE TO POINT THE WAY IN WHICH CONDITION (A) MAY BE MET. A SYMMETRY RELATIONSHIP IN REAL SPACE CAUSES AN EQUIVALENT SYMMETRY RELATIONSHIP IN RECIPROCAL SPACE, THE TRANSPOSED ROTATION MATRIX BEING APPLIED TO THE INDICES H, K, AND L, AND THE TRANSLATION FORMING A =FRINGE FUNCTION= WHICH MODIFIES THE PHASE. THE ACTUAL FOURIER SUMMATION IS ACCOMPLISHED BY SUMMING ALL SPACE GROUPS AS IF THEY WERE TRICLINIC USING THE METHOD OF FACTORING SHOWN IN APPENDIX VII, SECTION 3.7.

THE REFLECTION TAPE, HOWEVER, CONTAINS ONLY A UNIQUE SET OF REFLECTIONS PLUS THE NECESSARY INDICATORS TO MAKE POSSIBLE THE AUTOMATIC GENERATION OF SYMMETRY-RELATED REFLECTIONS. SUBROUTINE =GENCHK= OF THE DATA REDUCTION PROGRAM =DATRON= ANALYZES THE SPACE-GROUP SYMMETRY OPERATIONS FOR A SET OF ROTATION MATRICES (R) AND TRANSLATION VECTORS (T) AND STORES THEM IN A FORM USEFUL TO SUBROUTINE =GEN=. =GEN= APPLIES THE GENERATIONS TO EACH UNIQUE REFLECTION AND BUILDS A SET OF CODES WHICH DEFINE FOR EACH REFLECTION THE OPERATIONS NECESSARY TO GENERATE THE SYMMETRICALLY RELATED REFLECTIONS. THE OPERATIONS MAY INCLUDE SIGN CHANGES AND PERMUTATIONS OF H, K, AND L, AND PHASE ROTATIONS OF A AND B. SUBROUTINE =FOFUN= USES THE OUTPUT OF =GEN= TO DELIVER THE CORRECT GENERATED SET (PROPERLY COMBINED A(H,K,L), A(-H,K,L), A(H,-K,L), A(H,K,-L) AND SIMILAR B TERMS ARE REQUIRED) TO =FOSUM= THE FOURIER SUMMATION PROGRAM.

THE CALCULATIONS ARE DONE BY FACTORING THE THREE-DIMENSIONAL SUMMATION INTO THREE ONE-DIMENSIONAL SUMMATIONS, AFTER THE MANNER OF BEEVERS AND LIPSON. SUMMATION IS CARRIED OUT OVER ONE HEMI-SPHERE OF RECIPROCAL SPACE, SYMMETRY-RELATED REFLECTIONS BEING GENERATED FROM A UNIQUE SET OF OBSERVATIONS.

THE SYMMETRY OPERATIONS OF THE SPACE-GROUPS MAY BE WRITTEN IN TERMS OF ROTATION MATRICES (R) AND TRANSLATION VECTORS (T) (SEE EQUATION 1). WASERS RESULT, IN MATRIX NOTATION, IS GIVEN IN EQUATION (2).

TABLE 1.40-I GIVES ALL THE ALLOWED VALUES FOR =FRINGE FUNCTIONS= IN THE CRYSTALLOGRAPHIC SPACE-GROUPS. ALSO TABULATED ARE THE EFFECTS OF THE REAL AND IMAGINARY PARTS OF F(H). IN ADDITION TO THE PHASE CHANGE, THE PROBLEM OF THE GENERATION OF THE SYMMETRICALLY RELATED INDICES (R-PRIME H) MUST BE HANDLED. TO THIS END =GEN= DETERMINES A NUMBER (JDESIG) FOR EACH ACCORDING TO TABLE 1.40-II. IN THIS TABLE, (KK) IS CARRIED IN THE REFLECTION RECORD AS A RESULT CALCULATED BY =GEN=. =FOFUN= CALCULATES A-PRIME AND B-PRIME UNDER DIRECTION OF (KK).

FOR NON-DIAGONAL ROTATIONS THE MAGNITUDE OF H,K,L AS WELL AS THE SIGNS WILL BE ALTERED - IN THIS CASE =GEN= PLACES THE VALUES OF THE MAGNITUDE OF H-PRIME,K-PRIME,L-PRIME BETWEEN EACH SET OF (KK)-S AND (JDESIG)-S.

THE MAXIMUM NUMBER OF (JDESIG)-S USED FOR ANY ONE REFLECTION IS FOUR, BUT THE PARTICULAR VALUES USED DEPEND ON THE SYMMETRY OPERATIONS USED AND THE SIGNS OF THE REFLECTION INDICES SUPPLIED. THE PROGRAM TREATS THE LAST FOUR BY CHANGING THE SIGN OF B-PRIME AND SUBTRACTING FOUR FROM (JDESIG), SINCE (B-PRIME(-H,-K,-L)) = -(B-PRIME(H,K,L)).

IN THE DISCUSSION THAT FOLLOWS, THE CONCEPT OF =SCANNING= OR =SUMMATION= ORDER WILL BE USED- THUS, H(1) IS THE INDEX SUMMED OVER FIRST AND X(1) THE CORRESPONDING COORDINATE WILL BE USED. IT VARIES FROM PAGE-TO-PAGE (SECTION-TO-SECTION) IN THE OUTPUT. SIMILARLY, H(2) IS SUMMED SECOND AND X(2) VARIES VERTICALLY (LINE-TO-LINE) DOWN THE PAGE, WHILE H(3) IS SUMMED THIRD AND X(3) VARIES HORIZONTALLY (POINT-TO-POINT) ALONG THE LINE. ON THE OTHER HAND, THE NOTATION X, Y, Z, AND H, K, L REPRESENTS THE COORDINATES AND INDICES REFERRED TO THEIR CONVENTIONAL AXES. PROGRAM INPUT IS ALWAYS IN TERMS OF THE CONVENTIONAL DIRECTIONS, THE SCANNING ORDER BEING SPECIFIED ON THE =LAYOUT= CARD. IT IS SOMETIMES NECESSARY, HOWEVER, TO CONSIDER THE SCANNING ORDER, ESPECIALLY WITH REGARD TO PROGRAM LIMITATIONS WHICH ARE DESCRIBED UNDER =FOSUM=.

DESCRIPTION OF THE FOURIER PROGRAM

THE PROGRAM IS COMPOSED OF FOUR SUBROUTINES- =FOURR=, =FOSUM=, =FOFUN=, AND =PATPAT=. A BRIEF DESCRIPTION OF THE FUNCTION OF EACH SUBROUTINE WILL BE GIVEN.

=FOURR=. THE MAIN PROGRAM AS FAR AS THE X-RAY PROGRAM SYSTEM IS CONCERNED (OR THE FORTRAN MONITOR WITH NON-SYSTEM USAGE). IT READS THE CONTROL CARDS AND STORES THEIR PARAMETERS FOR THE REST OF THE PROGRAM.

THE FOURIER CONTROLLER (=FOURR=) PROGRAM ALSO READS THE LEADING SEVEN RECORDS OF THE BINARY REFLECTION TAPE AND LOADS PERTINENT DATA (F(000), V, ETC.) STORED THEREON. IT CHECKS FOR CONSISTENCY OF SOME OF THE VARIABLES AND ASSIGNMENTS FROM INSTRUCTION CARDS TO REDUCE THE POSSIBILITY OF CHANCE ERRORS. ONCE THESE FUNCTIONS ARE TAKEN CARE OF THE =FOURR= PROGRAM CALLS =FOFUN= WHICH RETURNS CONTROL TO =FOURR= WHEN THE FOURIER IS COMPLETED. THE CONTROLLER WILL PERMIT MORE FOURIERS TO BE CALCULATED FROM THE SAME OR OTHER BINARY TAPES OR ELSE RETURN CONTROL TO FORTRAN-MONITOR THROUGH THE X-RAY SYSTEM =CALLER= FEATURE.

=FOFUN=. THE SUBROUTINE WHICH CALCULATES COEFFICIENTS FOR =FOSUM=. WHEN ENTERED THE FIRST TIME =FOFUN= SETS THE =CALCULATION TYPE= SWITCHES AND THEN CALCULATES THE PROPER VALUE FOR F(000) AND THE ELECTRON-DENSITY SCALE FACTOR. IT PERMITS THE USE OF A SUBROUTINE =PATPAT= (I.E.- FOURIER USER-S PATCH) WHICH ALLOWS ANY KIND OF COEFFICIENT MANIPULATION ONE MAY DESIRE TO WRITE A FORTRAN SUBROUTINE TO DO. =FOFUN= AS IT STANDS IS WELL ENDOWED WITH OPTIONS -- 14 IN ALL --

(1) USERS FUNCTION. BY MEANS OF SUBROUTINE =PATPAT=. (PRESENT FORM OF =PATPAT= PROGRAMMED ONLY FOR CONVENTIONAL VECTOR MAP (PATTERSON) AS OF 20 AUG. 1962).

(2) PATTERSON. A = (FO**2) AS COEFFICIENT.

(3) VECTOR MAP. SHARPENED, ORIGIN REMOVED PATTERSON.

(4) FO FOURIER. SUBSTITUTE FO/2 FOR LESS-THANS AND THEN TEST ALL REFLECTION- IF (FO * RR - ABSF(FC)) LESS THAN ZERO, THEN REFLECTION IS USED, WHERE (RR) IS A REJECTION RATIO SUPPLIED IN THE =FOURR= CARD. IF AN (RR) IS NOT SUPPLIED, (RR) IS ARBITRARILY SET EQUAL TO ZERO SO THAT ALL REFLECTIONS ARE USED. SUBSTITUTE FC FOR FO FOR EXTINCT REFLECTIONS (IF ANY).

(5) FO FOURIER. EACH FO IS CORRECTED FOR DISPERSION RATIO AND CRITERIA OF TYPE 4 USED. (FO * RATIO * RR - ABSF(FC)) LESS-THAN ZERO.

(6) FO FOURIER. PHASE ANGLES DETERMINED FROM E2, THE PHASE OF THE SCALED UNITARY STRUCTURE FACTORS. ONLY THOSE REFLECTIONS OF =KNOWN= PHASE (I.E.- E2 EQUAL TO OR LESS-THAN ONE CYCLE). CRITERIA OF TYPE 4 ARE USED, REJECTING ALL LESS-THANS.

(7) FC SYNTHESIS. USES ALL REFLECTIONS WITH MAGNITUDES AND PHASES OF THE CALCULATED STRUCTURE FACTORS AS AMPLITUDES.

(8) DELTA-F. TEST OBSERVED REFLECTIONS- IF (FO * RR * ABSF(FC)) LESS THAN ZERO, REFLECTION IS USED, WHERE (RR) IS A REJECTION RATIO SUPPLIED IN THE =FOURR= CARD. IF AN (RR) IS NOT SUPPLIED, (RR) IS ARBITRARILY SET EQUAL TO ZERO THUS MAKING A ZERO-PERCENT RULE. TEST LESS-THANS- IF (FO - ABSF(FC)) LESS-THAN ZERO REFLECTION IS USED. REJECTS ALL EXTINCT REFLECTIONS (IF ANY). (E.G.- RR = 0.50 IS 50-PERCENT RULE, AND RR = 1.00 IS 100-PERCENT RULE).

(9) DELTA-F. FOR OBSERVED REFLECTIONS, EACH DELTA-F IS MULTIPLIED BY THE LEAST SQUARES WEIGHT- (W * (FO - ABSF(FC))). TEST LESS-THANS- IF (FO - ABSF(FC)) LESS THAN ZERO, REFLECTION IS USED. REJECT ALL EXTINCT REFLECTIONS (IF ANY).

(10) DELTA-F. EACH FC IS CORRECTED FOR DISPERSION RATIO AND CRITERIA OF TYPE 8 IS USED- FOR OBSERVED (FO * RATIO * RR - ABSF(FC)) LESS THAN ZERO, REFLECTION IS USED. FOR UNOBSERVEDS (FO * RATIO - ABSF(FC)) LESS THAN ZERO, REFLECTION USED. REJECT ALL EXTINCT REFLECTIONS (IF ANY).

(11) DELTA-F. OBSERVED REFLECTIONS ONLY. REJECT ALL LESS-THANS AND EXTINCT REFLECTIONS (IF ANY).

(12) DELTA-F. VARIABLE WEIGHTING APPLIED- WHERE W = (ABSF(FC)/FO), TO ALL OBSERVED REFLECTIONS AND LESS-THANS WHERE (ABSF(FC) GREATER THAN FMIN). REJECT LESS-THANS WHERE (ABSF(FC) LESS THAN FMIN) AND ALL EXTINCTIONS (IF ANY).

(13) E MAP. USES SCALED UNITARY STRUCTURE FACTORS (E1) AS COEFFICIENTS. PHASES PREDETERMINED FROM KARLE-HAUPTMAN STATISTICS. REJECT ALL REFLECTIONS WITH UNDETERMINED PHASE, REJECT WHEN THE MAGNITUDE OF (E) IS LESS THAN (RR), REJECT ALL LESS-THAN REFLECTIONS.

(14) E MAP. PHASES FROM A STRUCTURE FACTOR CALCULATION. REJECT WHEN THE MAGNITUDE OF (E) IS LESS THAN (RR), REJECT ALL LESS-THAN REFLECTIONS.

ONCE THE CALCULATION SWITCHES ARE SET =FOFUN= READS, REFLECTION BY REFLECTION, THE UNIQUE SET SUPPLIED ON THE BINARY REFLECTION TAPE. IT WILL REJECT ANY REFLECTION HAVING A (SIN THETA)/LAMBDA OR H OR K OR L GREATER THAN SPECIFIED ON THE =MAXHKL= CARD OR THE VALUE STORED ON THE TAPE AT DATA REDUCTION TIME IF NO =MAXHKL= CARD USED. A PROVISION HAS BEEN MADE TO PERMIT MULTIPLE TAPES- LOW DENSITY TAPE WILL HOLD APPROXIMATELY 13,000 REFLECTIONS PER REEL. ON THE FIRST PASS DOWN THE BINARY TAPE THE BCD LIST OF FC MAY BE MADE BY =FOFUN= IF THE USER SO DESIRES. =FOFUN= LISTS ALL THE REFLECTIONS ON THE TAPE, AND IT FLAGS THOSE REFLECTIONS REJECTED WITH =R=. THE CORRECT COEFFICIENTS ARE FORMED FOR

THE CURRENT REFLECTION AND =FOSUM= IS CALLED IN TO CALCULATE FIRST SUMS. FOR A GENERAL REFLECTION - WITH OPTIMUM SORTING - THE CALLING OF =FOSUM= IS TABULATED IN TABLE 1.40-III (NO SORTING IS REQUIRED EXCEPT TO GAIN MAXIMUM COMPUTING SPEED). ONCE ALL THE REFLECTIONS ON THE BINARY TAPE HAVE BEEN TREATED, =FOFUN= CALLS =FOSUM= TO CALCULATE THE SECOND AND THIRD SUMS.

=FOSUM=. THE FOURIER CALCULATION SUBROUTINE WHICH DOES THE ACTUAL FOURIER SUMMATION. IT CONTAINS PROVISION FOR BREAKING THE SUMMATION UP INTO AN OPTIMUM NUMBER OF PASSES IF THE WHOLE CALCULATION CANNOT BE ACCOMPLISHED IN A SINGLE PASS OF THE REFLECTION TAPE. AT PRESENT THE FOLLOWING LIMITATIONS APPLY-

(A) THE PRODUCT OF THE (MAXIMUM VALUES + 1) OF THE SECOND AND THIRD SUMMATION INDICES MAY NOT EXCEED 5000 (E.G.- H(2)MAX EQUALS 99 AND H(3) MAX EQUALS 49, OR H(2)MAX EQUALS 77 AND H(3)MAX EQUALS 63, ETC.).

(B) THE PRODUCT OF THE (THIRD SUMMATION INDEX + 1) AND THE NUMBER OF POINTS ALONG THE SECOND SUM DIRECTION MAY NOT EXCEED 2000 (NOTE THAT THE NUMBER OF POINTS DOES NOT NECESSARILY OR USUALLY EQUAL THE SECOND SUM GRID SPECIFICATION) (E.G.- AN H(3)MAX EQUAL TO 49 LIMITS POINTS SUCH THAT X(2) COULD BE (0 - 1/4) IN 159THS, (0 - 1/2) IN 79THS, ETC.).

(C) THE FINEST GRID WHICH MAY BE CALCULATED IN THE FIRST SUM DIRECTION IS 1/2627, IN THE SECOND SUM 1/400, AND 1/200 IN THE THIRD SUM DIRECTION.

(D) THE ABOVE RESTRICTIONS MAY BE RESCINDED ONLY BY REASSIGNMENT OF STORAGE AND RECOMPILATION -- SEE PROGRAM STATEMENTS ANS COMMENTS FOR DETAILS (A PROGRAM LISTING TAPE MAY BE OBTAINED THROUGH J. M. STEWART.)

BECAUSE OF THE PARTICULAR METHOD OF SUMMATION A VERY LARGE NUMBER OF REFLECTIONS CAN BE ACCOMMODATED AND THERE IS NO RESTRICTION PLACED ON THE FIRST SUMMATION INDEX.

NO INTERMEDIATE TAPES ARE WRITTEN. THE MAIN PART OF THE MEMORY HOLDS

SECOND SUM COEFFICIENTS FOR AS MANY LEVELS AS POSSIBLE -- IF ALL LEVELS CANNOT BE PROCESSED IN ONE PASS =FOSUM= DIVIDES THEM INTO TWO EQUAL PASSES AND SO ON. DURING THE SECOND SUM ONLY THE THIRD SUM COEFFICIENTS FOR ONE LAYER ARE STORED AT ANY GIVEN TIME AND ONLY ONE LINE OF ELECTRON DENSITIES IS CARRIED IN STORAGE. AS SOON AS THE LINES ARE FORMED THEY ARE WRITTEN ON THE BCD OUTPUT TAPE. IT IS POSSIBLE TO SUPRESS PRINTING VALUES BETWEEN SELECTED POSITIVE AND NEGATIVE CUT-OFF POINTS BY THE USE OF A =MAP= CARD.

THE FOURIER SUMMATION PROGRAM OPERATES BY =FOURH= READING THE CONTROL CARDS AND CALLING =FOFUN=. =FOFUN= PERFORMS ANY NECESSARY INITIALIZATIONS -- INITIALIZES =FOSUM= -- AND CALCULATES THE FIRST SUM BY CALLING =FOSUM= TO DO THE ACTUAL SUMMATION. THE END OF THE DATA IS SIGNIFIED WHEN =FOFUN= READS THE END-OF-REFLECTIONS RECORD (101010000000) ON THE BINARY INPUT REFLECTION TAPE. =FOFUN= THEN RETURNS CONTROL TO =FOSUM= TO COMPLETE CALCULATION OF THE FIRST SUM AND TO DO THE SECOND AND THIRD SUMS. AFTER COMPLETION OF THE SECOND AND THIRD SUMS =FOSUM= RETURNS CONTROL TO =FOFUN= WHICH RETURNS CONTROL TO THE CONTROLLER. THE CONTROLLER SEES IF MORE PASSES ARE REQUIRED AND IF NOT RETURNS CONTROL TO =CALLER=.

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FOURIER REFINEMENT PROGRAM

THE FOURIER REFINEMENT PROGRAM WAS WRITTEN BY JAMES R. HOLDEN.

THE PROGRAM CALCULATES STRUCTURE FACTORS FOR A SET OF ATOMIC PARAMETERS (MAXIMUM = 100 ATOMS PER CELL, RESTRICTED TO OVERALL ISOTROPIC TEMPERATURE FACTORS). THE PROGRAM THEN CALCULATES A 27-POINT FOURIER BLOCK, USING OBSERVED STRUCTURE FACTORS ONLY (NO LESS-THANS OR EXTINCTIONS), ABOUT EACH ATOMIC POSITION. THE GRID INTERVAL IS SPECIFIED ON THE =CYCLES= CARD, IN WHICH THE NUMBER OF REFINEMENT CYCLES ARE ALSO SPECIFIED.

THE PEAK MAXIMUM WITHIN THE 27-POINT BLOCK IS FOUND, AND THE ATOMIC COORDINATES ARE SHIFTED TO THE POSITION OF THE MAXIMUM. IF THE PEAK MAXIMUM LIES OUTSIDE OF THE 27-POINT BLOCK, THE ATOMIC COORDINATES ARE SHIFTED TO THE POINT OF MAXIMUM ELECTRON-DENSITY WITHIN THE BLOCK. AS THE SHIFTS BECOME SMALLER, FOR EACH ATOM, THE PROGRAM WILL REDUCE THE SIZE OF THE GRID INTERVAL.

PROVISION IS MADE FOR TERMINATION OF REFINEMENT BASED ON-

(1) A SPECIFIED NUMBER OF CYCLES.
(2) A MAXIMUM VALUE FOR DISCREPENCY INDEX, R, IS EXCEEDED.
(3) LESS THAN A SPECIFIED MINIMUM IMPROVED CHANGE IN R.

SINCE THE PROGRAM IS INTENDED FOR USE ONLY IN THE EARLY STAGES OF REFINEMENT, ATOM PARAMETERS CAN BE READ FROM THE REFLECTION TAPE, OR CARDS, OR BOTH. THERE IS NO ATTEMPT TO REFINE TEMPERATURE AND/OR SCALE PARAMETERS.

ONLY THE RESULTS OF THE LAST CYCLE ARE WRITTEN ON THE BINARY OUTPUT TAPE. IF THE REFINEMENT IS TERMINATED BEFORE THE SPECIFIED NUMBER OF CYCLES, THE NEW REFLECTION TAPE IS WRITTEN, IF POSSIBLE, AT THE TIME OF PROGRAM TERMINATION.

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SHELL PATTERSON PROGRAM

THE SHELL PATTERSON PROGRAM WAS WRITTEN BY JAMES R. HOLDEN.

THE PROGRAM WAS DESIGNED TO CALCULATE PATTERSON, SHARPENED PATTERSON, OR SHARPENED ORIGIN-REMOVED PATTERSON FUNCTIONS AS MERCATOR PROJECTION SHELLS OF SPECIFIED RADII. THE NUMBER OF DEGREES OF EQUATORIAL ANGLE (LONGITUDE) MAY BE SPECIFIED, AND THE LATITUDE IS ALWAYS FROM THE EQUATOR TO THE POLE. THE ORIENTATION OF THE MERCATOR PROJECTION DEPENDS ON THE FOURIER SUMMATION ORDER SPECIFIED ON THE =SHLPAT= CALLING CARD. THE ORIENTATION IS DESCRIBED ON THE OUTPUT. THE GRID INTERVAL (IN DEGREES) MAY BE SPECIFIED, BUT LONGITUDE AND LATITUDE GRID DEGREES ARE EQUAL.

IT IS IMPORTANT TO FOLLOW THE SUGGESTIONS REGARDING SUMMATION ORDER GIVEN IN THE =SHLPAT= CARD FORMAT SINCE THIS WILL CONSIDERABLY REDUCE COMPUTATION TIME.

BOND LENGTHS AND ANGLES PROGRAM

THE BOND LENGTHS AND ANGLES PROGRAM, =BONDLA=, IS DESIGNED TO CARRY OUT SEVERAL FUNCTIONS RELATED TO BOND LENGTHS AND ANGLES AND THE GENERATION OF =HYDROGEN= COORDINATES (WHERE =HYDROGEN= IS TAKEN TO MEAN THE CALCULATED POSITION OF AN ATOM AT A SPECIFIED DISTANCE FROM A SECOND ATOM).

(1) CALCULATE ALL =SIGNIFICANT= DISTANCES WITHIN THE SET OF ATOMS SUPPLIED, WHERE THE =SIGNIFICANT= DISTANCE IS SPECIFIED ON THE =BONDLA= CALLING CARD.

(2) CALCULATE ANGLES BETWEEN ATOMS IN THE SET WHICH ARE WITHIN THE SPECIFIED =SIGNIFICANT= DISTANCE FROM EACH OTHER.

(3) CALCULATE INTERATOMIC DISTANCES FOR SPECIFIED ATOMS IN THE SET.

(4) CALCULATE ANGLES BETWEEN THE LINES DEFINED BY TWO PAIRS OF SPECIFIED ATOMS.

(5) GENERATE SYMMETRICALLY RELATED SETS FROM SYMMETRY OPERATIONS SUPPLIED, AND CALCULATE BETWEEN STIPULATED LIMITS THE DISTANCES FROM THE ORIGINAL SET OF ATOMS TO THE GENERATED SET OF ATOMS.

(6) GENERATE COORDINATES FOR LINEAR, TRIGONAL, TETRAHEDRAL, AND TERMINAL TETRAHEDRAL =HYDROGEN= ATOMS.

NOTE 1 - IF APPROPRIATE STANDARD DEVIATIONS OF CELL DIMENSIONS AND COORDINATES ARE SUPPLIED, BOND LENGTH AND ANGLE STANDARD DEVIATIONS WILL BE CALCULATED FOR FUNCTIONS 1 THROUGH 5.

NOTE 2 - IF NO ATOM TYPES ARE SPECIFIED IN FUNCTION 6, THE GENERATED ATOMS WILL BE LABELED =H= AND SERIALIZED IN ORDER OF GENERATION

=ORFFE= BUSING-MARTIN-LEVY FUNCTION AND ERROR PROGRAM

THE FORTRAN CODING OF THE FUNCTION AND ERROR PROGRAM BY W.R.BUSING K.O.MARTIN AND H.A.LEVY (ORNL-TM-306, OAK RIDGE NATIONAL LABORATORY) HAS BEEN MODIFIED TO CONFORM WITH THE =X-RAY 63= SYSTEM BY J.R.HOLDEN. REFERENCE TO THE OAK RIDGE REPORT WILL BE FOUND TO BE HELPFUL.

THE SYSTEM VERSION OF THIS PROGRAM RETAINS ALL OF THE PARTS CONCERNED WITH THE CALCULATION OF FUNCTIONS AND THEIR ERRORS. NONE OF THE DATA CARDS OF THE ORIGINAL PROGRAM ARE USED BY THE SYSTEM VERSION. THIS VERSION DOES NOT ALLOW THE ATOM PARAMETER ERROR MATRIX TO BE READ FROM CARDS. THIS INFORMATION CAN ONLY BE OBTAINED FROM THE BINARY REFLECTION TAPE PRODUCED BY THE SYSTEM VERSION OF =ORFLS=. ALL OTHER FUNCTIONS OF THE ORIGINAL OAK RIDGE PROGRAM HAVE BEEN RETAINED.

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GENERAL DESCRIPTION

GIVEN THE UNIT CELL PARAMETERS OF A CRYSTAL TOGETHER WITH THE ATOMIC CO-ORDINATES AND/OR THE ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS, THIS PROGRA WILL COMPUTE VARIOUS FUNCTIONS OF THESE PARAMETERS SUCH AS THE DISTANCE BE-TWEEN TWO ATOMS, AN ANGLE DEFINED BY THREE ATOMS, THE PRINCIPAL AXES OF THE ANISTROPIC TEMPERATURE FACTOR, ETC. FURTHERMORE, IF THE ERRORS OF THE INPUT PARAMETERS ARE AVAILABLE TO THE PROGRAM IN THE FORM OF A VARIANCE-COVARIANCE MATRIX OBTAINED FROM THE INVERSE MATRIX OF A LEAST SQUARES REFINEMENT, THEN THE PROGRAM WILL ALSO COMPUTE THE STANDARD ERRORS OF THE VARIOUS FUNCTIONS WITH AND WITHOUT THE CONTRIBUTION OF THE CELL PARAMETER ERRORS. THIS PROGRAM MAY BE USED INDEPENDENTLY, READING ALL INPUT DATA FROM CARDS, OR IT MAY BE USED IN CONJUNCTION WITH THE LEAST SQUARES REFINEMENT PROGRAM, ORFLS, IN WHICH CASE MUCH OF THE INPUT IS TAKEN FROM THE BINARY OUTPUT TAPE OF A CYCLE OF LEAST SQUARES.

THE FUNCTIONS, WITHOUT STANDARD ERRORS, CAN BE CALCULATED FROM THE OUTPUT TAPES FROM OTHER PROGRAMS (E.G. FC, DIFSYN AND FOUREF).

MATHEMATICAL METHOD

THE FUNCTIONS WHICH THE PROGRAM COMPUTES ARE OF THE FORM

F = F (P1, P2, P3 ... A1, A2 ...A6)

WHERE THE P'S ARE THE ATOMIC PARAMETERS AND THE A'S ARE THE UNIT CELL PARA-METERS. EACH KIND OF F IS COMPUTED BY A SPECIAL SUBROUTINE FOR THIS PURPOSE

THE STANDARD ERROR OF F IS GIVEN BY

E = (E'**2+E''**2)**1/2

WHERE

E'**2 = SIGMA(I=1,N)SIGMA(J=1,N)((2-S(IJ))(DF/DP(I))(DF/DP(J)) V(IJ)

AND

E''**2 = SIGMA(I=1,6)SIGMA(J=1,6)(2-S(IJ))(DF/DA(I))(DF/DA(J)) U(IJ)

HERE V(IJ) IS AN ELEMENT OF THE VARIANCE-COVARIANCE MATRIX WHICH DESCRIBES TH ERRORS OF THE ATOMIC PARAMETERS, AND U(IJ) IS AN ELEMENT OF A SIMILAR MATRIX FOR THE UNIT CELL PARAMETERS.

WHEN ERRORS ARE TO BE COMPUTED, THE USER HAS THE OPTION OF OBTAINING V FROM THE BINARY OUTPUT TAPE OF ORFLS. IN THIS CASE THE PROGRAM STORES

V(IJ) = (SIGMA(W(OBS-CALC)**2/(M-N)) B(IJ)

WHERE B(IJ) IS AN ELEMENT OF THE INVERSE MATRIX OF THE NORMAL EQUATIONS, AND THE CONSTANT IN BRACKETS IS THE SUM OF THE WEIGHTED RESIDUALS SQUARED DIVIDED BY THE NUMBER OF DEGREES OF FREEDOM.

THE UNIT CELL ERRORS MAY BE PUT IN IN TWO WAYS. IF NO COVARIANCES ARE KNOWN THEN THE USER MAY SUPPLY ONLY THE SIX STANDARD ERRORS S(A(I)). THE PROGRAM THEN SETS

U(II) = S(A(I))**2

U(IJ) = 0, I NOT EQUAL TO J

ALTERNATIVELY THE 21 INDEPENDENT VALUES OF U(IJ) CAN BE READ FROM CARDS.

THE NECESSARY DERIVATIVES ARE COMPUTED NUMERICALLY BY ADDING AN INCREMEN DP(I) TO P(I) AND RE-ENTERING THE SUBROUTINE FOR F. THE DERIVATIVE IS THEN

DF/DP(I) = (F(P(1),P(2),..P(I)+DP(I),..)-F(P(1),P(2),..P(I)..))/DP(I)

THE INCREMENT USED IS DP(I) = (0.01)V(II)**1/2. THE DERIVATIVES WITH RESPECT TO THE CELL PARAMETERS ARE OBTAINED SIMILARLY.

THE PROGRAM IS ARRANGED SO THAT IT COMPUTES DERIVATIVES ONLY WITH RESPEC TO THE PARAMETERS ACTUALLY INVOLVED IN F. THE INFORMATION AS TO WHICH THESE ARE IS PROVIDED BY THE SUBROUTINES PRE1, PRE2, ETC., WHICH ARE SUPPLIED FOR EACH TYPE OF FUNCTION. DERIVATIVE COMPUTATIONS ARE ALSO OMITTED WITH RESPECT TO FIXED PARAMETERS WHICH ARE NOT REPRESENTED IN THE VARIANCE-COVARIANCE MATR (E.G., THE COORDINATES OF ATOMS IN SPECIAL POSITIONS).

NOTE THAT FOR THE DERIVATIVE COMPUTATION TO BE CORRECT ALL SYMMETRY TRAN FORMATIONS MUST BE MADE AFTER DP(I) HAS BEEN ADDED TO P(I). SIMILARLY ALL CO STRAINTS ON THE PARAMETERS MUST BE SET AFTER INCREMENTING. (SEE THE SECTION ENTITLED ''CONSTRAINTS ON THE PARAMETERS''.) IN OTHER WORDS, THE FUNCTION F ALWAYS COMPUTED DIRECTLY FROM THE FUNDAMENTAL PARAMETERS, THE ERRORS OF WHICH ARE DESCRIBED BY THE MATRICES, V AND U.

THE OUTPUT OF THE PROGRAM INCLUDES A DESCRIPTION OF THE FUNCTION, THE VALUE, F, OF THE FUNCTION, THE STANDARD ERROR, E, OF THE FUNCTION, AND E', TH STANDARD ERROR NOT INCLUDING THE EFFECT OF UNIT CELL ERRORS.

CONSTRAINTS ON THE PARAMETERS

IN ORDER TO INSURE THAT THIS PROGRAM CORRECTLY COMPUTES THE ERRORS OF VARIOUS FUNCTIONS IT IS NECESSARY FOR THE USER TO CONSIDER WHETHER THE SYMMET OF THE CRYSTAL INTRODUCES CONSTRAINTS EITHER ON THE CELL PARAMETERS, A, OR ON THE ATOMIC PARAMETERS, P. A SIMPLE CASE OCCURS WHEN THE SYMMETRY FORCES A PARAMETER TO HAVE A FIXED VALUE, AND THIS SITUATION IS CORRECTLY HANDLED BY

SPECIFYING THAT THE ERROR OF THIS PARAMETER IS ZERO. IN THE CASE OF ATOMIC PARAMETERS FROM A LEAST SQUARES REFINEMENT THIS IS PROBABLY AUTOMATIC SINCE THE DEPENDENT PARAMETERS WOULD NOT HAVE BEEN VARIED.

ERROR INDICATORS

DURING THE COURSE OF CALCULATION THE PROGRAM MAKES MANY TESTS FOR ERRORS WHICH MAY INDICATE THAT THE PROBLEM IS NOT SET UP CORRECTLY. IF THE ERROR IS ONE WHICH WOULD PROBABLY CAUSE ALL ANSWERS TO BE INCORRECT THE PROGRAM WRITES AN APPROPRIATE REMARK AND TRANSFERS TO THE ''EXIT ROUTINE''. IF, ON THE OTHER HAND, THE ERROR IS LIKELY TO CAUSE TROUBLE IN ONLY ONE ANSWER THEN THE PROGRAM DOES NOT HALT. INSTEAD OF THE INCORRECT ANSWER THE PROGRAM PUTS OUT ''***NG'' WHERE NG IS AN INTEGER, THE MEANING OF WHICH IS TABULATED BELOW. THE PROGRAM THEN PROCEEDS WITH THE NEXT FUNCTION TO BE COMPUTED.

ERROR RETURNS

NG	SUBPROGRAM	MEANING
1	ATOM,BETA	THE SYMMETRY POSITION SPECIFIED IS NEGATIVE OR GREATER THAN THE NUMBER OF SYMMETRY CARDS.
2	PRE	NO PRE ROUTINE HAS BEEN SUPPLIED FOR THE FUNCTION SPECIFIED.
3	FUN	NO FUN ROUTINE HAS BEEN SUPPLIED FOR THE FUNCTION SPECIFIED.
4	BETA	TEMPERATURE FACTORS ARE NOT IN ANISOTROPIC FORM, I.E. IC(9) IS LESS THAN 6
5	ATOM,BETA	THE PROGRAM IS LOOKING FOR A PARAMETER BE-BEFORE THE START OR BEYOND THE END OF THE LIST.
6	STOBB	THE CELL PARAMETER A(1), A(2), OR A(3) IS LESS THAN OR EQUAL TO ZERO.
7	EIGVAL	THE EIGENVALUES ARE IMAGINARY.
8	EIGVEC	ONLY NULL EIGENVECTORS ARE FOUND.
9	COSVV	ONE OF THE VECTORS IS NULL.
10	FUNXI	THE VECTOR IS NULL.
11	SUB 12, 14, 18	A NON-EXISTANT FUNCTION HAS BEEN SPECIFIED, I.E. XMODF(IN(I),100) IS GREATER THAN 20.

LEAST-SQUARES LINE AND PLANE PROGRAM

THE LEAST-SQUARES LINE AND PLANE PROGRAM, =LSQPL=, IS A PROGRAM TO CALCULATE 3-DIMENSIONAL LINES OR PLANES WITHOUT REGARD TO THE FIGURES DISTANCE TO THE ORIGIN. THIS PROGRAM WAS WRITTEN BY ROGER V. CHASTAIN.

THE METHOD OF CALCULATION IS THAT OF SCHOMAKER, ET AL, WITH THE EXCEPTION OF THE METHOD FOR OBTAINING THE ROOTS OF THE CUBIC EQUATIONS IN THE LAGRANGIAN MULTIPLIERS. SCHOMAKER, ET AL, USED AN ITERATIVE TECHNIQUE, WHEREAS THIS PROGRAM SOLVES FOR THE ROOTS DIRECTLY BY THE GENERAL SOLUTION EQUATIONS.

THE OPERATION OF THE PROGRAM CAN BE DESCRIBED AS FOLLOWS- FIRST THE NECESSARY DATA ARE READ FROM CARDS AND/OR TAPE, AND THEN THE EQUATION OF THE LINE OR PLANE IS CALCULATED. IT IS POSSIBLE TO CALCULATE THE EQUATION OF A PLANE OR LINE WITH A CENTER OF SYMMETRY AT THE ORIGIN BY SUPPLYING THE ATOMS IN ONE ASYMMETRIC UNIT ONLY AND CODING THE PROGRAM TO GENERATE EQUIVALENT ATOMS BEFORE PURSUING THE CALCULATION (THIS CODE IS IN THE CALLING CARD).

THE CALCULATION OF THE LEAST-SQUARES PLANE OR LINE IS OVER THE (N1) ATOMS (SPECIFIED IN THE CALLING CARD) ON THE FIRST (N1) =ATOM= CARDS IN THE DATA PLUS THE GENERATED CENTROSYMMETRIC ATOMS IF SO CODED. IF MORE THAN (N1) =ATOM= CARDS ARE SUPPLIED, THE EXCESS WILL BE IGNORED IN THE CALCULATION OF THE EQUATION, BUT WILL BE CONSIDERED IN THE CALCULATIONS OF THE DISTANCES OF ATOM FROM THE LINE OR PLANE.

FREQUENTLY ONE IS INTERESTED IN ANGLES BETWEEN PLANES AND LINES. =LSQPL= CAN BE CODED SO THAT, IF A SERIES OF =LSQPL= CALCULATIONS ARE SUBMITTED ONE RIGHT AFTER ANOTHER, THE ANGLES BETWEEN ALL PAIRS OF LINES AND PLANES WILL BE CALCULATED FOR THOSE LINES AND PLANES CODED NON-ZERO IN THE CALLING SEQUENCE. THE ORDER OF =LSQPL= CALCULATIONS ARE NOT IMPORTANT AS LONG AS THE =LSQPL= PROGRAM IS NOT REMOVED FROM CORE UNTIL ALL THE LINES AND PLANES HAVE BEEN CALCULATED FOR THE INTER-LINEAR AND INTER-PLANAR ANGLES DESIRED. (I.E. NO OTHER LINK IS CALLED BETWEEN PLANE CALCULATIONS.)

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PROGRAM FOR DELTA-F VS FO PLOT

THE PROGRAM =DELSIG= READS THE X-RAY SYSTEM REFLECTION TAPE AND GIVES VALUES OF DELTA-F AS A FUNCTION OF FO. THE PROGRAM WAS WRITTEN BY ROGER V. CHASTAIN.

THE OUTPUT FROM =DELSIG= HAS BEEN FOUND TO BE USEFUL FOR STUDYING NON-SYSTEMATIC EXTINCTION IN REFLECTIONS AND A PLOT OF DELTA-F VS FO MAY ALSO AID IN SELECTING A LEAST-SQUARES REFINEMENT WEIGHTING SCHEME.

IN OPERATION, =DELSIG= READS THE X-RAY SYSTEM REFLECTION TAPE AND SORTS REFLECTIONS IN THE ORDER OF INCREASING MAGNITUDES OF F-OBSERVED. ONCE THE TABLE OF ORDERED F-OBSERVEDS IS ESTABLISHED, THE F-OBSERVEDS ARE FURTHER SUB-DIVIDED EITHER AS-

(1) GROUPS OF EQUAL NUMBERS OF REFLECTIONS (I.E.- 15 REFLECTIONS PER GROUP, OR ANY OTHER DESIRED NUMBER), OR,

(2) GROUPS OF EQUAL RANGE IN F-OBSERVED (I.E.- FOR EACH GROUP, (FO(MAX) - FO(MIN)) IS A CONSTANT, AND THE NUMBER OF REFLECTIONS PER GROUP IS A VARIABLE DEPENDENT ON THE DISTRIBUTION OF MAGNITUDES OF F-OBSERVEDS.

FOR EACH GROUP THE AVERAGE F-OBSERVED AND DELTA-F IS CALCULATED AND WRITTEN ON THE OUTPUT TAPE. THE DELTA-F MAY BE AN ARITHMETIC AVERAGE OR A ROOT-MEAN-SQUARE AVERAGE.

=DELSIG= WILL ALSO INCLUDE IN THE OUTPUT A PLOT OF THE OUTPUT DATA, DELTA-F VS FO, IF THIS IS CODED IN THE =DELSIG= CALLING CARD. THE GRAPH CAN BE PLOTTED WITH 10(DELTA-F) MADE MODULO 100, OR WITH 10(DELTA-F) SCALED SO THAT THE MAXIMUM 10(DELTA-F) IS 100.

DATA REDUCTION PROGRAM (LINK 10000)

THE INITIAL CODING FOR THE DATA REDUCTION PROGRAM WAS WRITTEN BY JAMES N. STEWART DURING 1958-60 FOR THE IBM 704 AT THE OHIO STATE UNIV. MRS. MARY ANN JARSKI AND JAMES M. STEWART CONVERTED THE IBM 704 PROGRAM TO THE IBM 709, AND FURTHER EXPANDED THE CODING. THE BOND ABSORPTION CORRECTION WAS PROGRAMMED AND CHECKED-OUT BY BRUNO MOROSIN. THE FULL PROGRAM WAS FURTHER CHECKED OUT BY ROGER V. CHASTAIN.

THIS PROGRAM IS DESIGNED TO ORGANIZE THE RAW DATA NEEDED IN THE DETERMINATION OF A CRYSTAL STRUCTURE INTO A COHERENT COLLECTION STORED ON MAGNETIC TAPE SO THAT THE STRUCTURE FACTOR, AND REFINEMENT PROGRAMS WILL CALCULATE AUTOMATICALLY. THE PROGRAMS FORTRAN STATEMENTS ARE MADE USING ABBREVIATIONS FOR THE SYMBOLS USED BY BUERGER (1) AND LIPSON AND COCHRAN (2). THE CALCULATIONS PERFORMED ARE LISTED HERE WITH NO OTHER EXPLANATION. REFERENCE TO THE INTERNATIONAL TABLES (3) AS WELL AS THE PAPER ON THE LORENTZ AND POLARIZATION FACTOR FOR THE PRECESSION METHOD BY WASER (4) MAY BE FOUND HELPFUL.

THE PROGRAM REQUIRES THE FOLLOWING DATA-

(1) CELL DIMENSIONS AND F(000).
(2) ATOMIC FORM FACTORS (NEUTRON OR X-RAY).
(3) THE GENERAL SYMMETRY OPERATIONS OF THE SPACE GROUP, APART FROM LATTICE TRANSLATION AND CENTER OF SYMMETRY.
(4) IDENTIFICATION OF CELL AS CENTRIC OR ACENTRIC, AND LATTICE TYPE.
(5) DISPERSION CORRECTIONS (OPTIONAL).
(6) CAMERA DATA AND PHYSICAL ORIENTATION OF THE CRYSTAL.
(7) SCALE FACTORS TO BE APPLIED TO THE INTENSITY DATA (OPTIONAL).
(8) WEIGHTING DATA FOR LEAST-SQUARES (OPTIONAL).
(9) FILTER FACTORS IF NEEDED FOR SPECTROMETER DATA (OPTIONAL).
(10) ABSORPTION CORRECTIONS (OPTIONAL).
(11) REFLECTION DATA. H, K, AND L. I, F, OR F**2.

THE PROGRAM PERFORMS THE FOLLOWING SEQUENCE OF OPERATIONS-

(I) INITIALIZATION OF THE PROGRAM. ALL CONSTANTS ARE SET TO VALID =BEST= VALUES. TAPE ASSIGNMENTS ARE MADE. A TAPE LABELING CARD =LABEL= IDENTIFIES THE BINARY TAPE.

(II) THE CELL DIMENSIONS ARE READ AND CHECKED FOR REASONABLENESS- NO ZERO OR NEGATIVE AXIAL LENGTHS OR LENGTHS LESS THAN 1.0 A. NO COSINES WITH MAGNITUDE GREATER THAN 1.0 ARE PERMITTED. THE RECIPROCAL CELL CONSTANTS, THE METRIC TENSOR, AND INVERSE METRIC TENSOR ARE CALCULATED (1, PAGE 360).

(III) NEXT, THE SCATTERING FACTOR INFORMATION IS READ IN. THE VALUES FOR X-RAY FORM FACTORS ARE READ IN FOR A NUMBER OF VALUES OF SIN THETA/LAMBDA AND A TABLE IS STORED IN MEMORY FOR EACH ATOM-TYPE TO BE USED. THERE IS A MAXIMUM OF 16 ATOM-TYPES ALLOWED. THE X-RAY SCATTERING FACTORS, LIKE THE NEUTRON SCATTERING FACTORS, ARE GIVEN A DESIGNATION AT THIS TIME CONSISTING OF ONE TO SIX CHARACTERS (E.G.- N FOR NITROGEN, CU2+ FOR COPPER(II), ETC.). THE DESIGNATION IS STORED IN A =DICTIONARY= ON THE BINARY TAPE FOR THE USE OF THE FOLLOWING PROGRAMS. THESE DESIGNATIONS MUST NOT END IN A NUMERIC PUNCH. X-RAY FORM FACTORS MAY BE USED DIRECTLY FROM THE LITERATURE (5). THERE ARE STRINGENT REQUIREMENTS UPON THE ORDER AND RANGE OF THE ENTRIES, BUT NON-EQUAL INTERVALS ARE PERMISSIBLE. THE ACTUAL VALUES OF THE SCATTERING FACTORS AT EACH VALUE OF (SIN THETA)/LAMBDA FOR A GIVEN REFLECTION ARE DETERMINED BY A FOUR-POINT INTERPOLATION UTILIZING AITKEN-S METHOD (6). THE CONDITIONS WHICH MUST BE MET ARE- (SIN THETA)/LAMBDA MUST INCREASE MONOTONICALLY, F(J) SHOULD DECREASE MONOTONICALLY (HOWEVER, A 5-PERCENT INCREASE IN ANY INTERVAL IS PERMITTED TO ALLOW FOR THE OCCASSIONAL INFLECTION FOUND FOR SOME ELECTRON CONFIGURATIONS), THERE MUST BE AT LEAST TEN ENTRIES, AND LESS THAN 40 ENTRIES. IN ORDER TO INTERPOLATE AT THE HIGH VALUES OF (SIN THETA)/LAMBDA BE CERTAIN THAT THERE ARE AT LEAST TWO TABLE ENTRIES WITH A VALUE OF (SIN THETA)/LAMBDA GREATER THAN THE HIGHEST VALUE THAT IS ANTICIPATED IN THE REFLECTION DATA. THE PROGRAM CHECKS FOR THESE

CONDITIONS AND RETURNS ERROR REMARKS EXPLAINING ANY NON-AGREEMENT WITH THE PROGRAMMED CONDITIONS. THE VALUE FOR THE COHERENT SCATTERING OF NEUTRONS IS SUPPLIED AS A SINGLE NUMBER FOR EACH ATOM TYPE (7).

(IV) THE NEXT STEP IS THE BUILDING OF THE SYMMETRY OPERATIONS OF THE SPACE GROUP INTO MATRICES AND VECTORS WHICH MAY BE USED TO GENERATE ALL THE ATOMS IN THE CELL FROM ONE ASYMMETRIC SET. THE STRUCTURE FACTOR AND FOURIER PROGRAMS OPERATE ON THE BASIS OF P1 OR P1-BAR. THESE OPERATORS ARE READ IN THE FORM GIVEN IN THE FIRST PART OF VOLUME I OF THE INTERNATIONAL TABLES (3). THE PROGRAM CHECKS THE CARDS FOR POSSIBLE ERRORS IN PUNCHING AND STORES THEM IN TABLES IN FORTRAN MATRIX ORDER AS A 3X4 ARRAY. FOR EXAMPLE, WITH SPACE GROUP CMCM, CARDS ARE PUNCHED FOR THESE POSITIONS WHICH WILL BE CONVERTED TO THE MATRICES SHOWN IN EQUATION (1).

ONE MUST SUPPLY A SEPARATE CARD INDICATING WHETHER THE CELL IS CENTRIC OR ACENTRIC AND GIVING THE LATTICE TYPE SYMBOL-

P, R, A, B, C, I, OR F.

NOTE- =P= IS USED FOR RHOMBOHEDRAL SPACE GROUPS INDEXED AS RHOMBOHEDRAL AND =R= IS USED FOR RHOMBOHEDRAL SPACE GROUPS INDEXED AS HEXAGONAL. IN THE CENTRIC CASE WITH THE ORIGIN AT THE CENTER OF SYMMETRY ONLY THOSE OPERATIONS NOT INVOLVING THE CENTER SHOULD BE SUPPLIED. AFTER THE SYMMETRY OPERATIONS HAVE BEEN STORED IN A FORM SUITABLE FOR THE STRUCTURE FACTOR PROGRAM THEY ARE OPERATED UPON BY A SUBROUTINE =GENCHK= (GENERATION CHECKING SUBROUTINE) WHICH SORTS AND EXAMINES THE OPERATIONS TO CHECK FOR CRYSTALLOGRAPHIC VALIDITY.

(V) ONE MAY SUPPLY DISPERSION CORRECTION CARDS USING DATA FROM EITHER TEMPLETON (8) OR ROOF (9). THESE CARDS ARE OPTIONAL, AS IS THE APPLICATION OF THE DISPERSION CORRECTIONS AT =FC= TIME. IF THE DISPERSION DATA ARE NOT INCLUDED, IT WILL BE NECESSARY TO RE-REDUCE DATA TO GET THEM ON THE REFLECTION TAPE.

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(VI) THE CONDITIONS OF OBSERVATION ARE SUPPLIED NEXT. THIS CARD PROVIDES SPACE FOR WAVELENGTH, THE MAXIMUM (SIN THETA)/LAMBDA EXPECTED, THE MINIMUM OBSERVED INTENSITY, NEUTRON- OR X-RADIATION, THE CAMERA TYPE (ONLY POWDER, SPECTROMETER, WEISSENBERG, AND PRECESSION ARE ALLOWED), WHETHER OR NOT ONE WISHES TO APPLY 1/LP, OR TO TAKE THE SQUARE ROOT OF THE DATA BEING REDUCED.

AXIAL DESIGNATIONS MUST BE MADE FOR THOSE METHODS WHICH REQUIRE THE AXIS OF ROTATION AND/OR THE AXIS PARALLEL TO THE BEAM. FOR THE PRECESSION METHOD THE ANGLE BETWEEN THE AXIS MOST NEARLY HORIZONTAL AND THE HORIZONTAL ON THE FILM IS NECESSARY. THE CALCULATION OF 1/LP FOR X-RAY AND 1/L FOR NEUTRONS IS CARRIED OUT FOR EACH REFLECTION SO THAT NO TABLES ARE REQUIRED. THE FORMULAE USED ARE GIVEN IN EQUATIONS 2, 3, AND 4.

(VII) IF SPECTROMETER DATA ARE BEING PROCESSED, THEN FILTER FACTOR CARDS GIVING THE ABSORBANCY OF THE FILTERS AND AN INDEX CODE ARE SUPPLIED. FILTER =0= HAS A FACTOR OF 1.0 AUTOMATICALLY SO THAT FOR A REFLECTION MARKED =NO FILTER=, THE =CORRECT= FILTER FACTOR IS APPLIED.

(VIII) SCALE CARDS SERVE THE PRIMARY PURPOSE OF ADJUSTING THE SCALE OF THE RELATIVE INTENSITIES OF GROUPS OF REFLECTIONS. IN ADDITION THEY PERMIT TAGGING GROUPS OF REFLECTIONS AS ALL HAVING THE SAME SCALE FACTOR (MAXIMUM NUMBER OF GROUPS = 64). THE MINIMUM OBSERVED INTENSITY FOR THE GROUP, AND PROVISION FOR WEIGHTING, ARE SUPPLIED ON THIS CARD. IF NO SCALE CARD IS SUPPLIED THE PROGRAM ASSIGNS =1= AS THE REFLECTION GROUP INDEX AND USES 1.0 AS THE SCALE FACTOR AND NO LEAST-SQUARES WEIGHTING FACTORS ARE CALCULATED. HOWEVER, THE VALUE OF F-MINIMUM IS STORED ON THE TAPE IN THE WORD RESERVED FOR LEAST-SQUARES WEIGHT. THESE WEIGHTS CAN THEN BE CALCULATED AT SOME FUTURE TIME BY PROGRAM =WEIGHT= (LINK 10600). THE LEAST-SQUARES PROGRAMS ALLOW THE SETTING OF WEIGHTS = 1.0 IN THE CALLING CARD.

THERE IS A LEAST-SQUARES WEIGHTING SCHEME PROVIDED IN THE PROGRAM WHICH IS PATTERNED AFTER THE METHOD SUGGESTED BY HUGHES (10). IT IS CALLED BY A =2= IN THE SCALE CARD. THE FORTRAN CODING FOR THE UNIV. OF WASHINGTON SCHEME IS-

```
WEIGHT = Q1/MAX1F(SIGMA,Q2*FREL+Q3,Q4*FRELM+Q5)
```

WHERE WEIGHT = SQUARE ROOT OF WEIGHT TO BE USED IN LEAST-SQUARES.

Q1 = CONSTANT PUNCHED IN COLS. 33-37 OF =SCALE= CARD. (SET = 1.0 IF NOT SPECIFIED).

SIGMA = STANDARD DEVIATION OF MEASUREMENT, AND IS PUNCHED IN COLS 38-47 OF =REFLECTION= CARD.

Q2 = FRACTIONAL ERROR IN F-RELATIVE. PUNCHED IN COLS 38-42 OF =SCALE= CARD, AND INITIALIZED TO ZERO.

Q3 = ADDITIVE CONSTANT WHICH MAY BE APPLIED AT USERS DISCRETION. PUNCHED IN COLS 43-47 OF =SCALE= CARD, AND INITIALIZED TO 0.0.

Q4 = FRACTION OF F-MINIMUM WHICH IS TO BE CONSIDERED MINIMUM STANDARD DEVIATION. PUNCHED IN COLS 48-52 OF =SCALE= CARD AND INITIALIZED TO ZERO.

Q5 = ADDITIVE CONSTANT WHICH MAY BE APPLIED AT USERS DISCRETION. PUNCHED IN COLS 53-62 OF =SCALE= CARD, AND INITIALIZED TO 1.0.

THE SCHEME APPLIES WEIGHTING FUNCTION- WEIGHT=Q1/(J) IN WHICH (J) IS WHICHEVER OF THESE THREE FUNCTIONS IS A MAXIMUM- (1) SIGMA, (2) (Q2*FREL+Q3), OR (3) (Q4*FRELM+Q5). TO OBTAIN WEIGHTS LIKE THOSE SPECIFIED BY HUGHES (10)-

```
WEIGHT = 1.0 FOR F-REL LESS-THAN K
       = K/F-REL FOR F-REL GREATER-THAN OR EQUAL K
THEN SET  Q1 = Q5 = K
          Q2 = 1.0
          Q3 = Q4 = ZERO
```

TO OBTAIN WEIGHTS SIMILAR TO RESULTS OF =DELSIG= PROGRAM-

```
Q2 = SLOPE OF PLOT OF DELTA-F VS FO
Q1 = Q3 = (INTERCEPT OF PLOT)*(1/SCALE FACTOR)
Q4 = Q5 = ZERO
```

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NOTE- IN ORDER TO USE THE VALUE OF SIGMA FOR COUNTER DATA, Q3 AND Q5 MUST BE SET EQUAL TO A VERY SMALL NUMBER (BUT NOT ZERO) IN ORDER TO SUPERCEDE ANY PREVIOUSLY STORED VALUES OF Q3 AND Q5.

IF IT IS DESIRED THERE IS PROVISION FOR THE USER TO =PATCH= THE DATA REDUCTION PROGRAM BY WRITING A FORTRAN OR FAP SUBROUTINE ENTITLED =WTFN= (WEIGHT FUNCTION). THE =WTFN= CALLING SEQUENCE PLACES AT ITS DISPOSAL F-RELATIVE, F-RELATIVE(MINIMUM), ESTIMATED ERROR (AS SUPPLIED IN THE =SCALE= CARD), THE SCALE FACTOR, AND ARBITRARY PARAMETERS SUPPLIED IN THE =SCALE= CARD. THESE FACTORS ARE CALLED IN THE LISTED ORDER IN FLOATING POINT, AND THE DESIGNATION OF THE FORTRAN LOGICAL BCD OUTPUT TAPE IS SUPPLIED. THE CALLING SEQUENCE STEP-

1450 CALL WTFN (FREL, FRELM, CALE, SIGMA, Q1, Q2, Q3, Q4, Q5)

IS BY-PASSED UNLESS =KEYED-IN= BY CODING A =3= IN THE APPROPRIATE COLUMN OF THE =SCALE= CARD.

(IX) ABSORPTION CARDS SUPPLY INFORMATION SPECIFIC TO THE TYPE OF ABSORPTION CORRECTION BEING APPLIED. THE INFORMATION ON SPHERES AND CYLINDERS OF BOND (II) IS GIVEN IN VOLUME II OF THE INTERNATIONAL TABLES (3). THE DATA IS READ INTO THE COMPUTER ON CARDS AND INTERPOLATED FROM THE VALUE OF (SIN THETA)/LAMBDA BY AITKENS METHOD (6). DIFFERENT ABSORPTION CORRECTIONS ARE REQUIRED FOR EACH LEVEL, HOWEVER THE ANGULAR DEPENDENCE IS COMPUTER DETERMINED. THE ABSORPTION CORRECTIONS ARE HANDLED IN THE SUBROUTINES =ABSORB= AND =INABS=.

(X) FOR EACH UNIQUE REFLECTION OF THE SPACE GROUP UNDER CONSIDERATION H, K, L, AND EITHER F, F**2, OR I-RELATIVE MUST BE PROVIDED. THESE QUANTITIES ARE SUPPLIED BY THE SUBROUTINE =INPUT=. THE UNIV. OF WASH. IBM 709 =INPUT= ACCEPTS TWO TYPES OF INPUT FORMATS FOR REFLECTION DATA- ONE ASSUMING H, K, L, AND I WILL BE HAND-PUNCHED IN CARDS, AND THE OTHER ASSUMING MARK-SENSE CARDS IN CONJUNCTION WITH A MARK-SENSE REPRODUCER WILL BE USED. THE LATTER IS USEFUL FOR SPECTROMETER WORK WHERE THE INTENSITY CARDS ARE PREPARED BY THE =REFLECTION GENERATION AND CRYSTAL SETTING= PROGRAM, =GESET=.

A UNIQUE SET OF REFLECTIONS, NOT INCLUDING THOSE SYSTEMATICALLY ABSENT, MUST BE INCLUDED. IF A SHARPENED ORIGIN-REMOVED PATTERSON IS DESIRED THE SYSTEMATICALLY ABSENT REFLECTIONS SHOULD ALSO BE INCLUDED. IT IS MOST DESIRABLE, BUT NOT MANDATORY, THAT THE REFLECTIONS BE SORTED IN THE ORDER THAT WILL PERMIT FASTEST FOURIER SUMMATIONS AND THAT THE SYSTEMATICALLY ABSENT REFLECTIONS BE PLACED AFTER THE OBSERVED REFLECTIONS. THE FOURIER RUNS FASTEST IF THE REFLECTIONS WITH THE SAME ABSOLUTE VALUES OF H, K, AND L ARE GROUPED TOGETHER. THE FC RUNS FASTEST IF THE REFLECTIONS ARE SORTED SO THAT THE INDEX WITH THE SMALLEST RANGE VARIES SLOWEST, ETC. (IN THE TRICLINIC CASE, WHERE IT IS IMPOSSIBLE TO SATISFY BOTH CRITERIA, THE FORMER SHOULD BE GIVEN PRECEDENCE.) NOTE THAT FOR MAXIMUM EFFICIENCY, THE NEGATIVE VALUES SHOULD BE ASSIGNED TO INDICES ALONG SHORTER RECIPROCAL AXES.

FOR THE LESS-THAN REFLECTIONS (I.E.- THOSE REFLECTIONS WHOSE INTENSITIES ARE TOO WEAK TO BE MEASURED) A VALUE OF ZERO, OR A VALUE JUST BELOW THE LOWEST OBSERVED INTENSITY, IS PUNCHED IN THE INTENSITY CARD. THE =LESS-THANS= SERVE A USEFUL PURPOSE IN THE CALCULATIONS OF STRUCTURES AND PROVIDE ADDITIONAL, IF SOMEWHAT INACCURATE, DATA UPON WHICH TO BASE A STRUCTURE UNDER STUDY. IT IS NOT MANDATORY THAT THEY BE INCLUDED.

A NUMBER OF WAYS OF IDENTIFYING LESS-THANS HAVE BEEN PROVIDED. WHEN FILM DATA ARE BEING PROCESSED, THE TWO ALTERNATIVES DEPEND UPON WHETHER F**2, F, OR I IS THE FORM OF THE DATA SUPPLIED. (ONE) THE LESS-THAN CODE IS ASSIGNED ON THE BASIS OF A NUMERIC PUNCH IN THE INTENSITY CARD- ONE OR NINE (FOR IBM 650 COMPATIBILITY) DESIGNATING AN OBSERVED REFLECTION AND ANY OTHER NUMERIC PUNCH DESIGNATING A LESS-THAN (EIGHT WITH IBM 650) AND (TWO) A NUMERIC ZERO PUNCH OR BLANK IN THE CODE COLUMN IS VALID - IN THIS CASE THE VALUE OF THE INTENSITY MAY BE SUPPLIED AS ZERO, BLANK, OR LESS-THAN THE VALUE OF THE MINIMUM OBSERVED INTENSITY AS PUNCHED IN THE =CONDITION= OR =SCALE= CARD FOR THE REFLECTION TO BE CODED A LESS-THAN.

IN THE CASE OF A SPECTROMETER CARD, THE RELATIVE INTENSITY IS CALCULATED FROM THE REFLECTION COUNTS AND TIME, FILTER, ABSORBENCY, AND BACKGROUND COUNTS AND TIME. THE LESS-THANS ARE HANDLED MUCH THE SAME WAY AS FOR FILM DATA- THEY ARE IDENTIFIED BY CODE IN THE CARD, OR BY THE REFLECTION BEING WEAKER THAN THE BACKGROUND FOR THAT REFLECTION.

ON THE OUTPUT REFLECTION TAPE, A CODE OF =1= IS USED FOR OBSERVED REFLECTIONS, =2= FOR LESS-THANS, AND =3= FOR REFLECTIONS EXHIBITING SECONDARY EXTINCTION (WHICH ARE NOT MARKED AT DATA-REDUCTION TIME, BUT MAY BE IDENTIFIED LATER AT FC TIME). TABLE 1.100-I SUMMARIZES THE REFLECTION CODES.

THE VALUE OF (SIN THETA)/LAMBDA IS COMPARED WITH THE MAXIMUM ANTICIPATED VALUE PUNCHED IN THE =CONDITION= CARD TO CHECK THAT THE POINT IN RECIPROCAL SPACE WILL PASS INTO THAT PORTION OF THE SPHERE OF REFLECTION THAT CAN BE RECORDED BY THE CAMERA USED.

THE VALUES OF THE VARIOUS SCATTERING FACTORS ARE OBTAINED BY INTERPOLATION OF THE STORED LITERATURE VALUES. A COMPLETE LISTING OF THESE DATA FROM THE LITERATURE MAY BE FOUND IN THE =INTERNATIONAL TABLES= (3). A NUMBER OF ADDITIONAL DATA, MOST OF WHICH APPEARED IN THE LITERATURE SUBSEQUENT TO THE PUBLICATION OF THE =INTERNATIONAL TABLES=, ARE GIVEN IN TABLE 1.100-II. A NUMBER OF THE OLDER LITERATURE REFERENCES ARE ALSO LISTED IN REFERENCE 5, MAINLY AS A SOURCE FOR THE EARLIER STRUCTURE DETERMINATIONS.

THROUGH THE USE OF =FORMAT= AND =REFIN= CARDS IT IS POSSIBLE TO READ REFLECTION DATA IN MANY DIFFERENT FORMS. WHEN THE =CONDIT= CARD IS CODED TO EXPECT DATA IN A SPECIAL FORMAT A =FORMAT= CARD MAY BE SUPPLIED WHICH CONTAINS A VALID FORTRAN INPUT FORMAT STATEMENT BEGINNING WITH =(= AND ENDING WITH =)=. A =REFIN= CARD IS THEN USED TO SPECIFY THE DETAILS OF THE SOURCE OF THE DATA AS WELL AS ITS ORDER. IF THE DATA ARE BINARY, AND ARE ON A STANDARD FORTRAN WRITTEN BINARY TAPE, THE =REFIN= CARD MAY BE USED WITHOUT THE =FORMAT= CARD. THE NUMBER OF POSSIBILITIES ARE SO GREAT THAT ONLY AN ILLUSTRATIVE EXAMPLE IS GIVEN-

TO USE THE OUTPUT OF A PREVIOUS DATA REDUCTION AS INPUT TO A NEW DATA REDUCTION- IN PLACE OF THE REFLECTION DECK PLACE A =REFIN= CARD WHICH SPECIFIES THAT SEVEN RECORDS MUST BE SKIPPED AND THEN H, K, L, F-RELATIVE, LEVEL INDICATORS, AND WEIGHT ARE TO BE READ IN BINARY.

IF NECESSARY, THE CHOSEN 1/L OR 1/LP VALUE IS COMPUTED AND APPLIED. IF AN ABSORPTION CORRECTION IS TO BE MADE, IT IS DONE. THE WEIGHTING FACTOR FOR LEAST-SQUARES IS CALCULATED.

FOURIER CODES ARE GENERATED BY THE SUBROUTINE =GEN= USING THE SYMMETRY OPERATIONS PREPARED BY SUBROUTINE =GENCHK=. SEE FOURIER PROGRAM WRITE-UP (SECTION 1.40) FOR DETAILS CONCERNING THESE CODES. FINALLY, THE CALCULATED INFORMATION IS WRITTEN OUT ON TWO TAPES, A BCD LISTING TAPE AND THE BINARY =REFLECTION= TAPE WHICH SERVES AS INPUT TO THE OTHER PROGRAMS.

THE BINARY REFLECTION TAPE CONTAINS THE INFORMATION WHICH CONSTITUTES THE DATA WHICH ARE KNOWN ABOUT A CRYSTAL UNDER STUDY. THE REDUCTION OF DATA PROGRAM PLACES ON THE TAPE ONLY THOSE QUANTITIES WHICH ARE KNOWN BEFORE A STRUCTURE DETERMINATION IS STARTED, BUT IT LEAVES SPACE FOR PARAMETERS WHICH ARE DETERMINED AS THE SOLUTION PROGRESSES. THE FORMAT OF THE REFLECTION TAPE IS THEREFORE FIXED BY THE MOST GENERAL CALCULATION OR COMBINATION OF CALCULATIONS PROGRAMMED FOR THE SOLUTION OF STRUCTURES. A BINARY TAPE FORMAT IS LISTED IN APPENDIX IV, SECTION 3.4.

IN ADDITION TO ITS BINARY TAPE, REDUCTION OF DATA PREPARED A BCD TAPE FOR OFF-LINE LISTING. THIS LIST REPRESENTS THE RESULTS OF THE CALCULATIONS PERFORMED BY THE PROGRAM. IT SHOULD BE CAREFULLY SCANNED FOR EACH COMPOUND THAT IS TREATED IN ORDER TO MAKE SURE THAT THE BASIS FOR FURTHER CALCULATIONS IS SOUND.

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DATA MANIPULATION PROGRAM

THE =DATFIX= PROGRAM WAS WRITTEN BY JAMES R. HOLDEN.

THE DATA MANIPULATION PROGRAM SERVES FIRST TO GIVE AN ESTIMATE OF AN OVERALL ISOTROPIC TEMPERATURE FACTOR AND AN INTENSITY SCALE FACTOR FOR THE REFLECTION DATA. IT ALSO COMPUTES THE NORMALIZED STRUCTURE FACTORS, E, BASED UPON THE TEMPERATURE AND SCALE FACTORS OBTAINED.

THE METHOD OF CALCULATION OF THE ESTIMATED PARAMETERS IS BASED UPON THE NORMAL STATISTICS OF THE NORMALIZED STRUCTURE FACTORS (E). THE PROGRAM ITERATES STARTING WITH THE GIVEN VALUES OF TEMPERATURE AND SCALE FACTORS UNTIL THE SET OF NORMALIZED STRUCTURE FACTORS MEET THE FOLLOWING CONDITIONS =AS CLOSELY AS POSSIBLE= (1).

(A) E**2(HKL) = (FOBS**2(HKL)/EPSILON)*(SUM OVER ATOMS OF TEMPERATURE FACTOR CORRECTED (SCATTERING FACTOR **2))
WHERE FOBS MUST BE SCALED F-RELATIVE

(B) AVERAGE VALUE OF E**2 IS SET = 1.0 BY ITERATION.
THEORETICALLY, FOR A CENTROSYMMETRIC CRYSTAL THE FOLLOWING AVERAGES WILL OCCUR-
AVERAGE VALUE OF ABSF(E) = 0.798
AVERAGE VALUE OF E**2 = 1.0
AVERAGE VALUE OF ABSF(E**2 - 1) = 0.968

WHILE FOR ACENTRIC-
AVERAGE VALUE OF ABSF(E) = 0.886
AVERAGE VALUE OF E**2 = 1.0
AVERAGE VALUE OF ABSF(E**2 - 1) = 0.736

ONCE CONVERGENCE IS OBTAINED, THE SCALE INFORMATION IS PLACED IN THE =RESCALE= FACTOR BAND OF THE BINARY REFLECTION TAPE(RECORD 5, WORDS 86 THROUGH 149) AND THE ESTIMATED TEMPERATURE FACTOR DATA ARE PLACED IN THE CALCULATED CHANGE IN OVERALL ISOTROPIC TEMPERATURE FACTOR LOCATION ON THE BINARY REFLECTION TAPE (RECORD 5, WORD 85) WHERE IT IS AVAILABLE TO SUBSEQUENT PROGRAMS (E.G.- =FC=, =FCURR=, ETC.).

IT IS POSSIBLE, WITH THIS PROGRAM, TO ESTIMATE THE INDIVIDUAL LEVEL SCALE FACTORS. THESE, HOWEVER, MAY NOT BE VERY RELIABLE, ESPECIALLY IF THERE ARE FEW OBSERVATIONS IN A GIVEN LEVEL. THE PROGRAM THEREFORE PERMITS THE USER TO PLACE RESTRICTIONS ON VALUES OF THE TEMPERATURE AND SCALE FACTORS.

IN ADDITION TO FITTING THE TEMPERATURE AND SCALE FACTORS, IT IS POSSIBLE TO PERMIT THE VARYING OF THE POWER TO WHICH (SIN THETA)/LAMBDA IS RAISED IN THE EXPRESSION EXP(-(2*B*((SIN THETA)/LAMBDA)**X)) IN ORDER TO MORE CLOSELY MEET THE ABOVE CONDITIONS FOR THE STATISTICS OF (E).

THIS PROGRAM GENERATES A NEW TAPE WHICH IS A COPY OF THE REFLECTION TAPE WITH THE INCLUSION OF THE ESTIMATED TEMPERATURE AND SCALE FACTORS AND VALUE OF (E) FOR EACH REFLECTION STORED ON IT. THESE VALUES MAY THEN BE SORTED INTO TABLES FOR LISTING BY =ESORT=, AND IN CONJUNCTION WITH PROGRAM =MODIFY= MAY HAVE PHASES ASSIGNED TO (E). IT IS THEN POSSIBLE TO COMPUTE E-MAPS THROUGH THE USE OF =FOURR= PROGRAM.

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SEARCH AND MODIFY THE REFLECTION TAPE

THE =MODIFY= PROGRAM PERMITS THE MODIFICATION OR ALTERATION OF THE REFLECTION DATA ON THE BINARY TAPE. THE VARIOUS FUNCTIONS OF THE PROGRAM ARE-

(1) THE USER MAY SPECIFY ANY PARTICULAR QUANTITY IN ANY REFLECTION RECORD WHICH IS TO BE MODIFIED, AND REPLACE THIS QUANTITY BY THE NEW VALUE PUNCHED IN A CARD. THIS CARD MUST HAVE THE INDICES OF THE REFLECTION TO BE MODIFIED. REFERENCE TO APPENDIX IV (SECT 3.4) IS NECESSARY IN ORDER TO SPECIFY THE PARTICULAR QUANTITY IN THE REFLECTION RECORD (E.G.- =4= IS F-RELATIVE, =8= IS LEAST-SQUARES WEIGHT, =9= IS THE NORMALIZED STRUCTURE FACTOR (E), =10= IS THE PHASE OF THE NORMALIZED STRUCTURE FACTOR, =21= IS THE FIRST SCATTERING FACTOR, ETC.).

(2) PLACE A SPECIFIED PHASE ON A GIVEN REFLECTION.

(3) REPLACE F-RELATIVE FOR EVERY REFLECTION WITH F-CALCULATED TO WHICH A SPECIFIED RANDOM GAUSSIAN ERROR HAS BEEN APPLIED.

(4) PLACE THE PHASE OF F-CALCULATED IN PLACE OF THE PHASE OF THE UNITARY STRUCTURE FACTOR FOR ALL REFLECTIONS.

(5) RESCALE F-RELATIVE FOR ALL REFLECTIONS.

(6) TRANSFORM THE INDICES OF ALL THE REFLECTIONS.

WHEN PHASES HAVE BEEN DETERMINED BY A METHOD OTHER THAN THROUGH THE CALCULATION OF STRUCTURE FACTORS THE =MODIFY= PROGRAM PROVIDES A WAY TO PLACE THE DETERMINED PHASES ON THEIR CORRESPONDING REFLECTIONS. THESE PHASES ARE CARRIED (AS AN ANGLE IN CYCLES) IN E2 (WORD 10) ON THE BINARY TAPE REFLECTION RECORDS (SEE APPENDIX IV, SECTION 3.4). WHEN THE VALUE OF E2 IS GREATER THAN ONE CYCLE IT SERVES AS A SIGNAL THAT THE PHASE FOR THE REFLECTION IS UNKNOWN. =FOURR=, IN MODES 6, 13, AND 14, THEN USES THOSE REFLECTIONS FOR WHICH A KNOWN PHASE IS STORED.

MODIFY REQUIRES =MODREF= CARDS ONLY FOR THOSE REFLECTIONS FOR WHICH A =KNOWN= PHASE IS STORED SINCE =DATRON= INITIALIZED E2 = 2.0. THERE ARE TWO OPTIONS AVAILABLE FOR STORING PHASES-

(1) IF THE STRUCTURE IS CENTROSYMMETRIC, COL 16 OF THE =MODIFY= CARD MAY BE PUNCHED =2=, AND THE APPROPRIATE =MODREF= CARD COLUMN MAY BE PUNCHED (+1)/(0)/(-1) FOR (0 CYCLES)/(UNDETERMINED)/(0.5 CYCLES).

(2) IN THE ACENTRIC CASE, IT IS MANDATORY THAT THE WORD TO BE REPLACED MUST BE SPECIFIED IN THE =MODIFY= CARD AND THE ACTUAL PHASE IN CYCLES BE PUNCHED IN THE =MODREF= CARD. IN THIS CASE, COL 16 OF THE =MODIFY= CARD IS PUNCHED =1= AND COLS 18-19 MUST BE PUNCHED =10= TO INDICATE THAT E2 IS THE TENTH WORD OF THE REFLECTION RECORD.

THERE WILL BE MANY INSTANCES WHEN MODIFICATIONS (ESPECIALLY OF TYPE 6 IN THE LIST ABOVE) WILL REQUIRE DATA RE-REDUCTION IN ORDER TO MODIFY THE PROLOGUE RECORDS. REFERENCE TO THE DATA REDUCTION PROGRAM (SECTIONS 1.100 AND 2.100) SHOULD SERVE TO SHOW HOW THIS MAY BE CARRIED OUT.

SORT FOR KARLE-HAUPTMAN PHASE DETERMINATION

THE =ESORT= PROGRAM WAS WRITTEN BY CHARLES DICKINSON.

THIS PROGRAM IS INTENDED TO BE USED TO SORT THE NORMALIZED STRUCTURE FACTORS (E) INTO AN ORDER CONVENIENT FOR USE WITH THE KARLE-HAUPTMAN STATISTICAL PHASE DETERMINING METHODS (SYMBOLIC ADDITION PROCEDURE).

REFLECTIONS ARE READ FROM THE STANDARD BINARY REFLECTION TAPE. IF THE NORMALIZED STRUCTURE FACTOR (E) FOR A GIVEN REFLECTION IS GREATER THAN A MINIMUM VALUE SPECIFIED BY THE USER IT IS THEN SEPARATED INTO ITS PROPER CLASS DEPENDING UPON THE SYMMETRY OF THE INDICES (I.E.- HKL ALL EVEN IS PLACED IN CLASS GGG, H AND K EVEN AND L ODD IS PLACED IN GGU, ETC.). WITHIN THESE CLASSES THE REFLECTIONS ARE SORTED IN DECREASING MAGNITUDE OF THE ABSOLUTE VALUE OF E.

PROGRAM FOR LISTING STRUCTURE FACTOR DATA

=FCLIST= IS DESIGNED TO GIVE LISTS OF FC AND FO WITH THEIR CORRESPONDING H, K, AND L, AND, FOR ACENTRIC SPACE GROUPS, THE PHASE ANGLE ALPHA. THESE LISTS ARE DESIGNED TO BE AS SUCCINCT AS POSSIBLE AND IF PRINTED ON WHITE PAPER WITH A NEW RIBBON IN THE IBM 1401 WILL BE SUITABLE FOR PHOTOGRAPHY. THE FORMATS OF THE OUTPUT ARE DESIGNED TO MEET THE REQUIREMENTS FOR JOURNALS AND/OR THESIS COMMITTEES.

IN ORDER TO LIST WITH THIS PROGRAM THE REFLECTIONS MUST BE SORTED IN EXACTLY THE WAY THE LISTS ARE TO BE MADE. IF THIS WAS NOT DONE BEFORE DATA REDUCTION IT WILL BE NECESSARY TO TAKE APPROPRIATE STEPS TO PLACE THE REFLECTIONS IN ORDER BEFORE USING =FCLIST=. MANY OPTIONS ARE GIVEN, AND REFERENCE TO THE CARD FORMATS IN SECTION 2.110-8 SHOULD MAKE THESE CLEAR. THE PROGRAM WILL EITHER LIST FROM 650 FC DECKS, OR FROM A SYSTEM BINARY TAPE. IF THE REFLECTIONS OF THE BINARY TAPE ARE NOT PROPERLY SORTED, USE THE =BYEBYE= PROGRAM TO GENERATE A SET OF 650 FC CARDS WHICH CAN THEN BE SORTED IN THE CORRECT ORDER BEFORE USING =LISTFC=.

DONNAY-TAKEDA CRYSTAL TRANSFORMATION PROGRAM

TRANSFORMATIONS OF CRYSTAL SETTINGS AND SPACE GROUP SYMBOLS

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-1963-

INTRODUCTION

THE GENERAL RULES BY WHICH A CRYSTAL SETTING IS TRANSFORMED IN THIS PROGRAM ARE

(1) WHENEVER POSSIBLE THE CELL EDGES SHOULD COINSIDE WITH SYMMETRY DIRECTIONS OF THE LATTICE.

(2) SYMMETRY-EQUIVALENT EDGES SHOULD BE CHOSEN, IF POSSIBLE.

(3) THE CELL SHOULD BE THE SMALLEST POSSIBLE CELL THAT OBEYS CONDITIONS (1) AND (2).

(4) CELL EDGES THAT CANNOT BE SYMMETRY DIRECTIONS SHOULD BE THE SHORTEST POSSIBLE LATTICE TRANSLATIONS COMPATIBLE WITH CONDITION (2).

(5) CELL EDGES, THE NAMING OF WHICH IS NOT GOVERNED BY THE LATTICE SYMMETRY, SHOULD OBEY THE INEQUALITIES C LESS THAN A LESS THEN B.

(6) THE AXES OF CO-ORDINATES SHOULD BE DIRECTED, ALONG THE CELL EDGES, SO AS TO FORM A RIGHT-HANDED SYSTEM, WITH NON-ACUTE INTER-EDGE ANGLES ALPHA AND BETA.

THE RULES FOR EACH CRYSTAL SYSTEM ARE DESCRIBED IN DETAIL IN THE INTRODUCTION OF THE 2ND EDITION OF CRYSTAL DATA (DONNAY ET AL 1963).

EACH CRYSTAL SYSTEM OTHER THAN CUBIC, TETRAGONAL AND HEXAGONAL S.S (I.E., EXCLUDING RHOMBOHEDRAL) IS TREATED BY THIS PROGRAM IN A SEPARATE SUBROUTINE. THE RHOMBOHEDRAL SUBROUTINE TRANSFORMATIONS THE CELL TO THE CORRESPONDING HEXAGONAL CELL. IN THE ORTHORHOMBIC SUBROUTINE THE MAIN PROBLEM IS TO REORIENT THE SPACE-GROUP SYMBOL IN ACCORDANCE WITH ONE OF THE SIX POSSIBLE TRANSFORMATIONS (B GREATER THAN A GREATER THAN C). THE MONOCLINIC SUBROUTINE HAS TO FIND THE REDUCED MESH IN THE PLANE (UNIQUE SETTING) OF THE CELL WITH A GREATER THAN C, BETA NON-ACUTE AND AT THE SAME TIME TO REORIENT THE SPACE-GROUP SYMBOL. IN THE TRICLINIC SUBROUTINE, TO FIND THE SHORTEST THREE TRANSLATIONS IS THE MAIN PROBLEM, PROVIDED THE GIVEN CELL IS A PRIMATIVE ONE, THE EDGES ARE RELABELED TO OBEY C GREATER THAN A GREATER THAN B, WITH ALPHA AND BETA NON-ACUTE.

THE EXISTING PROGRAM WRITTEN BY MISS D. PILLING IN ENGLAND, ONLY PERFORMS CELL REDUCTIONS. IT DOES NOT DEAL WITH SPACE-GROUP SYMBOLS OR CENTERED LATTICES OF THE TRICLINIC SYSTEM. OUR PROGRAM SOLVES THESE PROBLEMS, MOREOVER, IT DOES REORIENTATION AND REWRITTING OF THE SPACE-GROUP SYMBOL IN ACCORDANCE WITH THE PRIORITY RULE OF THE SYMMETRY ELEMENTS.

THE PROGRAM MAKES MANY LOGICAL DESISIONS SUCH AS HOW TO CONVERT AN UNCONVENTIONAL SETTING TO THE CONVENTIONAL ONE, TO REORIENT THE SPACE-GROUP SYMBOL. FORTRAN IS NOT ALWAYS CONVENIENT FOR THIS PURPOSE ESPECIALLY WHEN DEALING WITH SPACE-GROUP SYMBOLS, NEVERTHELESS, WHEREVER PRACTICAL, THE PROGRAM IS WRITTEN IN FORTRAN. SEVERAL SUBROUTINES WHICH BECAME CUMBERSOME AND INEFFICIENT IN FORTRAN WERE WRITTEN IN FAP, WITH THE HELP OF DR. J. N. STEWART OF THE UNIVERSITY OF MARYLAND. THESE FAP SUBROUTINES PROCESS THE ALPHANUMERICAL INFORMATION BY ''A'' FORMAT SPECIFICATIONS. FOR EXAMPLE THE LINEAR OUTPUT FORM OF THE TRANSFORMATION MATRIX IS PREPARED BY A FAP SUBROUTINE. THE CELL DIMENSIONS ARE READ FORST BY ''A'' SPECIFICATION AND AFTER DETERMINING THE NUMBER OF DECIMAL PLACES AFTER THE DECIMAL POINT, THE PROGRAM CONVERTS THEM TO FLOATING POINT NUMBERS BY A FAP SUBROUTINE. THE OUTPUT FORMAT IS SELECTED TO PRINT THE TRANSFORMED DATA IN ACCORDANCE WITH THE HIGHEST ACCURACY OF THE ORIGINAL DATA.

DESCRIPTION OF THE METHOD

THE PRINCIPLES OF THE METHOD USED IN THIS PROGRAM ARE GIVEN IN DETAIL BY J. D. H. DONNAY (1954) AND BY M. J. BUERGER (1957, 1960).

(1) MAIN ROUTINE

THE FIRST STEP OF THE MAIN ROUTINE IS TO CONVERT ALL DATA, NUMERICAL VALUES AS WELL AS SPACE-GROUP SYMBOL FROM INPUT TO INTERNAL FORM AN TO CHECK THAT THE DATA ARE COMPATIBLE WITH THE CRYSTAL SYSTEM. THE SECOND STEP IS TO CALL THE SUBROUTINE OF THE APPROPRIATE CRYSTAL SYSTEM, RHOMBH, ORTHOR, MONOCL AND TRICLI. THEN THE TRANSFORMED RESULTS ARE CHECKED. FOR MONOCLINIC AND ANORTHIC FOR EXAMPLE, ONE CHECK IS BASED ON THE CONSTANCY OF THE CELL VOLUME BEFORE AND AFTER REDUCTION. FINALLY THE OUTPUT FORM IS PREPARED, GIVING THE TRANSFORMED VALUES OF A/B, C/B,A,B,C, (OR C/A,A,C FOR A RHOMBOHEDRAL CELL). CARE IS TAKEN NOT TO LOOSE ANY OF THE ACCURACY OF THE ORIGINAL DATA BY ADUTP. NEXT THE REORIENTED SPACE-GROUP SYMBOL AND THE TRANSFORMATION MATRIX IN LINEAR FORM AS PRINTED, FINALLY FOLLOWED BY THE ORIGINAL DATA.

IF A CELL HAS ONE OR MORE 90 DEGREE ANGLES OR IF IT HAS EQUAL EDGES, IT IS HANDLED BY ONE OF TWO SUBROUTINES NAMED RANCL AND SAME. THEN CONTROL IS TRANSFERRED TO READ THE NEXT CARD.

(2) SUBROUTINES OF RHOMBOHEDRAL SYSTEM.

RHOMBH THE CELL (ARH , ALPHA) IS TRANSFORMED TO HEXAGONAL (C/A,A,C) THROUGH THE EXPRESSIONS

$$\cos P = 1/(3)^{0.5}\tan(\mathrm{ALPHA}/2)$$

$$C/A = ((3)^{0.5}/2)\tan(P)$$

$$A = 2A(\mathrm{RH})\sin(\mathrm{ALPHA}/2)$$

$$C = 3A(\mathrm{RH})\cos(\mathrm{ALPHA}/2)\sin(P)$$

(3) SUBROUTINES OF ORTHORHOMBIC SYSTEM.

ORTHOR USING THE KNOWN ROUTINE TO FIND THE LARGEST VALUE IN AN ARRAY, THE PROGRAM ARRANGES CELL EDGES AND SYMMETRY ELEMENTS OF THE SPACE GROUP IN THE SEQUENCE A GREATER THEN B GREATER THAN C, SETTING THE INDEX OF TRANSFORMATION ITR. ITR TELL WHICH OF THE SIX POSSIBLE TRANSFORMATIONS APPLIE AFTER THAT, A AND B ARE INTERCHANGED. BY MEANS OF COMPUTED GO TO STATEMENTS, USING ITR AS AN INDEX, IT SETS THE TRANSFORMATION MATRIX INTERNALLY AND REORIENTS THE SPACE-GROUP SYMBOL THROUGH THE SUBROUTINE SMTR WHICH TAKES CARE OF THE INTERCHANGE OF AXES. FINALLY ORTHOR CALLS SUBROUTINES EX221 AND CONVO.

CONVO REWRITES THE SPACE-GROUP SYMBOL TO OBEY THE PRIORI RULE OF THE INTERNATIONAL TABLES, M, A, B, C, D, N EXCEPT THAT IBCA IS USED INSTEAD OF IBBA. IN THE CASE OF ''DOUBLE-GLIDE PLANES'' E.G. I ( ) ( ) ( ), B AND C GLIDE PLANES ALTERNATE PARALLEL TO (100), ETC. FOR EACH CENTERED LATTICE LISTED IN TABLE 1, IF THE BOTTOM LETTER IS WRITTEN, IT REWRITES THE TOP ONE B INSETAD OF C, ETC.

TABLE 1

(L STANDS FOR LATTICE MODE 1, 2, 3, FOR AXIAL DIRECTIONS X, Y, Z)

L	1	2	3
A	B		
	C	.	.
B		A	
	.	C	.
C			A
	.	.	B
I	B	A	A
	C	C	B

EX221 SOME OF THE SPACE-GROUP SYMBOLS LISTED IN TABLE 2, ARE WRITTEN WITH 2 INSTEAD OF 21 . THIS SUBROUTINE EXAMINES THE SPACE-GROUP SYMBOL AND CHECKS WHETHER 21 SHOULD OR SHOULD NOT REPLACE 2. E.G., IF PMC2 IS WRITTEN, IT MUST BE REWRITTEN AS PMC21. THIS IS PERFORMED IN A SINGLE ROUTINE ACCORDING TO LOC.

TABLE 2

(L STANDS FOR LATTICE MODE 1, 2, 3, FOR THE AXIAL DIRECTIONS X, Y, Z)

L	1	2	3	L	1	2	3	L	1	2	3
P	M	C(N)	2_1	P	B(N)	2_1	M	P	2_1	M	A(N)
	B	C(N)	2_1		B(N)	2_1	A		2	C	A(N)
	C	M(A)	2_1		M(C)	2_1	B		2_1	C	M(B)
	N	M(A)	2_1		M(C)	2_1	N		2_1	N	M(B)
C	M	C	2_1	B	M	B	2_1	A	5_1	M	A
	C	M	1		B	M	1		1	A	M

SMTR THE SUBROUTINE CHANGES THE BRAVAIS LATTICE SYMBOL BL1 TO BL2 OR VICE-VERSA AND ALSO CHANGES THE GLIDE-PLANE SYMBOL GP1 TO GP2 OR VICE-VERSA IN THE ORTHORHOMBIC SYSTEM. FOR EXAMPLE, SUPPOSE AMAA HAS TO BE REORIENTED AFTER INTERCHANGING THE A AND B AXES. THE CALLING ROUTINE HAS ALREADY REWRITTEN AAMA. NOW SMTR, WITH ARGUEMENTS BL1 = A, BL2 = B, GP1 = A, GP2 = B, IS CALLED TO REWRITE BBMB.

(4) SUBROUTINES OF MONOCLINIC SYSTEM.

MONCL THE SUBROUTINE FIRST EXAMINES ALPHA, BETA, GAMMA. IF THE UNCONVENTIONAL SETTING (C UNIQUE) IS FOUND, IT REWRITES THE DATA IN THE CONVENTIONAL SETTING (B UNIQUE) REORIENTS THE SPACE-GROUP (B CENTERED TO C, B GLIDE PLANE TO C GLIDE PLANE) REGISTERS THE NEW-FROM-OLD TRANSFORMATION MATRIX 100/00-1/010 BY CALLING THE SUBROUTINE TRANS. A SUBROUTINE CONVM IS CALLED TO REWRITE ANY UNCONVENTIONAL SPACE-GROUP SYMBOL TO THE CONVENTIONAL ONE. THE MONOCLINIC SUBROUTINE THEN EXAMINES BETA. FOR BETA, IT ALWAYS TAKES THE SUPPLEMENT OF BETA. IF THE DATA COME FROM AN OLD MORPHOLIGICAL PAPER, THE ANGLE BETA WAS DEFINED AS THE ACUTE ANGLE (BETWEEN THE AXES +C AND -A) THE COMMENT S MEANS THAT THE SUPPLEMENT IS TAKED INSTEAD. NOWADAYS BETA IS THE ANGLE BETWEEN +C AND +A, AND IT USUALLY IS OBTUSE IF IT IS ACUTE IN A CRYSTAL PAPER, THE TRANSFORMATION TAKES IT INTO ACCOUNT AND THE COMMENT T RECALLS THE FACT.

THIRD STEP, IF C IS GREATER THAN A, THE C AND A AXES ARE INTERCHANGED BY CHAC, WHICH ALSO REORIENTS THE SPACE-GROUP SYMBOL AND CALLS SUBROUTINE TRANS. THESE THREE STEPS FACILITATE THE NEXT STEPS, WHICH ARE THE REDUCTION OF THE CELL AND THE LAST REORIENTATION OF THE SPACE-GROUP.

AFTER CALCULATING THE SCALAR PRODUCTS AND THE MESH AREA ARO, IT CALLS SHORT AND SPREO TO FIND THE SECOND SHORTEST TRANSLATION IN THE PLANE (ASSUMING C TO BE THE SHORTEST) AND TO REORIENT THE SPACE-GROUP. IF A HAS BECOME SMALLER THAN C , THE MONOCLINIC SUBROUTINE AGAIN CALLS SHORT AND SPREO. AFTER A SECOND REDUCTION, IF AGAIN A BECOMES SMALLER THAN C , CHAC IS CALLES TO INTERCHNAGE A AND C .

TWO THINGS MUST NOW BE DONE (1) TO TEST THE CONDITION FOR REDUCED CELL (2) TO CONFIRM THE CONSTANCY OF THE MESH AREA AFTER REDUCTION.

FOR THE LAST CHECK.....

THE VALUES OF CELL EDGES AND ANGLES, OBTAINED FROM THE FINAL REDUCED SCALAR PRODUCTS, ARE CONFRONTED (IN THE SUBROUTINE CHECK) WITH THE VALUES OBTAINED DIRECTLY FROM THE ORIGINAL VECTORS BY THE TRANSFORMATION MATRIX THAT WAS CALCULATED IN THE SUBROUTINE NWAX.

LITERATURE CITED

(1) DONNAY,J.D.H., =CRYSTAL DATA=, 2ND ED., ACA MONOGRAPH NO. 5.

(2) BUERGER,M.J., ZEIT. KRIST. (1957). VOL 109, PAGE 42.

(3) IBID., (1960). VOL 113, PAGE 52.

CALCULATE R OVER PROJECTION

THE =RPLANE= PROGRAM WAS WRITTEN BY JAMES R. HOLDEN.

THE =RPLANE= PROGRAM IS DESIGNED TO PERMIT THE CALCULATION OF THE VALUE OF R = (SUM DELTA-F)/(SUM FO) FOR A GIVEN ORIENTATION OF A MOLECULE FOR ZONAL PROJECTIONS. THE MOLECULAR COORDINATES ARE TREATED BY BEING TRANSLATED BY SPECIFIC INCREMENTS PARALLEL TO THE ZONAL AXES. STRUCTURE FACTORS ARE CALCULATED FOR EACH OF THE TRANSLATIONALLY RELATED COORDINATES AND THE R VALUE IS PUBLISHED. THERE IS A LIMIT OF 200 ATOMS IN THE UNIT CELL.

THE BEGINNING POINT OF THE COORDINATE TO BE VARIED, THE FINAL POINT, AND THE INCREMENT CAN BE SPECIFIED FOR EACH OF THE ZONAL DIRECTIONS. THE PROGRAM THEN CALCULATES EVERY POINT WITHIN THE BLOCK SO SPECIFIED.

THE OUTPUT IS IN THE FORM OF A MAP GIVING THE VALUES OF R FOR EACH POINT IN THE SPECIFIED BLOCK WITH LABELED COORDINATES.

R LIST PROGRAM

THE R LIST PROGRAM WAS WRITTEN BY WILLIAM KEEFE AND J. M. STEWART.

THE PROGRAM CALCULATES VARIOUS MEASURES OF THE RELIABILITY OF STRUCTURES. IN ALL 11 DIFFERENT MEASURES OF AGREEMENT BETWEEN OBSERVED AND CALCULATED STRUCTURE FACTORS ARE PREPARED. THE OUTPUT OF THE PROGRAM LIS THE QUANTITIES CALCULATED. PROVISION HAS BEEN MADE TO LIST R'S FOR ALL THE USUAL ZONES, LAYERS, AND GROUPS OF REFLECTIONS. IN ADDITION TO THE CONVENTIONAL SCALE GROUPS ONE MAY LIST BY GROUPS OF SINE THETA BY LAMBDA, EITHER IN EQUAL INCREMENTS OF THAT QUANTITY OR IN EQUAL NUMBERS OF REFLECTION AS THAT QUANTITY INCREASES. FOR EACH SET OF R VALUES THERE ARE LISTED NUMBER OF REFLECTIONS IN THE VARIOLS CATEGORIES.. OBSERVED, EXTINCT, LESS-THAN, AND LESS-THAN CALCULATING ABOVE THE THRESHOLD VALUE.

A BREIF SUMMARY OF THE R VALUES CALCULATED.....

R1	SUM DELTA F/SUM F OBSERVED
R2	SUM DELTA F/SUM F OBSERVED (INCLUDES LESS-THANS)
R3	LESS-THANS ONLY
R4, R5, R6	REPEATS R1, R2, AND R3 USING SQUARED QUANTITIES
R7	LIKE R1 BUT INCLUDES REFLECTION MULTIPLICITY
R8	LIKE R1 BUT INCLUDES EFFECT OF DISPERSION CORRECTION
R9	(DELTA B) IS THE SLOPE OF LN(FO/FC) AGAINST SIN SQUARED THETA OVER LAMBDA SQUARED
R10	(SCALE) THE RATIO OF SUM FC TO SUM FO (LESS-THANS INCLUDED AT ONE HALF VALUE)
R11	AN APPROXIMATION OF THE STANDARD ERROR OF AN OBSERVATION OF UNIT WEIGHT (SQRTF((WLF)**2/NO))

LOCATION OF PEAKS IN FOURIER MAPS

THE PROGRAM WAS WRITTEN BY MARGARET O. DAYHOFF AND J. M. STEWART.

=PEAKPK=EXAMINES A FOURIER OR PATTERSON MAP AND RETURNS THE COORDINATES AND DENSITY OF THE MAXIMA. THREE ADDITIVE ONE DIMENSIONAL PARABOLIC INTERPOLATIONS ARE MADE TO FIND THE COORDINATES AND THE DENSITY OF THE TRUE PEAK. THE MAXIMUM DEVIATION OF THIS APPROXIMATION TO A ONE DIMENSIONAL GAUSSIAN CURVE IS .003 GRID UNITS AND .02 PERCENT DENSITY FROM THE TRUE VALUE.

THE FOURIER OR PATTERSON MAP IS READ INTO CORE, ONE LAYER AT A TIME, INCLUDING AS MANY AS 20,000 POINTS PER LAYER. THE LAYER IS SCANNED FOR GRID PEAKS. NEAR EACH OF THESE, THE TRUE PEAK LOCATION AND DENSITY IS DETERMINED AND THE VALUES STORED. MAXIMA ALONG THE BOUNDARY SURFACE OF THE MAP ARE ACCEPTED AS BEING IN THE SURFACE. AS SUCCESSIVE LAYERS ARE READ IN, RECORDS KEPT OF THE LOCATION, DENSITY AND LAYER NUMBERS OF EACH PEAK IN THE LAST TWO LAYERS IN WHICH IT HAS BEEN FOUND. AS SOON AS THE DENSITY OF A PEAK DECREASE THE INTERPOLATION BETWEEN THREE SUCCESSIVE LAYER PEAKS IS MADE AND COORDINATE AND DENSITY ARE PRINTED OUT. IF THREE PEAKS ARE AVAILABLE, A PARABOLIC FIT I MADE. IF ONLY TWO HAVE BEEN FOUND, THE LARGER OF THE TWO IS ASSUMED TO BE TH EXACT POSITION.

IDENTICAL PEAKS FROM EACH LAYER MUST BE MATCHED. IF SPECIAL RESOLUTION OF PEAKS IS DESIRED, THE DISTINCTION BETWEEN THE LAYER COORDINATES OF TWO SUCCESSIVE PEAKS MAY BE SET DURING THE SEARCH.

VALUES FOR A MAXIMUM OF 100 PEAKS CAN BE STORED AT ANY GIVEN TIME DURING THE SEARCH. IF PEAKS BECOME TOO NUMEROUS IN ANY GIVEN LAYER, THE EXCESS IS LOST. THIS MAY HAPPEN IF THE CUTOFF OF DENSITY IS SET TOO LOW OR IF TOO MANY PEAKS ARE SEARCHED FOR IN ONE PASS. PEAKS ARE ELIMINATED FROM THE LISTS WHEN THEY ARE NO LONGER DETECTABLE IN THE LATEST LAYER. GRID POINTS BELOW CUTOFP(ARE SKIPPED OVER. IF ANY GRID POINTS ARE BELOW CUTOFP(2), (HOLES) A SIGNAL I SET. IF THE NUMBER OF PEAKS READ OUT BECOMES GREATER THAN INUMB, PEAK-PICKIN IS TERMINATED.

AS MANY AS NPEAKS PEAKS ARE STORED. SYMMETRICALLY RELATED PEAKS ARE ELIM INATED AFTER EACH ADDITION. IF NPEAKS IS EXCEEDED, THE LOWEST PEAK ALREADY STORED IS REPLACED.

THE THREE PROJECTIONS OF ATOMS IN THE UNIT CELL ARE PRINTED OUT.

THE MATRIX OF CONNECTIONS BETWEEN ATOMS IN THE WHOLE MOLECULE IS GENERATE

CONVERT SYSTEM REFLECTION TAPE TO NON-SYSTEM INPUT FORMATS

THE FUNCTION OF THE =BYEBYE= PROGRAM IS TO ALLOW ONE TO READILY CONVERT THE X-RAY SYSTEM REFLECTION TAPE TO ANY FORMAT DESIRED. AT THE PRESENT TIME =BYEBYE= IS CONSTRUCTED WITH THREE SWITCHES FOR THE FOLLOWING FORMATS-

(1) U. OF W. IBM 650 SYSTEM REFLECTION DECK FORMAT.

THESE DECKS HAVE SIGNS-OVER-UNITS. DECIMAL PLACES AS SHOWN ARE NOT PUNCHED IN CARDS. COLUMNS MUST NOT BE BLANK OR ALPHABETIC.

1- 4	XXXX	DECK IDENTIFICATION CODE, OR ZEROS.
5	X	8 IF EXTINCTION, OTHERWISE 9
6	X	8 IF UNOBSERVED, OTHERWISE 9
7-10	00XX	H INDEX (SIGN-OVER-UNITS)
11-16	00XXXX	1.0/WEIGHT
17-20	00XX	K INDEX (SIGN-OVER-UNIT)
21-26	X.XXXXX	(SIN THETA)/LAMBDA
27-30	00XX	L INDEX (SIGN-OVER-UNIT)
31-35	00000	ZEROS
36-40	XXXX.X	F-RELATIVE (FOR UNOBSERVED, FREL = FMIN = MINIMUM OBSERVABLE F AT THIS VALUE OF (SIN THETA)/LAMBDA.
41-42	00	ZEROS
43-46	XX.XX	SCATTERING FACTOR, TYPE ONE, F(1)
47-50	XX.XX	F(2)
51-52	00	ZEROS
53-56	XX.XX	F(3)
57-60	XX.XX	F(4)
61-62	00	ZEROS
63-66	XX.XX	F(5)
67-70	XX.XX	F(6)
71-72	00	ZEROS
73-76	XX.XX	F(7)
77-80	XX.XX	F(8)

WHENEVER THE LEVEL INDICATOR ON THE REFLECTION TAPE CHANGES VALUE, A =CONSTANTS= CARD IS INSERTED IN THE 650 REFLECTION DECK. THE FORMAT OF THE =CONSTANTS= CARD IS- (9A,16X,I1,3X,I2)

1- 9	CONSTANTS	
10-25		BLANKS
26	X	NUMBER OF SCATTERING FACTORS
27-29	BLANKS	
30-31	XX	LEVEL NUMBER
32-72		BLANKS

THE LAST CARD OF THE DECK IS AN X-40 TRAILER CARD WHICH HAS EACH COLUMN NON-BLANK AND AN 11-PUNCH IN COLUMN 40.

(2) U. OF W. IBM 650 SYSTEM FC DECK FORMAT.

THESE DECKS HAVE SIGNS-OVER-UNITS. DECIMAL PLACES AS SHOWN ARE NOT PUNCHED IN CARDS. COLUMNS MUST NOT BE BLANK OR ALPHABETIC.

1- 2	XX	TRIAL NUMBER OR ZEROS
3	X	8 IF 2FC LESS-THAN FO OR FC LESS THAN FMIN OTHERWISE 9
4	X	8 IF FC LESS THAN FO OR FC LESS THAN FMIN OTHERWISE 9
5	X	8 FOR FO WITH EXTINCTION, OTHERWISE 9.
6	X	8 FOR FO UNOBSERVED, OTHERWISE 9.
7-10	00XX	H INDEX
11-16	XX.XXXX	DISPERSION RATIO, OR ZEROS
17-20	00XX	K INDEX
21-26	X.XXXXX	(SIN THETA)/LAMBDA
27-30	00XX	L INDEX
31-36	000000	ZEROS
37-40	XXX.X	F-OBSERVED
41-46	000000	ZEROS
47-50	XXX.X	F-CALCULATED
51-56	000000	ZEROS
57-60	XXX.X	DELTA-F = ABSF(FO)-ABSF(FC)
61-65	00000	ZEROS
66-70	X.XXXX	COS ALPHA = A/ABSF(FC)
71-75	00000	ZEROS
76-80	X.XXXX	SIN ALPHA = B/ABSF(FC) (SIN ALPHA = ZERO FOR CENTRIC CASE)

THE FC DECK IS PRECEEDED BY A =650= CARD HAVING =650= IN COLS 1-3 AND BLANKS IN COLS 4-72. THE FC DECK IS FOLLOWED BY AN X-40 TRAILER.

(3) ORXLS - BUSING-LEVY IBM 704 FULL-MATRIX LEAST-SQUARES REFINEMENT PROGRAM DATA TAPE FORMAT. REFER TO THE OAK RIDGE NATIONAL LABORATORY WRITE-UP OF =ORXLS= FOR THE TAPE FORMAT.

IF ONE DESIRES ANY OTHER FORMAT, HE MAY EITHER MODIFY THE PROGRAM =BYEBYE= TO ACCEPT CODING OF (ICHOOS) = 4 IN COL 23 OF THE =BYEBYE= CARD OR ELSE HE MAY WRITE HIS OWN EQUIVALENT OF =BYEBYE=. THE READER IS REFERRED TO SECTION 1.1 IN THIS MANUAL FOR GUIDANCE IN CODING PROGRAMS WITH THE SYTEM AND FOR INSTRUCTIONS ON HOW TO LOAD A NEW SYSTEM PROGRAM USING THE =LOADER= FEATURE.

PART II - USERS GUIDE (INPUT DATA)

A. CARD ORDER SUMMARY

REFER TO THE APPROPRIATE SECTION OF THIS PART FOR DETAILED LISTINGS OF SUBROUTINES REQUIRED FOR THE PROGRAMS. THESE LISTINGS WILL BE IN THE =2.XX-C= SECTION FOR EACH PROGRAM. A SUMMARY OF ALL SUBROUTINES IN THE X-RAY PROGRAM SYSTEM IS GIVEN IN APPENDIX I, SECTION 3.1-A.

IN THIS SECTION, A =*= INDICATES AN OPTIONAL CARD. GENERALLY, THE IDENTIFYING SIX CARD COLUMNS ARE MADE AS A MNEMONIC OF THE CARD FUNCTION IN THE PROGRAM. A SUMMARY OF ALL CARD FORMATS IS GIVEN IN APPENDIX II, SECTION 3.2.

EACH COMPUTER LABORATORY HAS LABORATORY SPECIFIC RUN CARDS FOR JOB SUBMISSION. EXAMPLES OF CARD ORDERS FOR IBM 709 COMPUTER RUNS AT THE RESEARCH COMPUTER LABORATORY AT THE UNIVERSITY OF WASHINGTON ARE GIVEN IN APPENDIX VI, SECTION 3.6. THESE EXAMPLES FOLLOW THE USERS MANUAL OF THE RESEARCH COMPUTER LABORATORY (EDITION OF APRIL 1963) AND ALSO SERVE AS EXAMPLES FOR JOB SUBMISSION IN OTHER INSTALLATIONS.

THE VARIOUS PROGRAMS ARE LINKED BY A SCHEME LIKE THE FORTRAN-CHAIN SYSTEM. THE LINK LABELS AND THE CALLING CARDS FOR EACH PROGRAM ARE GIVEN IN APPENDIX V, SECTION 3.5.

THE ELEVEN OPERATION CARDS (SEE SECTION 1.0-A) RECOGNIZED AT ANY TIME BY THE =CALLER= PROGRAM MAY BE INSERTED WITHIN A DATA DECK AT THE USERS DISCRETION. PREFERRED TIMES OF INSERTION ARE GIVEN IN SECTION 2.0-B. THESE CARDS ARE NOT EXHAUSTIVELY CITED (IF AT ALL) IN ANY OF THE CARD ORDER SUMMARIES IN PART II INASMUCH AS THEIR USE BECOMES SELF-EVIDENT.

B. PREFERRED TIMES FOR OPERATION CARD INSERTION

ALL OF THE OPERATION CARDS ARE ACCEPTABLE AT ANY TIME AT THE USERS DISCRETION, BUT THEY ARE MOST USEFUL AS FOLLOWS-

REMARK - USED ANY TIME A REMARK IS DESIRED ON OUTPUT TAPE.

TITLE - USED BEFORE CALLING CARD OF PROGRAM TO CORRECTLY STORE PAGE TITLE.

TAPES - USED BEFORE CALLING CARD OF PROGRAM TO ASSIGN TAPE UNITS IF LABORATORY STANDARD DESIGNATIONS ARE NOT DESIRED (REFER TO SECTION 1.0-A FOR DETAILS).

PRINTR - BEFORE CALLING CARD OF PROGRAM WHICH WILL WRITE SPECIAL OUTPUT.

OPRATR - USED WHENEVER OPERATOR COMMUNICATION OR INTERVENTION IS NEEDED.

PAUSE - USUALLY USED DIRECTLY FOLLOWING AN =OPRATR= CARD TO ALLOW THE MACHINE OPERATOR TIME TO ACT ON THE =OPRATR= CARD.

ENDFIL - WHENEVER IT IS DESIRED TO SEPARATE FILES ON THE OUTPUT TAPE -- USUALLY USED BETWEEN PROGRAMS.

ENDTAP - AFTER THE =END= CARD OR A PROGRAM WHOSE OUTPUT WAS ON A SPECIAL TAPE.

IGNORE - USED BEFORE A =*DATA= CARD.

SAVE - USED WHEN A FRESHLY GENERATED TAPE IS TO BE SAVED. IT IS USUALLY USED AFTER A =*DATA= CARD AND JUST BEFORE A =FINISH= CARD. THIS CARD ASSURES THAT THE TAPE(S) SPECIFIED IS MECHANICALLY SEPARATED FROM THE COMPUTOR(7090-7094 ONLY). NO TAPES SHOULD EVER BE SPECIFIED THAT ARE TO BE READ IN SUCCEEDING CALCULATIONS OR THAT DO NOT ACTUALLY REQUIRE OPERATOR INTERVENTION.

FINISH - =ABSOLUTE= TERMINATION OF A RUN. NEVER USE THIS CARD AFTER AN =IGNORE= CARD OR IN THE MIDDLE OF A RUN. ALWAYS USE THIS CARD WITH A MONITOR THAT HAS NO END-OF-FILE BETWEEN JOBS (E.G.- BELL MONITOR).

REFER TO SECTION 1.0-A FOR MORE DETAILS CONCERNING OTHER USES OF THE OPERATION CARDS.

C. CARD FORMATS FOR OPERATION CARDS.

THE OPERATION CARDS ARE COLLECTED IN THIS SECTION FOR USER CONVENIENCE. THESE CARDS ARE DESCRIBED IN MORE DETAIL REGARDING THEIR USES IN SECT 1.0-A. THESE CARDS MAY BE USED AT ANY TIME IN ANY OF THE PROGRAMS IN THE SYSTEM.. PREFERRED TIMES FOR INSERTION ARE SUGGESTED IN SECT 2.0-B1.

```
*DATA   - USED BY MONITOR AND =CALLER= TO DENOTE BEGINNING OF DATA
          DECK.  REQUIRED IN ALL PROGRAMS.
          FORMAT (A1,5XA6)
               1     *              (ASTERISK)
             2- 6                   (BLANK)
             7-10     DATA
            11-72                   (BLANK)

ENDFIL  - ENDFILE OUTPUT TAPE.  OPERATION CARD.  CAUSES END-OF-FILE
          TO BE WRITTEN ON THE BCD OUTPUT TAPE (NTOUT).
          FORMAT (A6)
             1- 6     ENDFIL
             7-72                   (IGNORED)

ENDTAPE - END OUTPUT TAPE.  OPERATION CARD.  WRITES MESSAGE =END OF
          OUTPUT TAPE= ON TAPE =NTOUT=.  WRITES 20 END-OF-TAPE MARKS ON
          TAPE =NTOUT=.  REWINDS TAPE =NTOUT=.  REDEFINES =NTOUT= TO
          =NTOUTN= (IF NTOUT=NTOUTN, ENDTAP CARD IS IGNORED).
          FORMAT (A6)
             1- 6     ENDTAP
             7-72                   (IGNORED)

FINISH  - =ABSOLUTE= TERMINATION CARD (NEVER USE AFTER AN =IGNORE= CARD
          OR IN THE MIDDLE OF A RUN).
          FORMAT (A6)
             1- 6     FINISH
             7-72                   (IGNORED)

IGNORE  - IGNORE INPUT.  OPERATION CARD.  CAUSES FOLLOWING CARD TO BE
          IGNORED (SKIPPED UNCONDITIONALLY) AND SUBSEQUENT CARDS TO BE
          SKIPPED UNTIL A =*DATA= CARD IS REACHED.  (USED PRINCIPALLY
          JUST BEFORE A =*DATA= CARD).
          FORMAT (A6)
             1- 6     IGNORE
             7-72                   (IGNORED)

OPRATR  - OPERATOR INSTRUCTION CARD.  OPERATION CARD.  OCCURRANCE OF ONE
          OR MORE =OPRATR= CARDS CAUSES THE CONTENTS TO BE WRITTEN ON-
          LINE AS AN INSTRUCTION TO THE COMPUTER OPERATOR.  (THE INSTRUC-
          TIONS ARE ALSO LISTED OFF-LINE LIKE =REMARK= CARD.)
          FORMAT (12A6)
             1- 6     OPRATR
             7-72     INSTRUCTION TO COMPUTER OPERATOR  (11A6)
```

```
PAUSE  - STOP COMPUTER.  OPERATION CARD.  CAUSES COMPUTER TO WRITE ON-
         LINE MESSAGE =PRESS START TO CONTINUE= AND STOPS.  USED MAINLY
         AFTER =OPRATR= CARD TO WAIT FOR OPERATOR TO CARRY OUT INSTRUCT.
         FORMAT (A6)
           1- 6     PAUSE$
           7-72                    (IGNORED)

PRINTR - PRINTER INSTRUCTION CARD.  OPERATION CARD.  OCCURENCE OF ONE
         OR MORE  PRINTR  CARDS CAUSES THE CONTENTS TO BE WRITTEN OFF-
         LINE AS AN INSTRUCTION TO THE PRINTER OPERATOR AND CAUSES THE
         PRINTER TO BE STOPPED.  THE PRINTER WILL ALSO STOP AGAIN,
         INDICATING THE END OF THE JOB AND TO RETURN THE PRINTER TO
         ITS NORMAL CONDITION.
         FORMAT (12A6)
           1- 6     PRINTR      (A6)
           7-72     INSTRUCTION TO OFF-LINE PRINTER OPERATOR. (11A6)

REMARK - REMARK CARD.  OPERATION CARD.  A REMARK CARD IS USED TO
         INSERT A REMARK ONTO THE BCD OUTPUT TAPE AT ANY TIME FOR
         INCLUSION ON THE OFF-LINE LISTING.
         FORMAT (12A6)
           1- 6     REMARK      (A6)
           7-72     ALPHANUMERIC INFORMATION FOR REMARK  (11A6)

SAVE   - SAVE CARD.  REWIND AND UNLOAD (7090,7094) FUNCTION CARD.  THIS CARD
         IS USED TO PREVENT THE LOSS OF A NEWLEY GENERATED TAPE.  IT CAUSES
         THE SPECIFIED LOGICAL TAPE TO BE MECHANICALLY REMOVED FROM THE
         COMPUTOR.
         FORMAT (A6,12I3)
           1- 6     SAVE$$
           7- 9
          10-12
          .....
          40-42
                    NUMBERS OF THE LOGICAL TAPES TO BE UNLOADED.  THE
                    FIRST BLANK FEILD TERMINATES THE SCAN OF THE CARD.

TAPES  - TAPE ASSIGNMENT CARD.  OPERATION CARD.  A BLANK FIELD OR
         ZEROS IN COLS 7-42 IMPLIES NO CHANGE IN ASSIGNMENT FOR THE
         TAPE DESIGNATED BY THAT FIELD.
         FORMAT (A6,12I3)
           1- 6     TAPES$
                    NEW LOGICAL TAPE NUMBER FOR ----
           7- 9     $XX          NTIN     BCD INPUT TAPE (FROM CARD READER)
          10-12     $XX          NTOUT    BCD OUTPUT TAPE (TO PRINTER)
          13-15     $XX          NTAPEA   BINARY DATA TAPE (REFLECTIONS)
          16-18     $XX          NTAPEB   BINARY DATA TAPE (STRUCT.FACTORS)
          19-21     $XX          NTAPEC   BCD CARD OUTPUT (TO PUNCH)
          22-24     $XX          NTAPED   SPECIAL BCD OUTPUT (OPTIONAL PRNT)
          25-27     $XX          NTAPEE   SPECIAL UTILITY OUTPUT TAPE
          28-30     $XX          NTAPEF   SPECIAL UTILITY INPUT TAPE
          31-33     $XX          NTAPEG   UNDESIGNATED INPUT-OUTPUT
          34-36     $XX          NTAPEH   UNDESIGNATED INPUT-OUTPUT
          37-39     $XX          NTAPEI   UNDESIGNATED INPUT-OUTPUT
          40-42     $XX          NTAPEJ   UNDESIGNATED INPU T-OUTPUT
          43-72                  (IGNORED)

TITLE  - TITLE CARD.  OPERATION CARD.  PRINTS TITLE ON EACH PAGE OF
         OFF-LINE OUTPUT.
         FORMAT (12A6)
           1- 6     TITLE$      (A6)
           7-72     ALPHANUMERIC INFORMATION FOR PAGE TITLE.
```

D. STATEMENT REGARDING STANDARDIZATION OF CARD FORMATS AND INCLUSION OF SUBROUTINES IN THE =X-RAY 63= SYSTEM.

THE FOLLOWING STATEMENT REGARDING FORTRAN CONVENTIONS IS APPLICABLE TO ALL SECTIONS OF THIS WRITE-UP RELATING TO CARD FORMATS.

FAMILIARTY WITH FORTRAN CONVENTIONS REGARDING INTEGER, FIXED, FLOATING AND BCD INPUT IS A NECESSARY ADJUNCT TO UNDERSTANDING THESE CARD FORMATS. A DOLLAR SIGN ($) INDICATES A BLANK COLUMN MUST BE PRESENT, EXCEPT AS SPECIFICALLY ALLOWED BY FORTRAN CONVENTIONS. COLUMNS NOT SPECIFIED MAY CONTAIN ANY LEGAL HOLLERITH PUNCHES. A PLUS SIGN IMPLIES A PLUS OR MINUS SIGN. IN EACH CARD THE FIRST SIX COLUMNS REPRESENTS CARD TYPE IDENTITY. THESE COLUMNS ARE INVIOLABLE. EACH PROGRAM DEPENDS UPON THEM TO IDENTIFY UNEQUIVOCALLY THE CARD FUNCTION.

NOTE THAT THE PROGRAMS WILL FUNCTION CORRECTLY IF THESE FORMATS ARE PUNCHED EXACTLY AS LISTED. FIELDS MAY BE MODIFIED ONLY WITHIN THE FORTRAN CONVENTIONS.

THE FOLLOWING STATEMENT REGARDING INCLUSION OF SUBROUTINES IN THE VARIOUS PROGRAMS OF THE =X-RAY 63= SYSTEM IS GIVEN HERE (USING THE =BEGIN= PROGRAM AS AN EXAMPLE). THE SEVERAL LISTS IN THIS WRITE-UP DO NOT INCLUDE THE SUBROUTINES IN THE UTILITY PACKAGE (SEE SECT 2.0-F) AND IF ANY OF THESE PROGRAMS ARE TO BE USED INDEPENDENTLY OF THE SYSTEM THESE SUBROUTINES MUST BE INCLUDED.

THE SUBROUTINES INCLUDED WITH =BEGIN= ARE GIVEN BELOW. MORE DETAILED INFORMATION CONCERNING ALTERNATE ENTERING MODES AND INTERNAL STRUCTURE MAY BE FOUND IN APPENDIX I, SECT 4.1. ALL BINARY DECKS ARE IDENTIFIED BY A CODE NAME AND SEQUENTIAL CARD NUMBERS IN COLS. 73-80. ALL FORTRAN LIBRARY ROUTINES CALLED BY =BEGIN= ARE INCLUDED IN THE BINARY PROGRAM DECKS TO PRECLUDE PROGRAM MALFUNCTION DUE TO LABORATORY SPECIFIC FORTRAN LIBRARY CHANGES.

ROUTINES ENDING WITH =UW= ARE FROM RCL-IBM LIBRARY, SUMMER 1962.

E. UTILITY PACKAGE ROUTINES.

THIS IS A LIST OF THE SYSTEM ROUTINES WHICH ARE COMMON TO ALL OF THE =X-RAY 63= PROGRAMS. IF ANY OF THE SYSTEM PROGRAMS ARE TO BE USED INDEPENDENTLY, THESE ROUTINES MUST BE INCLUDED WITH THE ROUTINES LISTED FOR THE PROGRAM IN PART II OF THIS SYSTEM WRITE-UP.

CALLER	CONTROL SUBROUTINE FOR X-RAY SYSTEM.
EFTUW	FORTRAN ENDFILE TAPE (9EFT)
EXEMW	REPLACES FORTRAN EXECUTION ERROR ROUTINE (9XEM).
FPTUW	FORTRAN FLOATING POINT TRAP (9FPT)
IOBUW	FORTRAN INPUT-OUTPUT BINARY (9IOB)
IOHUW	FORTRAN INPUT-OUTPUT HOLLERITH (9IOH).
~~IOSW~~	~~MODIFIED FORTRAN INPUT-OUTPUT SUPERVISOR (9IOS).~~
NAME	LEFT-JUSTIFY ALL NON-BLANK CHARACTERS IN BCD WORD
RERW	MODIFIED FORTRAN TAPE READ ERROR (9RER)
RWTUW	FORTRAN REWIND TAPE (9RWT)
SPHW	MODIFIED FORTRAN STORAGE TO PRINTER HOLLERITH (9SPH).
STBUW	FORTRAN STORAGE-TO-TAPE BINARY (9STB)
STHW	MODIFIED FORTRAN STORAGE TO TAPE HOLLERITH (9STH).
TESUW	FORTRAN TEST LAST WRITE (9TES).
TIME	READS CLOCK. LABORATORY SPECIFIC ROUTINE TO GIVE MIN. IN FLOAT. POIN DIFFERENT ROUTINE FOR EACH SHOP. TIMEMD READS THE LOCS STORAGE CLOCK
TSBUW	FORTRAN TAPE-TO-STORAGE BINARY (9TSB)
WERW	MODIFIED FORTRAN TAPE WRITE ERROR (9WER).

A. CARD ORDER SUMMARY FOR =LOADER= PROGRAM (LINK 100.

LOADER CALLS PROGRAM. GIVES SIX CHARACTER TAPE IDENTIFICATION AND UNIT UPON WHICH NEW SYSTEM TAPE IS TO BE GENERATED.

*BEGIN USED TO DENOTE THE BEGINNING OF UTILITY SUBROUTINE PACKAGE. ONLY REQUIRED IF UTILITY PACKAGE IS TO BE ALTERED.

*LINK USED TO DENOTE BEGINNING OF BINARY DECK OF A SPECIFIED LINK.

END END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

READS =NTPROG= AND WRITES THE TAPE SPECIFIED IN THE =LOADER= CARD.

B. CARD FORMATS FOR =LOADER= PROGRAM.

```
LOADER - CALL SYSTEM UPDATE PROGRAM
         FORMAT (A6,1X,A6,I3)
           1- 6       LOADER
             7        $          BLANK
           8-13                  NEW TAPE ID (E.G. =7MAY63=)
          14-16       XXX        =LOGICAL= TAPE NUMBER UPON WHICH THE NEW
                                   SYSTEM TAPE IS TO BE GENERATED
          17-72                  (IGNORED)

BEGIN  - MARKS THE BEGINNING OF BINARY DECKS OF UNIVERSALLY USED
         SUBROUTINES THAT WILL BE STORED IN LOW CORE.
         FORMAT (A6)
           1- 6       BEGIN$
           7-72                  (IGNORED)

LINK   - TO MARK BEGINNING OF A LINK.
         FORMAT (A6,I5)
           1- 6       LINK$$
           7-11       XXXXX      LINK NUMBER AS SPECIFIED IN =CALLER= (SEE
                                   APPENDIX V)
          12-72                  (IGNORED)
```

C. PROGRAM DECK AND SUBROUTINES FOR =LOADER= PROGRAM.

LINK 100	=LOADER= PROGRAM
BEGIN	PROGRAM FOR UPDATING AND/OR LOADING SYSTEM TAPE.
IOUW	FORTRAN INPUT-OUTPUT UNIT TABLE (9IOU).
SYSCOM	SUBROUTINE TO INITIALIZE SYSTEM COMMON STORAGE.

D. PROGRAM LOADING SEQUENCE FOR =NOCALL= OPERATION.

LIST OF =LOADER= PROGRAM SUBROUTINES REQUIRED AS CARD DECKS TO RUN UNDER THE FORTRAN MONITOR AS A PRIMARY SOURCE TO GENERATE AN X-RAY SYSTEM TAPE FROM THE BINARY DECKS OF PROGRAMS AND SUBROUTINES. ONCE THESE PROGRAMS HAVE BEEN UTILIZED, THE PROGRAM TAPE ITSELF CAN FULFIL THE =LOADER= FUNCTION.

NOCALL	CUT-DOWN VERSION OF =CALLER= FOR NON-CHAIN OPERATION.
ERREC	ERROR RECORD SUBROUTINE.
SYSCOM	SUBROUTINE TO INITIALIZE SYSTEM COMMON.
IOUW	INPUT-OUTPUT ROUTINE. REPLACES FORTRAN (9IOU). U OF W SPECIFIC.
BEGIN	SYSTEM =BEGIN= ROUTINE AND BSS LOADER (PROGRAM TAPE GENERATOR).
IOHUW	FORTRAN INPUT-OUTPUT HOLLERITH (9IOH)
IOSW	MODIFIED FORTRAN INPUT-OUTPUT SUPERVISOR (9IOS).
SPHW	MODIFIED FORTRAN STORAGE TO PRINTER HOLLERITH (9SPH).
STHW	MODIFIED FORTRAN STORAGE TO TAPE HOLLERITH (9STH).
TESUW	FORTRAN TEST LAST WRITE (9TES)
WERW	MODIFIED FORTRAN TAPE WRITE ERROR (9WER).

A. CARD ORDER SUMMARY FOR STRUCTURE FACTOR PROGRAM.

FC — CALLING CARD FOR STRUCTURE FACTOR PROGRAM.

*LABEL — TAPE HEADING. TAPE IDENTIFICATION INFORMATION.

*GRID — FOURIER GRID CARD. REQUIRED ONLY IF =ATOMG= OR =BNORMG= CARDS ARE USED. THIS CARD NEED BE USED ONLY ONCE FOR ANY GIVEN GRID SPECIFICATION. IT IS THEN STORED ON THE BINARY TAPE UNTIL CHANGED BY A SUBSEQUENT =GRID= CARD.

*EDIT — EDIT CARD FOR MODIFYING REFLECTIONS.

*SCALE — SCALE CARD. F-RELATIVE SCALE FACTORS FOR VARIOUS GROUPS OF REFLECTIONS, OR MULTIPLICATIVE F-RELATIVE SCALE FACTOR TO CHANGE ALL STORED FACTORS BY A CONSTANT VALUE. GROUPS FOR WHICH NO =SCALE= CARD APPEARS WILL BE SCALED BY THE CONSTANT ON THE BINARY TAPE.

*MAXHKL — FOR MAKING TAPES WITH LIMITED DATA (IDENTICAL WITH SIMILAR FOURIER CARD). THE =NTAPEB= WILL NOT CONTAIN REFLECTIONS OUTSIDE THE SPECIFIED MAXIMA.

IF AN =END= CARD APPEARS AT THIS POINT, STRUCTURE FACTORS WILL BE CALCULATED FROM PARAMETERS STORED ON THE INPUT TAPE.
IF ANY ATOMIC PARAMETERS ARE SUPPLIED ON CARDS, ALL PARAMETERS FOR ALL ATOMS MUST BE SUPPLIED ON CARDS.

FOR OVERALL TEMPERATURE FACTOR, A SINGLE =B=, =BIJ=, =UIJ=, =BETA=, =BNORM=, OR =BNORMG= CARD MUST BE THE FIRST PARAMETER CARD. IF IN THE INDIVIDUAL TEMPERATURE FACTOR MODE, EACH =ATOM= OR =ATOMG= CARD MUST BE FOLLOWED BY A TEMPERATURE FACTOR CARD (EXCEPT THAT ISOTROPIC =B= COULD BE PUNCHED IN =ATOM= OR =ATOMG= CARD). BE SURE THAT THE ATOM IDENTITY CODE IN COLS 8-13 OF =ATOM= OR =ATOMG= CARD IS IDENTICALLY THE SAME AS THE IDENTITY CODE ON THE FOLLOWING TEMPERATURE FACTOR CARD. NOTE THAT THE PROGRAM RECOGNIZES =B=, =BIJ=, =UIJ=, =BETA=, =BNORM=, AND =BNORMG= CARDS AND CONVERTS THEM INTERNALLY SO THAT THESE CARDS MAY BE DIFFERENT FOR EACH ATOM.

ATOM — ATOM PARAMETER CARD IN FRACTIONAL COORDINATES.

ATOMG — ATOM PARAMETER CARD IN FOURIER GRID COORDINATES. THIS CARD REQUIRES A =GRID= CARD (ABOVE).

B ISOTROPIC TEMPERATURE FACTOR CARD.

BIJ ANISOTROPIC TEMPERATURE FACTOR CARD.

UIJ ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRATION IN CRUICKSHANK NOTATION.

BETA ANISOTROPIC TEMPERATURE FACTOR CARD.

BNORM ANISOTROPIC TEMPERATURE FACTOR CARD RELATED TO AXES OF VIBRATION ELLIPSOID.

BNORMG ANISOTROPIC TEMPERATURE FACTOR CARD RELATED TO AXES OF VIBRATION ELLIPSOID REFERRED TO FOURIER GRID COORDINATES. REQUIRES A =GRID= CARD (A8C0E).

IF MORE THAN ONE TEMPERATURE FACTOR SPECIFICATION APPEARS FOR A GIVEN ATOM. THE PROGRAM SAVES ONLY THE LAST TEMPERATURE FACTOR READ, WITH THE FOLLOWING EXCEPTION= IF A =BNORM= OR =BNORMG= CARD IS READ ITS CONTRIBUTION TO THE ANISOTROPIC TEMPERATURE FACTOR IS ADDED TO ANY PREVIOUS ANISOTROPIC SPECIFICATION. ANY NUMBER OF =BNORM= OR =BNORMG= CARDS MAY BE USED FOR THEIR ADDITIVE CONTRIBUTIONS.

END END CARD. CAUSES THE PROGRAM TO SUMMARIZE AND RETURN CONTROL TO NEXT PROGRAM SEGMENT.

(OR)

END-TRACE END CARD TO INITIATE SNAPSHOT TRACE OF EXECUTION OF =FCALC= AND A CORE DUMP FOR PROGRAM CHECKING BEFORE RETURNING CONTROL TO NEXT PROGRAM SEGMENT.

THE STRUCTURE FACTOR PROGRAM HAS A =USERS PATCH= PROVISION. WHEN SWITCHED IN BY =CALCOS(7)= THIS SUBROUTINE IS CALLED AT INITIALIZATION TIME BY=

```
TSX     SETFCP,4
```

AND AGAIN JUST BEFORE EACH REFLECTION IS WRITTEN OUT BY=

```
TSX     FCPACH,4
TSX     DF
TSX     FO
```

THE TWO QUANTITIES IN THE CALLING SEQUENCE ARE NOT IN COMMON STORAGE. THIS PROCEDURE IS NOT GENERALLY RECOMMENDED UNLESS THE PROGRAMMER IS VERY CONVERSANT WITH FORTRAN AND FAP CODING SINCE CAREFUL STUDY OF THE PROGRAM STATEMENTS AND COMMENTS WILL BE NECESSARY. BE SURE TO OBSERVE THE =CAVEAT TWIDDLER= CONCERNING COMMON STORAGE. PATCHING IS ACCOMPLISHED THROUGH THE =LOADER= PROGRAM.

B. CARD FORMATS FOR STRUCTURE FACTOR PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
FC      - SET-UP CARD FOR STRUCTURE  FACTOR CALCULATION.
          FORMAT (A6,1X,A6,8X,8I4,F6.0,I4)
            1- 6     FC$$$$
              7      $              BLANK
            8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
           14-21                    BLANK
           22-25     $$$X           RESCALE CODE.  (1)/(2) FOR USE (OLD)/(NEW)
                                      F RELATIVE SCALE FACTORS.
           26-29     $$$X           FIXAT.  (1)/(2)/(3)  FOR  (NO PARTIAL
                                      CONTRIBUTION)/(PARTIAL CONTRIBUTION)/
                                      (USE PREVIOUS FC AS PARTIAL CONTRIB.)
           30-33     $$$X           HI-FI.  (1)/(2)  FOR  (LO-FI)/(HI-FI) TRIG
                                      AND EXPONENTIAL FUNCTIONS.
           34-37     $$$X           DISPERSION CORRECTION.  (1)/(2)  FOR
                                      (DO NOT APPLY)/(APPLY WHERE NECESSARY)
           38-41     $$$X           USER PATCH. (1)/(2) FOR (BYPASS)/(APPLY)
           42-45     $$$X           (1)/(2) FOR (NORMAL)/(CRIPPLE AUTOMATIC
                                      SCALING OF ATOMS AT SYMMETRY CENTERS FOR
                                      CENTRIC ONLY)
           46-49     $$$X           FC SCALE FACTOR.  (1)/(2)  FOR  (NORMAL)/
                                      (SPECIAL).
           50-53     $$$X           FOR OVERALL T.F. ALWAYS COMPUTES CORRECT.
                                      TO OVERALL B.  (1)/(2) FOR (USE OLD)/
                                      (USE NEW) VALUE FOR B.
                                      FOR INDIVIDUAL T.F. (1)/(2)  FOR
                                      (DO NOT)/(DO) COMPUTE OVERALL B.
           54-59     $XXXX.         SPECIAL FC SCALE FACTOR.  (NUMBER OF
                                      ASYMMETRIC UNITS OR MOLES, IF OTHER
                                      THAN THAT DETERMINED BY LATTICE TYPE.)
           60-63     $$$I           BLANK, ZERO, OR ONE CAUSES PARAMETERS TO
                                      LIST ON BCD OUTPUT TAPE. TWO WILL CAUSE
                                      PARAMETERS AND FC TO LIST.  THREE
                                      SUPRESSES BOTH.  (IT IS BEST TO LIST FC
                                      AT FOURIER OR DIFFERENTIAL SYNTHESIS
                                      TIME BY CODING THE =FOURR= OR =DIFSYN=
                                      CARD TO LIST FC, THEREBY SAVING ABOUT
                                      1/3 OF CALCULATION TIME MOVING TAPES.)
           64-72                    ANY LEGAL PUNCHING DESIRED, OR BLANKS.

LABEL   - TAPE LABELING CARD.  USED TO IDENTIFY BINARY TAPE.
          FORMAT (12A6)
            1- 6      LABEL$
            7-72     ALPHANUMERIC INFORMATION TO BE USED AS TAPE LABEL

GRID    - FOURIER GRID CARD.
          FORMAT (A6,1X,A6,3I4)
            1- 6     GRID$$
              7      $              BLANK
            8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
           14-17     $XXX           NUMBER OF GRID INTERVALS ALONG THE X
                                      AXIAL DIRECTION.
           18-21     $XXX           GRID INTERVALS ALONG Y AXIAL DIRECTION
           22-25     $XXX           GRID INTERVALS ALONG Z AXIAL DIRECTION
           26-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
EDIT    - EDIT CARD FOR MODIFYING REFLECTIONS AT FC TIME.
          FORMAT (A6,1X,5I5,2F10.5)
            1- 6     EDIT$$
              7      $              BLANK
            8-12     XXXXX          H OF REFLECTION NEEDING CHANGE.
           13-17     XXXXX          K OF REFLECTION NEEDING CHANGE.
           18-22     XXXXX          L OF REFLECTION NEEDING CHANGE.
                       NOTE= LEAVING ANY ONE OF FIELDS IN COLS. 23-52
                                BLANK WILL CAUSE FCALC TO USE OLD VALUES
           23-27     XXXXX          NEW JCODE STATUS 1/2/3 FOR OBSERVED/
                                      UNOBSERVED/EXTINCT
           28-32     XXXXX          NEW LEVEL INDICATOR (1 TO 64 ALLOWED)
           33-45     XXXX.XXXXX      NEW FRELATIVE AS (F10.5)
           43-52     XXXX.XXXXX      NEW LEAST SQUARES WEIGHT
           53-72     ANY LEGAL DESIRED PUNCHING, OR BLANKS.

SCALE   - SCALE CARD FOR F RELATIVE DATA
          FORMAT (A6,F10.4,I4,F10.4,I2,3F10.4)
            1- 6     SCALE$
            7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
           17-20     $$XX          GROUP IDENTIFICATION (1-64)     (I4)
                                     A GROUP IDENTITY OF ZERO WILL APPLY
                                     OVERALL F-RELATIVE SCALE TO STORED
                                     VALUES OF SCALE FACTORS. SCALE CARDS
                                     LOADED AFTER GROUP=ZERO WILL NOT BE
                                     AFFECTED.
           21-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

MAXHKL  - LIMITS FOR FOURIER SUMMATION.
          FORMAT (A6,1X,A6,3I4,2F8.4)
            1- 6     MAXHKL
              7      $              BLANK
            8-13                      COMPID, COMPOUND IDENTIFICATION CODE.
           14-17     $XXX           MAXIMUM H TO BE USED     (I4)
           18-21     $XXX           MAXIMUM K TO BE USED
           22-25     $XXX           MAXIMUM L TO BE USED
           26-33     $X.XXXXX       MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                     NO LIMIT)    (F8.4)
           34-41     $X.XXXXX       MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                     NO LIMIT)    (F8.4)
           42-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
              7      $              BLANK
            8-13                     ATOM NAME - CONSISTS OF TWO PARTS. THE
                                       FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                       THE ATOM-TYPE NAME (SEE FORMFX). THE
                                       REST OF THE WORD, UP TO A TOTAL OF SIX
                                       COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                       OF THE PARTICULAR ATOM. THIS SECOND PART
                                       MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX       X    FRACTIONAL COORDINATE     (F8.4)
                                       DECIMAL POINT MUST BE PUNCHED IN ORDER
                                       TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX       Y
           30-37     $XX.XXXX       Z
           38-43     $X.XXX         INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                       MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                       ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                       TEMPERATURE FACTOR CARD IS USED, SINCE
                                       THIS WORD IS THEN IGNORED.
           44-48     $X.XX          INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                       BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX       STANDARD DEVIATION IN X.  (OPTIONAL - THIS
                                       IS REQUIRED ONLY IF PROGRAMS TO BE
                                       USED REQUIRE THE INFORMATION.)
           57-64     $X.XXXXX       STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX       STANDARD DEVIATION IN Z.
```

```
ATOMG   - ATOM PARAMETER CARD BASED ON GRID POINTS.
          FORMAT (A6,1X,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOMG$
            7-72                    SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                      EXPRESSED AS GRID VALUES FROM FOURIER
                                      MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                      CARDS MUST BE PRECEDED BY A LEADING
                                      GRID CARD.

B       - ISOTROPIC TEMPERATURE FACTOR CARD.
          FORMAT (A6,1X,A6,F8.4)
            1- 6     B$$$$$
              7      $               BLANK
            8-13                     COMPID IF OVERALL TEMPERATURE FACTOR.
            8-13                     NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
           14-21     $XX.XXXX        B
           22-61                     MUST BE BLANK.
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BIJ     - ANISOTROPIC TEMPERATURE FACTOR CARD.  IN FORTRAN NOTATION
                     8*(PI**2)*U(I,J)=B(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BIJ$$$
              7      $               BLANK
            8-13                       NAMEAT.
           14-21     $XX.XXXX        B11   (F8.4)
           22-29     $XX.XXXX        B22
           30-37     $XX.XXXX        B33
           38-45     $XX.XXXX        B12
           46-53     $XX.XXXX        B13
           54-61     $XX.XXXX        B23
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

UIJ     - ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRATION
                     SEE D.W.J.CRUICKSHANK,ACTA CRYST,VOL 9,747-758 (1956)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     UIJ$$$
            7-61     FORMAT IDENTICAL WITH BIJ CARD.
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BETA    - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                     2*(PI**2)*ASTAR(I)*ASTAR(J)*U(I,J)=BETA(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BETA$$
            7-61     FORMAT IDENTICAL WITH BIJ CARD
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
BNORM  - ANISOTROPIC TEMPERATURE FACTOR CARD, WHERE TEMPERATURE FACTOR
                 IS EXPRESSED IN TERMS OF B(I) USING THREE PRINCIPAL
                 AXES OF THE ELLIPSOID OF VIBRATION, AND THE E(I,J)
                 ARE VECTORS WHICH EXPRESS THE DIRECTIONS OF TWO OF
                 THE THREE PRINCIPAL AXES OF THE VIBRATION ELLIPSOID.
                 THE THIRD IS ASSUMED TO BE NORMAL TO THESE TWO.
         FORMAT (A6,1X,A6,9F6.4)
           1- 6     BNORM$
              7     $              BLANK
           8-13                      NAMEAT.
          14-18     X.XXXX         B1   (F6.4)
          19-25     X.XXXX         B2
          26-31     X.XXXX         B3
          32-37     X.XXXX         E11
          38-43     X.XXXX         E12
          44-48     X.XXXX         E13
          49-54     X.XXXX         E21
          55-60     X.XXXX         E22
          61-66     X.XXXX         E23
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BNORMG - ANISOTROPIC TEMPERATURE FACTOR CARD. LIKE THE =BNORM= CARD
                 EXCEPT COEFFICIENTS ARE BASED ON GRID POINTS.
         FORMAT (A6,1X,A6,9F6.4)
           1- 6     BNORMG
           7-66     FORMAT IDENTICAL WITH BNORM CARD.
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.


END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
              7     $              BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

END-TRACE - END CARD TO INITIATE SNAPSHOT TRACE.
         FORMAT (A6,A5)
           1- 6       END$$$
           7-11       TRACE
          12-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR STRUCTURE FACTOR PROGRAM.

LINK 1000 PARAMETER LOADER FOR FC.

FCONE	PARAMETER LOADING PROGRAM FOR STRUCTURE FACTOR CALCULATION.
ATN	DISCARDS RIGHT DIGITS FROM ATOM NAME, LEFT JUSTIFIES ATOM NAME DESIGNATION, AND LOOKS UP ATOM TYPE NUMBER FROM DICTIONARY.
DOT	DOT PRODUCT BETWEEN TWO VECTORS.
EDIT	USERS PATCH TO ALLOW EDITING OF SELECTED REFLECTIONS PRIOR TO THE CALCULATION OF FC.
ERASE	WRITES BLANK TAPE FOR RECORDS TO BE REWRITTEN.
ORDNL	HAS SENSE ENOUGH TO PUT PROPER SUFFIX ON OUTPUT NUMBERS. (I.E.= 22NDS INSTEAD OF 22THS (WHICH LOOKS SILLY)).
PMV	MATRIX VECTOR PRODUCT.
PSV	SCALAR VECTOR PRODUCT.
PVMV	VECTOR MATRIX VECTOR PRODUCT.
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
SQUASH	PACKS UP THE ATOM PARAMETER STORAGE DEPENDING UPON THE TYPE OF TEMPERATURE FACTOR DATA TO BE CALCULATED.
UCROSS	NORMALIZED CROSS PRODUCT BETWEEN TWO VECTORS.
UNITV	NORMALIZED VECTOR.

LINK 1001 FC STATISTICS PROGRAM.

FCTWO	TAPE WRITING AND STATISTICS CALCULATING PROGRAM FOR STRUCTURE FACTOR PROGRAM.
DMPUW	FORTRAN DUMP ROUTINE (9DMP)
ERASE	WRITE BLANK TAPE FOR RECORDS TO BE REWRITTEN.
FCALC	CALCULATION OF STRUCTURE FACTORS.
FCINPU	READS REFLECTION DATA FOR FC SUBROUTINE.
FCOUTP	WRITE REFLECTION DATA FOR FC SUBROUTINE.
FCPACH	DUMMY WHICH ALLOWS PATCHING OF FC JUST BEFORE THE FINAL WRITE OUT OF THE REFLECTION DATA.
FCSUMS	ACCUMULATES SUMS FOR R AND RESCALE. IN OVERALL TEMPERATURE FACTOR MODE, CALCULATES CORRECTION TO ISOTROPIC TEMP. FACTOR.
GENRAT	GENERATION OF SYMMETRIC ATOMS FROM SPACE GROUP CONSIDERATIONS.
LOGUW	FORTRAN FLOATING POINT LOG ROUTINE (9LOG)
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
TRACE	SNAPSHOT TRACE FOR CHECK-OUT CONVENIENCE.
XMIX	CONVERT FLOATING POINT NUMBER TO FIXED POINT NUMBER.

C. PROGRAM DECK AND SUBROUTINES FOR DIFFERENTIAL SYNTHESIS PROGRAM.

LINK 2000 DIFFERENTIAL SYNTHESIS PROGRAM

DIFSYN	PROGRAM FOR DIFFERENTIAL SYNTHESIS (LINK 2000)
ATN	LOOK-UP ATOM NAME IN ATOM-TYPE DICTIONARY
ERASE	WRITES BLANK TAPE FOR RECORDS TO BE RE-WRITTEN
EXPAND	SUBROUTINE TO EXPAND ATOM PARAMETERS FOR INDIVIDUAL ANISOTROPIC TEMPERATURE FACTOR DATA
FCOUTP	WRITE REFLECTION DATA FOR FC SUBROUTINE
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SOLVPM	SUBROUTINE TO SOLVE PARAMETER SHIFTS
SOLVTM	SUBROUTINE TO SOLVE TEMPERATURE FACTOR SHIFTS
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
SQUASH	PACKS ATOM PARAMETERS STORAGE DEPENDING ON TEMPERATURE FACTOR
XPFUW	FORTRAN FLOATING POINT EXPONENTIAL ROUTINE (9XPF)

A. CARD ORDER SUMMARY FOR SYSTEM =ORFLS=

ORFLS	CALLING CARD FOR BUSING-MARTIN-LEVY LEAST-SQUARES
*SCALE	SCALE CARD FOR F RELATIVE DATA
*ATOM	ATOM PARAMETER CARD
*B	ISOTROPIC TEMPERATURE FACTOR CARD
*BETA	ANISOTROPIC TEMPERATURE FACTOR CARD
*BIJ	ANISOTROPIC TEMPERATURE FACTOR CARD
*REF	TURN ON REFINEMENT
*NOREF	SHUT OFF REFINEMENT
*NOTEMP	SHUT OFF REFINEMENT OF ALL TEMPERATURE FACTORS
*NOSCAL	SHUT OFF REFINEMENT OF SPECIFIED SCALE FACTORS
END	END CARD

* THESE CARDS ARE OPTIONAL.

(NOTE 1) THE =B=, =BETA=, OR =BIJ= CARDS (IF ANY) FOR A GIVEN ATOM MUST FOLLOW EXACTLY BEHIND THE =ATOM= CARD FOR THAT ATOM.

(NOTE 2) ALL ATOM, TEMPERATURE FACTOR, AND SCALE INFORMATION MUST BE LOADED BEFORE ANY REFINEMENT INSTRUCTIONS

(NOTE 3) THIS PROGRAM HAS NEVER HEARD OF OVERALL TEMPERATURE FACTORS.

(NOTE 4) IF NO ATOM PARAMETERS ARE LOADED THE ONES ON THE BINARY TAPE ARE USED. IF ANY ARE LOADED FROM CARDS ONLY THOSE FROM THE CARDS ARE USED.

(NOTE 5) IF ALL REFINEMENT RESTRICTION CARDS ARE LEFT OUT REFINEMENT WILL BE ON ALL SCALE, POSITIONAL, AND TEMPERATURE PARAMETERS. HOWEVER, NO SCATTERING FACTORS OR MULTIPLICITY FACTORS WILL BE SET TO REFINE.

***** READS =NTAPEA= AND WRITES =NTAPEB= *****

ONLY IF THE PROGRAM IS SET TO PUNCH CARDS (COLS 32-34 OF =ORFLS= CARD WRITES THESE IMAGES IN THE BCD MODE ON =NTAPEC=, THE PUNCH TAPE.

B. CARD FORMATS FOR SYSTEM =ORFLS=

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
ORFLS  - CALLING CARD FOR BUSING-MARTIN-LEVY LEAST-SQUARES PROGRAM.
         FORMAT (A6,1X,A6,1I3, 3F4.3,I3)
           1- 6       ORFLS$
             7        $          BLANK
           8-13                  COMPID - COMPOUND IDENTIFICATION CODE
          14-16       $$X        NUMBER OF CYCLES TO BE CALC.  (NC)
          17-19       $$X        (1)/(2) FOR (ISOTROPIC)/(ANISOTROPIC)(ITF)
                                   PROGRAM CONVERTS IF REQUIRED. AVERAGE
                                   DIAGONAL ELEMENT USED IN ANISOTROPIC
                                   CONVERSION
          20-22       $$X        (BLANK)/(1)/(2) FOR REFINEMENT BASED ON
                                   (F)/(F**2)/(F CORRECTED FOR DISPERSION)
                                   (IFSQ)
          23-25       $$X        (BLANK)/(1) FOR USE (SCALE)/(RESCALE)
                                   FACTORS FROM TAPE     (IRESC)
          26-28       $$X        (BLANK)/(1) FOR (LC-FI)/(HI-FI) TRIG
                                   FUNCTIONS       (IFI)
          29-31       $$X        (BLANK)/(1) FOR (WEIGHTS FROM TAPE)/(ALL
                                   WEIGHTS EQUAL 1.0)      (IW)
          32-34       $$X        (BLANK)/(1)/(2)/(3) FOR (NO CARDS)/(PUNCH
                                   CARDS)/(PUNCH CARDS AND IGNORE NON
                                   POSITIVE DEFINITE TEST)/(SET BACK THE T.F.
                                   WHICH GO NON-POS-DEF)          (IT)
          35-37       $$X        (BLANK)/(1) FOR (DO NOT)/(DO) LIST THE
                                   REFLECT. INFO. DURING LAST CYCLE (ILIST)
          38-40       $$X        BLANK= DO NOT LIST.
                                   1 = LIST THE REFLECT. FOR WHICH WEIGHTED
                                       DELTA-F IS GREATER THAN  RR  (IREJ)
                                   2 = LIST REJECTED REFLECT. AND ALSO THE
                                       CORRELATION MATRIX FOR EACH CYCLE
          41-43       $$X        (BLANK)/(1)/(2) FOR (NO)/(USE)/(USE PREV-
                                   IOUS FC) FIXED ATOM CONTRIB. (IP)
          44-46       $$X        (BLANK)/(1) FOR (X-RAY)/(NEUTRON) (INEU)
          47-50       .XXX       DAMPING OR ENHANCING FACTOR FOR PARAMETER
                                   SHIFTS (BLANK OR 0.0 = 1.0)
          51-54       .XXX       RR TO CONTROL LIST (BLANK = 2.0)
          55-58       .XXX       REJECT FROM CONSIDERATION IN SHIFTS REFLECTIONS
                                 WHOSE WEIGHTED DELTA-F IS LARGER. (BLANK = 10**
          59-61       $$X        (BLANK)/(1) (NO)/(SPECIAL) SYMMETRY PATCH
                                 REQUIRED.
          62-72                  (IGNORED)

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6     SCALE$
           7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20     $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                 A GROUP IDENTITY OF ZERO WILL APPLY
                                 OVERALL F-RELATIVE SCALE TO STORED
                                 VALUES OF SCALE FACTORS. SCALE CARDS
                                 LOADED AFTER GROUP=ZERO WILL NOT BE
                                 AFFECTED.
          21-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
               7     $              BLANK
            8-13                    ATOM NAME - CONSISTS OF TWO PARTS. THE
                                      FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                      THE ATOM-TYPE NAME (SEE FORMFX). THE
                                      REST OF THE WORD, UP TO A TOTAL OF SIX
                                      COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                      OF THE PARTICULAR ATOM. THIS SECOND PART
                                      MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX    X    FRACTIONAL COORDINATE    (F8.4)
                                      DECIMAL POINT MUST BE PUNCHED IN ORDER
                                      TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX    Y
           30-37     $XX.XXXX    Z
           38-43     $X.XXX      INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                      MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                      ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                      TEMPERATURE FACTOR CARD IS USED, SINCE
                                      THIS WORD IS THEN IGNORED.
           44-48     $X.XX       INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                      BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX    STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                      REQUIRED BY PROGRAM BEING USED.)
           57-64     $X.XXXXX    STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX    STANDARD DEVIATION IN Z.

B       - ISOTROPIC TEMPERATURE FACTOR CARD.
          FORMAT (A6,1X,A6,F8.4)
            1- 6     B$$$$$
               7     $              BLANK
            8-13                    NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
           14-21     $XX.XXXX    B
           22-61                 NUST BE BLANK.
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BETA    - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                    2*(PI**2)*ASTAR(I)*ASTAR(J)*U(I,J)=BETA(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BETA$$
            7-61     FORMAT IDENTICAL WITH BIJ CARD
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BIJ     - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                    8*(PI**2)*U(I,J)=B(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BIJ$$$
               7     $              BLANK
            8-13                      NAMEAT.
           14-21     $XX.XXXX    B11   (F8.4)
           22-29     $XX.XXXX    B22
           30-37     $XX.XXXX    B33
           38-45     $XX.XXXX    B12
           46-53     $XX.XXXX    B13
           54-61     $XX.XXXX    B23
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
REF     - REFINE ON NAMED PARAMETER CARDS.
          FORMAT (A6,1X,A6,11A3)
            1- 6        REF$$$
               7        $              BLANK
            8-13                       ATOM ID (IF THIS FIELD IS LEFT BLANK THIS
                                         CARD ACTS ON ALL ATOMS).
                                         (IF ONLY A SCATTERING FACTOR DESIGNATION IS
                                         PUNCHED THIS CARD ACTS UPON ALL ATOMS OF THE
                                         SCATTERING FACTOR TYPE PUNCHED.)
          IF THE FOLLOWING FIELDS ARE ALL LEFT BLANK (OR NOT PUNCHED FROM
          THE FOLLOWING VALID LIST) THIS CARD ACTS ON THE NAMED ATOM.
          WITHIN ANY OF THESE ELEVEN FIELDS THE FOLLOWING SYMBOLS WILL
          HAVE MEANING=
            S     SCATTERING FACTOR
            M     MULTIPLICITY FACTOR
            X,Y,Z,  X,Y,Z ATOMIC PARAMETERS
            B     ISOTROPIC TEMPERATURE FACTOR
            B11,B22,B33,B12,B13,B23  ANISOTROPIC TEMPERATURE FACTORS
            B     TURNS ON ALL SIX TEMPERATURE FACTORS IF IN THE
                    ANISOTROPIC MODE
           14-16        XXX            (SYMBOL FROM ABOVE LIST)
           17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43
           44-46        XXX            (SYMBOL FROM ABOVE LIST)
           47-72                       (IGNORED)

NOREF   - DO NOT REFINE ON NAMED PARAMETER CARDS.
          FORMAT (A6,1X,A6,11A3)
            1- 6        NOREF$
               7        $              BLANK
            8-13                       ATOM ID (IF THIS FIELD IS LEFT BLANK THIS
                                         CARD ACTS ON ALL ATOMS).
          IF THE FOLLOWING FIELDS ARE ALL LEFT BLANK (OR NOT PUNCHED FROM
          THE FOLLOWING VALID LIST) THIS CARD ACTS ON THE NAMED ATOM.
          WITHIN ANY OF THESE ELEVEN FIELDS THE FOLLOWING SYMBOLS WILL
          HAVE MEANING=
            S     SCATTERING FACTOR
            M     MULTIPLICITY FACTOR
            X,Y,Z,  X,Y,Z ATOMIC PARAMETERS
            B     ISOTROPIC TEMPERATURE FACTOR
            B11,B22,B33,B12,B13,B23  ANISOTROPIC TEMPERATURE FACTORS
            B     SHUTS OFF ALL SIX TEMPERATURE FACTORS IF IN THE
                    ANISOTROPIC MODE
           14-16        XXX            (SYMBOL FROM ABOVE LIST)
           17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43
           44-46        XXX            (SYMBOL FROM ABOVE LIST)
           47-72                       (IGNORED)

NOTEMP  - CAUSES ALL TEMPERATURE FACTOR REFINEMENT TO BE SHUT OFF.
          FORMAT (A6)
            1- 6        NOTEMP
            7-72                       (IGNORED)

NOSCAL  - CAUSES ALL SCALE FACTOR REFINEMENT TO BE SHUT OFF.
          FORMAT (A6)
            1- 6        NOSCAL         (OR =NOSCALE= IF IT WILL MAKE YOU HAPPY)
            7-16                       (IGNORED)
           17-20        $$XX           (-1)/(BLANK)/(SCALE GROUP INTEGER)
                                       (APPLY OVERALL)/(SHUT OFF ALL)/(SHUT OFF
                                       SPECIFIED GROUP)
           21-72                       (IGNORED)

END     - END CARD.
          FORMAT (A6)
            1- 6        END$$$
               7        $              BLANK
            8-72        ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR =ORFLS= PROGRAM.

LINK 3600 BUSING-MARTIN-LEVY FULL-MATRIX LEAST-SQUARES

ORFLS	BUSING-MARTIN-LEVY FULL-MATRIX LEAST-SQUARES PROGRAM (LINK 3600)
ATNUM	GET ATOM TYPE NUMBER FROM ATOM AND DICTIONARY NAME
ERASE	WRITES BLANK TAPE FOR RECORDS TO BE RE-WRITTEN
ORBET	RESET RELATIONSHIP FOR BETAS WHEN SPECIAL POSITION PATCHING IS REQUIRED (USER SUPPLIED SPECIAL POSITION PATCH).
ORCAL	CALCULATES STRUCTURE FACTORS AND DERIVATIVES
ORFUN	USES SYSTEM CODES TO GENERATE REFLECTIONS
ORIN	READ BINARY REFLECTION TAPE
OROUT	WRITE BINARY REFLECTION TAPE
ORPAC	CORRECTION FOR SPECIAL POSITIONS.
ORPT	COPY PARAMETERS FROM ONE STORAGE ARRAY TO ANOTHER
ORPRE	SETTING-UP OF PRELIMINARY DATA FROM REFLECTION TAPE
ORRES	RESET RELATIONSHIPS FOR POSITIONAL PARAMETERS WHEN SPECIAL POSITIONAL PATCHING IS REQUIRED (USER SUPPLIED SPECIAL PATCH)
ORSBT	COPY PARAMETERS FROM ONE STORAGE ARRAY TO ANOTHER
ORSMI	SYMMETRIC MATRIX INVERTER
ORTES	TEMPERATURE FACTOR EVALUATION
ORTRIG	TRIG FUNCTION ADOPTED FROM SYSTEM =FCALC= SUBROUTINE
ORWT	WRITE NEW PARAMETERS ON FRONT OF BINARY INPUT TAPE
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
XPFUW	FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)

A. CARD ORDER SUMMARY FOR FOURIER SYNTHESIS PROGRAM.

FOURR	CALLING CARD FOR FOURIER PROGRAM.
*FZERO	CHANGE VALUE OF F(0,0,0) FROM THAT SUPPLIED AT DATA REDUCTION
*MAXHKL	LIMITS FOR FOURIER SUMMATIONS.
*MAP	PRINT CONTROL CARD
*GRID	FOURIER GRID CARD (OPTIONAL IF A *GRID* CARD HAS BEEN USED AT ANY PREVIOUS FC CALCULATION TIME).
*REMARK	ANY NUMBER OF REMARK CARDS MAY BE USED TO INSERT REMARKS ON THE OUTPUT TAPE
*PRINTR	INSTRUCTION CARD FOR OFF-LINE PRINTER OPERATOR. USUALLY USED TO INSTRUCT OPERATOR TO TURN-OFF AUTOMATIC OVERFLOW FOR PAGE RESTORING
LAYOUT	DESCRIPTION OF FOURIER MAP
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

* THESE CARDS ARE OPTIONAL. THE ORDER OF *TITLE*, *FZERO*, *MAXHKL*, *GRID*, *REMARK*, AND *PRINTR* IS OPTIONAL. *LAYOUT* AND *END* MUST FOLLOW AFTER THESE CARDS.

***** READS *NTAPEB* AND WRITES *NTAPEO* *****
***** OPTIONALLY WRITES A BINARY COPY OF MAP ON *NTAPEE* *****

(NOTE 1) THE BINARY INPUT TAPE *NTAPEB* WILL BE REWOUND BEFORE AND AFTER EACH FIRST-SUM PASS. IF *NTAPEO* IS NOT THE MONITOR OUTPUT TAPE, THERE WILL BE AN END-OF-FILE AFTER THE OUTPUT FOR EACH MAP.

FOURIER MAP AND THE TAPE *NTAPEO* WILL BE REWOUND AT THE END OF THE RUN, BUT NOT AT THE END OF THE FOURIER.

(NOTE2) IF ANY REFLECTION EXCEEDS THE LIMITS OF H, K, L, OR (SIN THETA)/LAMBDA PUNCHED IN THE *MAXHKL* CARD, THE REFLECTION IS IGNORED. HOWEVER, THE MAXIMA FOR H2 AND H3 SHOULD BE NO LARGER THAN NECESSARY, FOR THEY CONTROL THE EXTENT OF THE CALCULATION TO BE DONE IN THE SECOND AND THIRD SUMS AS WELL AS THE LAYOUT OF STORAGE. THE DATA REDUCTION PROGRAM STORES THE CORRECT VALUES FOR USE OF FULL REFLECTION DATA.

B. CARD FORMATS FOR FOURIER PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
FOURR  - CALLING CARD FOR FOURIER PROGRAM (LINK 4000)
         FORMAT(A6,1X,A6,6X,3I3,F9.5,F4.2)
           1- 6     FOURR$
             7      $            BLANK
           8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
          14-19                   BLANK
          20-22     $$X          (BLANK)/(1)  FOR (NO)/(YES) LIST FC.
          23-25     $XX          CALCULATION TYPE  (I3)    REFER TO
                                   SECT 1.40 FOR DETAILS.
                                   1=USER FUNCTION BY MEANS OF  PATPAT.
                                   2=PATTERSON  (A=FO**2)
                                   3=VECTOR MAP (SHARPENED,ORIGIN REMOVED
                                      PATTERSON).
                                   4=FO FOURIER BY REJECTION TEST WITH
                                      (FO*RR-FC) WITH FMIN/2 FOR LESS-THANS
                                   5=FO FOURIER, FO CORRECTED FOR DISPERS.
                                      RATIO AND CRITERIA (4) USED.
                                   6=FO FOURIER, PHASE ANGLES DETERMINED
                                      FROM UNITARY STRUCTURE FACTORS.
                                   7=FC FOURIER, USES ALL REFLECTIONS.
                                   8=DELTA F, BY REJECTION TEST (FO*RR-FC)
                                      FOR OBSERVED, (FO-FC) FOR LESS-THANS.
                                   9=DELTA F, WITH LEAST SQUARES WEIGHT
                                      APPLIED TO DELTA F   W*(FO-FC).
                                      TEST LESS-THANS BY  (FMIN-FC).
                                  10=DELTA F, FO CORRECTED FOR DISPERSION
                                      RATIO AND CRITERIA (8) USED.
                                  11=DELTA F, OBSERVED REFLECTIONS ONLY.
                                  12=DELTA F, VARIABLE WEIGHTING W=(FC/FO)
                                      OR 1.0 WHICHEVER IS LESS AND REJECT
                                      LESS-THANS CALCULATING LESS-THAN.
                                  13=E MAP. PHASES FROM STATISTICS.
                                  14=E MAP. PHASES FROM FC.
          26-28     $$X          (BLANK)/(1)  USE (OLD)/(NEW) F RELATIVE
                                   SCALE FACTORS.
          29-37     XXX.XXXXX    ELECTRON DENSITY SCALE FACTOR.  BLANKS
                                   GIVES OUTPUT AS 10*(2/V)*SIGMA F. FACTOR
                                   PUNCHED REPLACES  10.
          38-41     X.XX         REJECTION RATIO USED BY CRITERIA TESTS OF
                                   (4) AND (8). IF LEFT BLANK RR SET EQUAL
                                   TO ZERO TO INCLUDE ALL REFLECTIONS.
          42-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

MAXHKL - LIMITS FOR FOURIER SUMMATION.
         FORMAT (A6,1X,A6,3I4,2F8.4)
           1- 6     MAXHKL
             7      $            BLANK
           8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
          14-17     $XXX         MAXIMUM H TO BE USED   (I4)
          18-21     $XXX         MAXIMUM K TO BE USED
          22-25     $XXX         MAXIMUM L TO BE USED
          26-33     $X.XXXXX     MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                   NO LIMIT)   (F8.4)
          34-41     $X.XXXXX     MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                   NO LIMIT)   (F8.4)
          42-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
FZERO  - PUT IN ANY VALUE OF F(000) DESIRED.
         FORMAT (A6,7X,F9.5)
           1- 6     FZERO$
           7-13                BLANKS
          14-22     XXX.XXXXX   VALUE OF F(000) DESIRED.
          23-72     ANY DESIRED LEGAL PUNCHING, OR BLANKS.

LAYOUT - DESCRIPTION OF MAP FOR FOURIER, PATTERSON, ETC..
         FORMAT (A6,1X,A6,9I4,1X,3I1,I4,I2)
           1- 6     LAYOUT          (A6)
             7              $      BLANK
           8-13                    COMPID, COMPOUND IDENTIFICATION CODE.

                    (THE NEXT NINE FIELDS ARE PUNCHED  (I4).)

          14-17     $XXX            NUMBER OF POINTS CALCULATED IN X DIRECTION
          18-21     $XXX            ORIGIN VALUE OF X (IN GRID COORDINATES).
          22-25     $XXX            INCREMENT ALONG X (IN GRID COORDINATES).
          26-29     $XXX            NUMBER OF POINTS CALCULATED IN Y DIRECTION
          30-33     $XXX            ORIGIN VALUE OF Y (IN GRID COORDINATES).
          34-37     $XXX            INCREMENT ALONG Y (IN GRID COORDINATES).
          38-41     $XXX            NUMBER OF POINTS CALCULATED IN Z DIRECTION
          42-45     $XXX            ORIGIN VALUE OF Z (IN GRID COORDINATES).
          46-49     $XXX            INCREMENT ALONG Z (IN GRID COORDINATES).
             50             $      BLANK
             51             X      SCANNING INDEX FOR X DIRECTION.  (I1)
             52             X      SCANNING INDEX FOR Y DIRECTION.  (I1)
             53             X      SCANNING INDEX FOR Z DIRECTION.  (I1)

                    THE SCANNING INDEX FOR A GIVEN DIRECTION IS 1 IF THAT
          COORDINATE GOES FROM PAGE TO PAGE IN THE MAP (FIRST SUM), 2 IF
          IT IS DOWN THE PAGE (SECOND SUM), AND 3 IF IT IS ACROSS THE
          TOP OF THE PAGE (THIRD SUM).

          54-57        $$XX       LINE WIDTH.  (I4)

                    LINE WIDTH W IS THE NUMBER OF POINTS ALONG X3 (THE
          THIRD SCANNING DIRECTION) TO APPEAR ON ONE PAGE.  IF THE
          NUMBER OF POINTS ALONG X3 IS GREATER THAN W + 1, W POINTS
          APPEAR ON THE FIRST PAGE AND THE NUMBER OF POINTS REMAINING
          TO BE PRINTED WILL BE DECREASED BY W. AS SOON AS THE NUMBER OF
          POINTS REMAINING ALONG X3 IS EQUAL TO OR LESS THAN W + 1, ALL
          REMAINING POINTS WILL BE PRINTED ON THIS PAGE. THE MAXIMUM
          PERMISSIBLE VALUE FOR W IS 30.
          (FOR LISTING ON A 120-CHAR. PRINTER (IBM 717), MAX. W IS 27.)
                    AS AN EXAMPLE, IF THE NUMBER OF POINTS ALONG X3 IS
          21 AND W IS 20, ONE PAGE WILL BE LISTED WITH 21 POINTS PER
          LINE.  IF THERE ARE 61 POINTS ALONG X3 AND W IS 30, 30 POINTS
          WILL APPEAR ON THE FIRST PAGE AND 31 ON THE SECOND.
                    IF THIS FIELD IS BLANK, OR W IS OUTSIDE THE RANGE
          10 TO 30, THE PROGRAM WILL COMPUTE AN OPTIMUM VALUE OF W.)

          58-59          $X       SPACE CONTROL INDEX.   (I2)

                    THE SPACE CONTROL INDEX MAY BE 1, 2, 3, 4, FOR SINGLE
          DOUBLE, TRIPLE, OR QUADRUPLE SPACING, RESPECTIVELY. (TRIPLE
          OR QUADRUPLE SPACING REQUIRE EXTRA COMPUTING AND PRINTING
          TIME, AS BLANK LINES MUST BE PRINTED.)
          ANY NUMBER OTHER THAN ONE OF THESE WILL CAUSE DOUBLE SPACING.

          60-72          $        BLANK
```

```
MAP     - PRINT CONTROL CARD.
          FORMAT (A6,1X,A6,3I4)
            1- 6     MAP$$$
               7     $              BLANK
            8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
           14-17       $X           (1)/(2)/(3)  FOR (IGNORE CARD)/(SUPRESS THE
                                      PRINTING OF NUMBERS WITHIN THE RANGE
                                      SPECIFIED)/(WRITE MAP IN BINARY ON =NTAPEE=
                                      AS WELL AS FUNCTION 2)
           18-21      XXXX          UPPER LIMIT TO ESTABLISH PRINT
                                      SUPPRESSION
           22-25      XXXX          LOWER LIMIT WITH SIGN TO ESTABLISH PRINT
                                      SUPPRESSION
           26-72                    MUST BE BLANK

GRID    - FOURIER GRID CARD.
          FORMAT (A6,1X,A6,3I4)
            1- 6     GRID$$
               7     $              BLANK
            8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
           14-17     $XXX           NUMBER OF GRID INTERVALS ALONG THE X
                                      AXIAL DIRECTION.
           18-21     $XXX           GRID INTERVALS ALONG Y AXIAL DIRECTION
           22-25     $XXX           GRID INTERVALS ALONG Z AXIAL DIRECTION
           26-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

END     - END CARD.
          FORMAT (A6)
            1- 6     END$$$
               7     $              BLANK
            8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR FOURIER SYNTHESIS PROGRAM.

LINK 4000 FOURIER SUMMATION PROGRAM.

FOURR	PROGRAM FOR FOURIER SYNTHESIS.
FOFUN	FOURIER REFLECTION READING, GENERATOR, AND FOSUM FEEDER.
FOSUM	TRICLINIC FOURIER SUMMATION PROGRAM.
MAP	SPECIAL FOURIER PRINT FEATURES
MODPOS	SUB-ROUTINE TO CONVERT A POSITIVE OR NEGATIVE NUMBER INTO A POSITIVE MODULO VALUE.
ORDNL	HAS SENSE ENOUGH TO PUT PROPER SUFFIX ON OUTPUT NUMBERS. (I.E.= 22NDS INSTEAD OF 22THS (WHICH LOOKS SILLY)).
PATPAT	PATCH WHICH PERMITS CALCULATION OF ANY TYPE OF PATTERSON.
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
TIME	SUBROUTINE TO READ CLOCK.
XRND	SUB-ROUTINE TO PROPERLY ROUND JUST-FIXED FLOATING POINT NUMBERS.

A. CARD ORDER SUMMARY FOR FOURIER REFINEMENT PROGRAM.

FOUREF	PROGRAM CALLING CARD.
*GRID	GRID SPECIFICATION
*SCALE	LEVEL SCALE OR OVERALL AS FOR FC (LINK 1000)
*B	OVERALL ISOTROPIC TEMPERATURE FACTOR
*ATOM	(SEE NOTE 1)
*ATOMG	(SEE NOTE 1)
*DATOMS	(SEE NOTE 1)
CYCLES	SPECIFIES NUMBER OF REFINEMENT CYCLES.
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

(NOTE 1) THESE ATOM CARDS SUPERCEDE ATOMS ON THE REFLECTION TAPE WITH IDENTICAL NAME, OR PERMIT ADDING ATOMS WITH DIFFERENT NAMES.

THIS PROGRAM READS =NTAPEA= AND WRITES FINAL FC ON =NTAPEB=.

B. CARD FORMATS FOR FOURIER REFINEMENT PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
FOUREF - FOURIER REFINING PROGRAM CALLING CARD
         FORMAT (A6,1XA6,1X3I1,2I2)
           1- 6       FOUREF
             7        $          BLANK
           8-13                  COMPID - COMPOUND IDENTIFICATION CODE
            14                   BLANK
         (15-17)                 SUMMATION ORDER
            15        X          (1)/(2)/(3) IF H IS (FIRST)/(SECOND)/
                                   (THIRD) SUM INDEX
            16        X          (1)/(2)/(3) FOR K SUM INDEX
            17        X          (1)/(2)/(3) FOR L SUM INDEX
                                   IT IS IMPORTANT FOR SPEED THAT (3) VARY
                                   LEAST RAPIDLY AND (1) MOST RAPIDLY.
          18-19       $X         (0 OR BLANK)/(1)/(2) FOR (SET ALL SCALES
                                   =1.0)/(USE SCALE FACTORS FROM TAPE)/(USE
                                   RESCALE FACTORS FROM TAPE)
          20-21       $X         (0 OR BLANK)/(1) FOR (READ NO ATOM PARAM.
                                   FROM TAPE)/(READ ATOM PARAM. FROM TAPE)
                                   WITH CODE=1 SOME OR ALL PARAMETERS MAY
                                   BE SUPERCEDED BY CARDS
          22-72                  (IGNORED)

GRID   - FOURIER GRID CARD.
         FORMAT (A6,1X,A6,3I4)
           1- 6       GRID$$
             7        $          BLANK
           8-13                  COMPID, COMPOUND IDENTIFICATION CODE.
          14-17       $XXX       NUMBER OF GRID INTERVALS ALONG THE X
                                   AXIAL DIRECTION.
          18-21       $XXX       GRID INTERVALS ALONG Y AXIAL DIRECTION
          22-25       $XXX       GRID INTERVALS ALONG Z AXIAL DIRECTION
          26-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6       SCALE$
           7-16       $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20       $$XX       GROUP IDENTIFICATION (1-64)    (I4)
                                   A GROUP IDENTITY OF ZERO WILL APPLY
                                   OVERALL F-RELATIVE SCALE TO STORED
                                   VALUES OF SCALE FACTORS. SCALE CARDS
                                   LOADED AFTER GROUP=ZERO WILL NOT BE
                                   AFFECTED.
          21-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.

B      - ISOTROPIC TEMPERATURE FACTOR CARD.
         FORMAT (A6,1X,A6,F8.4)
           1- 6       B$$$$$
             7        $          BLANK
           8-13                  COMPID IF OVERALL TEMPERATURE FACTOR.
           8-13                  NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
          14-21       $XX.XXXX   B
          22-61                  MUST BE BLANK.
          62-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
               7     $            BLANK
            8-13                  ATOM NAME - CONSISTS OF TWO PARTS. THE
                                    FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                    THE ATOM-TYPE NAME (SEE FORMFX). THE
                                    REST OF THE WORD, UP TO A TOTAL OF SIX
                                    COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                    OF THE PARTICULAR ATOM. THIS SECOND PART
                                    MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX   X    FRACTIONAL COORDINATE    (F8.0)
                                    DECIMAL POINT MUST BE PUNCHED IN ORDER
                                    TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX   Y
           30-37     $XX.XXXX   Z
           38-43     $X.XXX       INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                    MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                    ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                    TEMPERATURE FACTOR CARD IS USED, SINCE
                                    THIS WORD IS THEN IGNORED.
           44-48     $X.XX        INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                    BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX     STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                    REQUIRED BY PROGRAM BEING USED.)
           57-64     $X.XXXXX     STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX     STANDARD DEVIATION IN Z.

ATOMG   - ATOMIC PARAMETER CARD BASED ON GRID POINTS.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOMG$
            7-72                  SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                    EXPRESSED AS GRID VALUES FROM FOURIER
                                    MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                    CARDS MUST BE PRECEDED BY A LEADING
                                    GRID CARD.

DATOMS - MOLECULE SHIFT CARD
          FORMAT (A6,3F8.0)
            1- 6       DATOMS
            7-14       XX.XXXXX   X DIRECTION SHIFT
           15-22       XX.XXXXX   Y DIRECTION SHIFT
           23-30       XX.XXXXX   Z DIRECTION SHIFT
           31-72                  (IGNORED)

CYCLES - NUMBER OF ITERATIONS AND CRITEREA
          FORMAT (A6,I3,3F5.3,3F8.4)
            1- 6       CYCLES
            7- 9       XXX        MAXIMUM NUMBER OF CYCLES (0 OR BLANK = 5)
           10-14       X.XXX      MAXIMUM ALLOWED VALUE OF R (DECIMAL FRACT)
                                    (0 OR BLANK = 1.0)
           15-19       X.XXX      MINIMUM IMPROVED CHANGE IN R TO CONTINUE
                                    CYCLING
           20-24       X.XXX      REJECTION RATIO FOR FC/FO LESS THAN THIS
                                    VALUE (0 OR BLANK = 0.001)
           25-32       XXX.XXXX GRID INTERVAL IN X DIRECTION FOR FIRST
                                    CYCLE (THIS VALUE IS REDUCED ON EACH
                                    SUCCEEDING CYCLE FOR ATOMS WHICH ARE AT
                                    PEAKS)  (0 OR BLANK = 0.001*CELL EDGE)
           33-40       XXX.XXXX INITIAL GRID INTERVAL FOR Y DIRECTION
           41-48       XXX.XXXX INITIAL GRID INTERVAL FOR Z DIRECTION
           49-72                  (IGNORED)

END     - END CARD.
          FORMAT (A6)
            1- 6     END$$$
               7     $            BLANK
            8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR FOURIER REFINEMENT PROGRAM.

LINK 5000 FOURIER REFINEMENT PROGRAM

FOREF	FOURIER REFINEMENT PROGRAM (LINK 5000)
ATNUM	GET ATOM TYPE NUMBER FROM ATOM AND DICTIONARY NAME
COOR	SYMMETRY GENERATOR
EDCAL	FOURIER BLOCK CALCULATOR
PKCAL	PEAK CALCULATOR
SCNUM	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SFCAL	STRUCTURE FACTOR CALCULATOR
SQRUM	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
TABLE	GENERATES TABLE OF TRIG FUNCTIONS
TIME	READS CLOCK AT U. OF W. (TIMEM, TINCL, ETC., MAY BE SUBSTITUTED)
XPFUM	FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)

A. CARD ORDER SUMMARY FOR SHELL PATTERSON PROGRAM.

SHLPAT	CALLING CARD FOR PROGRAM
*SCALE	SCALE F RELATIVE
RADIUS	GIVES THE RADII AND GRID INTERVALS OF SPHERES. AS MANY RADIUS CARDS AS DESIRED MAY BE USED.
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

INPUT FROM =NTAPE8= AND OUTPUT ON =NTAPE0=.

B. CARD FORMATS FOR SHELL PATTERSON PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
SHLPAT - CALLING CARD FOR SHELL PATTERSON PROGRAM
         FORMAT (A6,2XA6,1X3I1,2I2,F10.5)
           1- 6       SHLPAT
             7        $          BLANK
           8-13                  COMPID - COMPOUND IDENTIFICATION CODE
            14        $          BLANK
         (15-17)                 SUMMATION ORDER
            15        X          (1)/(2)/(3) IF H IS (FIRST)/(SECOND)/
                                   (THIRD) SUMMATION INDEX
            16        X          (1)/(2)/(3) FOR K SUMMATION INDEX
            17        X          (1)/(2)/(3) FOR L SUMMATION INDEX
                                   IT IS VERY IMPORTANT WHERE SPEED IS A
                                   CONSIDERATION THAT THE INDEX DESIGNATED
                                   (3) VARY LEAST RAPIDLY AND THE INDEX
                                   MARKED (1) VARY MOST FREQUENTLY.
          18-19       $X         (0)/(1)/(2) FOR (PATTERSON F**2.0,SHARP.
                                   PATTERSON E**2)/(SHARP. PATTERSON WITH
                                   ORIGIN REMOVED (E**2)-1) AS COEFFICIENTS
          20-21       $X         (0)/(1)/(2) FOR SCALE OF (1.0)0(SCALE)/
                                   (RESCALE). RELEVANT ONLY FOR F**2.
          22-31       XXXX.XXXXX   SCALING OF RESULTS
          32-72                  (IGNORED)

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6     SCALE$
           7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20     $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                   A GROUP IDENTITY OF ZERO WILL APPLY
                                   OVERALL F-RELATIVE SCALE TO STORED
                                   VALUES OF SCALE FACTORS. SCALE CARDS
                                   LOADED AFTER GROUP=ZERO WILL NOT BE
                                   AFFECTED.
          21-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

RADIUS - SPECIFIES SIZE OF PATTERSON SHELL TO BE CALCULATED.
         FORMAT (A6,2X10F6.0)
           1- 6       RADIUS
             7        $          BLANK
           8-13       XXXXX.     STARTING VALUE OF THETA(1) IN DEGREES
                                   (THE EQUATORIAL ANGLE, LONGITUDE)
          14-19       XXXXX.     FINAL VALUE OF THETA(1) IN DEGREES
          20-25       XXXXX.     GRID INTERVAL FOR BOTH LONGITUDE AND
                                   LATITUDE IN DEGREES
          26-31       XXXXX.     FIRST RADIUS (MUST NOT BE ZERO OR BLANK)
          32-37       XXXXX.     SECOND (AND SUBSEQUENT) RADII IF DESIRED
                                   (FIRST BLANK OR ZERO MARKS END)
          38-43       XXXXX.     THIRD RADIUS
          44-49       XXXXX.     FOURTH RADIUS
          50-55       XXXXX.     FIFTH RADIUS
          56-61       XXXXX.     SIXTH RADIUS
          62-67       XXXXX.     SEVENTH RADIUS
          68-72       $$$$$      BLANKS

END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $          BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR SHELL PATTERSON PROGRAM.

LINK 5500 SHELL PATTERSON PROGRAM

SHLP	SHELL PATTERSON PROGRAM (LINK 5500)
REFLN	REFLECTION READING SUBROUTINE
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)

A. CARD ORDER SUMMARY FOR =BONDLA= PROGRAM.

BONDLA	CALLING CARD FOR =BONDLA= PROGRAM.
*CELL	CELL DIMENSIONS.
*CELLSD	STANDARD DEVIATIONS OF THE CELL DIMENTSIONS.
*GRID	FOURIER GRID CARD.
*SYMTRY	SYMMETRY OPERATION CARD. FORMAT LIKE THAT REQUIRED FOR DATA REDUCTION PROGRAM, EXCEPT =BONDLA= WILL ACCEPT ANY ADDITIONAL UNIT MULTIPLE TRANSLATION IN AXIAL DIRECTIONS.
*ATOM	ATOM PARAMETER CARDS IN FRACTIONAL COORDINATES.
*ATOMG	ATOM PARAMETER CARDS IN FOURIER GRID COORDINATES.
*BOND	CALCULATE A SPECIFIED =BOND= DISTANCE.
*ANGLE	CALCULATE A SPECIFIED =BOND= ANGLE.
*HLIN	GENERATE A LINEARLY-BONDED =HYDROGEN= ATOM.
*HTRIG	GENERATE A TRIGONALLY-BONDED =HYDROGEN= ATOM.
*HTET	GENERATE TWO TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS.
*HTERM	GENERATE THREE TERMINAL TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS
END	END CARD TO INITIATE CALCULATION.

* INDICATES OPTIONAL CARDS.

NOTE 1 - THE CARD ORDER HAS NO RESTRICTIONS WITH THE VARIOUS OPTIONAL CARDS EXCEPT WITH THE RESTRICTIONS OF NOTES 2 AND 3.

NOTE 2 - A =GRID= CARD MUST PRECEDE ANY =ATOMG= CARDS (IF USED) UNLESS A =GRID= CARD HAS BEEN READ BY A PREVIOUS PROGRAM AND INPUT DATA IS BEING TAKEN FROM THE BINARY REFLECTION TAPE.

NOTE 3 - THE PRESENCE OF THE =CELL= CARD IMMEDIATELY FOLLOWING THE =BONDLA= CARD PRECLUDES THE READING OF THE BINARY REFLECTION TAPE.

***** READS =NTAPEB= IF DATA TAKEN FROM REFLECTION TAPE *****
***** WRITES BCD CARD IMAGES ON =NTAPEC= IF ATOMS GENERATED *****

B. CARD FORMATS FOR =BONDLA= PROGRAM.

```
BONDLA - CALLING CARD FOR =BONDLA= PROGRAM (LINK 6000).
         FORMAT (A6,1X,A6,3(1XI4),3F6.2)
           1- 6      BONDLA
             7       $            BLANK
           8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
          14-15      $X           (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                    =INTRAMOLECULAR= DISTANCES.
          16-17      $X           (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                    =INTRAMOLECULAR= ANGLES. (IGNORED IF
                                    COL 15 IS BLANK.)
          18-19      $X           (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                    =INTERMOLECULAR= DISTANCES
          20-25      XXX.XX       MINIMUM =SIGNIFICANT= DISTANCE TO BE
                                    PRINTED.
          26-31      XXX.XX       MAXIMUM =SIGNIFICANT= DISTANCE TO BE
                                    PRINTED.
          32-37      XXX.XX       TEMPERATURE FACTOR TO BE PLACED ON GENERA-
                                    TED ATOMS (IF ANY). BLANK OR ZERO WILL
                                    CAUSE TEMPERATURE FACTOR OF BONDED
                                    =HEAVY= ATOM TO BE USED.
          38-72                   BLANKS

CELL   - CELL CONSTANT CARD.
         FORMAT (A6,1X,A6,3F8.3,3F9.5,F7.0)
           1- 6      CELL$$
             7       $            BLANK
           8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
          14-21      $AAA.AAA     A CELL DIMENSION  (F8.3)
          22-29      $AAA.AAA     B CELL DIMENSION  (F8.3)
          30-37      $AAA.AAA     C CELL DIMENSION  (F8.3)
          38-46      $+A.AAAAA    COS ALPHA  (F9.5)
          47-55      $+A.AAAAA    COS BETA (F9.5)
          56-64      $+A.AAAAA    COS GAMMA (F9.5)
          65-71      $AAAAA.      F(0,0,0)  (F7.0)

CELLSD - STANDARD DEVIATIONS OF CELL DIMENSIONS.
         FORMAT (A6,1X,A6,3F8.3,3F9.5)
           1- 6      CELLSD
             7       $            BLANK
           8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
          14-21      $AAA.AAA     STANDARD DEVIATION OF =A= AXIAL LENGTH.
          22-29      $AAA.AAA     STANDARD DEVIATION OF =B= AXIAL LENGTH.
          30-37      $AAA.AAA     STANDARD DEVIATION OF =C= AXIAL LENGTH.
          38-46      $+A.AAAAA    STANDARD DEVIATION OF COS ALPHA.
          47-55      $+A.AAAAA    STANDARD DEVIATION OF COS BETA.
          56-64      $+A.AAAAA    STANDARD DEVIATION OF COS GAMMA.
          65-72                   BLANKS

GRID   - FOURIER GRID CARD.
         FORMAT (A6,1X,A6,3I4)
           1- 6      GRID$$
             7       $            BLANK
           8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
          14-17      $XXX         NUMBER OF GRID INTERVALS ALONG THE X
                                    AXIAL DIRECTION.
          18-21      $XXX         GRID INTERVALS ALONG Y AXIAL DIRECTION
          22-25      $XXX         GRID INTERVALS ALONG Z AXIAL DIRECTION
          26-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
SYMTRY - SYMMETRY OPERATION CARD.
         THE SYMMETRY OF THE SPACE GROUP IS INDICATED BY SUPPLYING THE
         SET OF GENERAL EQUIVALENT POSITIONS. EACH EQUIVALENT POSITION
         IS SPECIFIED ON A SEPARATE SYMTRY CARD.
                   A SIMPLE RULE IS THAT ANY GENERAL EQUIVALENT POSITION
         IN THE INTERNATIONAL TABLES MAY BE WRITTEN VERBATIM WITH THE
         FOLLOWING CONVENTIONS, (1) MINUS SIGNS PRECEDE THE NEGATIVE
         QUANTITY, E.G. -X FOR X-BAR,  (2) FRACTIONS ARE WRITTEN WITH
         THE SLASH, E.G. 1/2 FOR ONE-HALF,  (3) BLANKS ARE IGNORED.
         NOTE-  1/2-X  OR  -X+1/2  ARE BOTH ACCEPTABLE FORMATS.
                   AS AN EXAMPLE SPACE GROUP C2/M COULD HAVE THE
         FOLLOWING FOUR CARDS.
         SYMTRY     X,     Y,     Z
         SYMTRY     X + 1/2,     -Y + 1/2,     Z
         SYMTRY     X + 1/2,     Y + 1/2,     Z
         SYMTRY     X,     -Y,     Z
         FORMAT (12A6)
         1 - 6      SYMTRY
         7 - 72     GENERAL EQUIVALENT POSITION

ATOM   - ATOM PARAMETER CARD.
         FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
           1- 6     ATOM$$
             7      $              BLANK
           8-13                     ATOM NAME - CONSISTS OF TWO PARTS. THE
                                      FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                      THE ATOM-TYPE NAME (SEE FORMFX). THE
                                      REST OF THE WORD, UP TO A TOTAL OF SIX
                                      COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                      OF THE PARTICULAR ATOM. THIS SECOND PART
                                      MUST BE NUMERIC. BLANKS ARE IGNORED.
          14-21     $XX.XXXX    X     FRACTIONAL COORDINATE    (F8.4)
                                      DECIMAL POINT MUST BE PUNCHED IN ORDER
                                      TO SUPERCEDE FORMAT.
          22-29     $XX.XXXX    Y
          30-37     $XX.XXXX    Z
          38-43     $X.XXX      INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                      MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                      ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                      TEMPERATURE FACTOR CARD IS USED, SINCE
                                      THIS WORD IS THEN IGNORED.
          44-48     $X.XX       INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                      BE ZEROS OR BLANK TO BE IGNORED.
          49-56     $X.XXXXX    STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                      REQUIRED BY PROGRAM BEING USED.)
          57-64     $X.XXXXX    STANDARD DEVIATION IN Y.
          65-72     $X.XXXXX    STANDARD DEVIATION IN Z.

ATOMG  - ATOMIC PARAMETER CARD BASED ON GRID POINTS.
         FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
           1- 6     ATOMG$
           7-72                     SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                      EXPRESSED AS GRID VALUES FROM FOURIER
                                      MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                      CARDS MUST BE PRECEDED BY A LEADING
                                      GRID CARD.

BOND   - CALCULATE A SPECIFIED =BOND= DISTANCE.
         FORMAT (A6,2(1XA6))
           1- 6       BOND$$
             7        $          BLANK
           8-13                   ATOM ID FOR FIRST ATOM.
             14       $          BLANK
          15-20                   ATOM ID FOR BONDED ATOM
          21-72                   BLANKS
```

```
ANGLE  - CALCULATE A SPECIFIED =BOND= ANGLE.
         FORMAT (A6,4(1X,A6))
           1- 6        ANGLES
              7        $          BLANK
           8-13                   ATOM ID FOR FIRST BONDED ATOM
             14        $          BLANK
          15-20                   ATOM ID FOR SECOND BONDED ATOM
             21        $          BLANK
          22-27                   ATOM ID OF THIRD BONDED ATOM
             28        $          BLANK
          29-34                   ATOM ID OF FOURTH BONDED ATOM
          35-72                   BLANKS
                       THE ANGLE CALCULATED IS THAT BETWEEN THE LINES
                       DEFINED BY A1-A2 AND A3-A4.  A1 AND A3 MAY BE
                       IDENTICAL TO GIVE =USUAL= BOND ANGLES.

HLIN   - GENERATE A LINEARLY-BONDED =HYDROGEN= ATOM.
         FORMAT (A6,2(1X,A6),8X,F6.3,1X,A6)
           1- 6        HLIN$$
              7        $          BLANK
           8-13                   ATOM ID OF FIRST DEFINING ATOM
             14        $          BLANK
          15-20                   ATOM ID OF SECOND DEFINING ATOM TO WHICH
                                    =HYDROGEN= IS TO BE =BONDED=.
          21-27                   BLANKS
          28-34        $XX.XXX    DISTANCE OF =HYDROGEN= FROM SECOND DEFIN-
                                    ING ATOM (MAY BE NEGATIVE, E.G.- FOR THE
                                    HYDROGEN-BOND CASE).  ZERO OR BLANK WILL
                                    USE 1.075 ANGSTROM UNITS.
             35        $          BLANK
          36-41                   ATOM ID FOR GENERATED =HYDROGEN= ATOMS.
                                    BLANK GIVES SERIALIZED IDENTIFICATION.
          42-72                   BLANKS.

HTRIG  - GENERATE A TRIGONALLY-BONDED =HYDROGEN= ATOM.
         FORMAT (A6,3(1X,A6),1X,F6.3,1X,A6)
           1- 6        HTRIG$
              7        $          BLANK
           8-13                   ATOM ID OF FIRST ATOM DEFINING BOND
             14        $          BLANK
          15-20                   ATOM ID OF SECOND ATOM DEFINING BOND, AND
                                    ATOM TO WHICH =HYDROGEN= IS ATTACHED.
             21        $          BLANK
          22-27                   ATOM ID OF THIRD ATOM DEFINING BOND.
             28        $          BLANK
          29-34        XX.XXX     BONDING DISTANCE. ZERO OR BLANK WILL USE
                                    1.075 ANGSTROM UNIT.
             35        $          BLANK
          36-41                   ATOM ID FOR GENERATED =HYDROGEN= ATOMS.
                                    BLANK GIVES SERIALIZED IDENTIFICATION.
          42-72                   BLANKS.
```

```
HTET    - GENERATE TWO TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS.
          FORMAT (A6,3(1X,A6),1X,F6.3,2(1X,A6))
            1- 6        HTET$$
              7         $          BLANK
            8-13                   ATOM ID OF FIRST ATOM DEFINING BOND
             14         $          BLANK
            8-13                   ATOM ID IF TERMINAL ATOM TO WHICH THE
                                     THREE =HYDROGEN= ATOMS ARE BONDED.
           15-20                   ATOM ID OF SECOND ATOM DEFINING BOND, AND
                                     ATOM TO WHICH =HYDROGENS= ARE ATTACHED.
             21         $          BLANK
           22-27                   ATOM ID OF THIRD ATOM DEFINING BOND.
             28         $          BLANK
           29-34        XX.XXX     BONDING DISTANCE. ZERO OR BLANK WILL USE
                                     1.075 ANGSTROM UNITS.
             35         $          BLANK
           36-41                   ATOM ID FOR FIRST GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
             42         $          BLANK
           43-48                   ATOM ID FOR SECOND GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
           49-72                   BLANKS.

HTERM   - GENERATE THREE TERMINAL TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS.
          FORMAT (A6,3(1X,A6),1X,F6.3,3(1X,A6))
            1- 6        HTERM$
              7         $          BLANK
            8-13                   ATOM ID OF FIRST ATOM DEFINING TETRAHEDRAL
                                     CHAIN FOR ORIENTATION OF =HYDROGEN=S.
             14         $          BLANK
           15-20                   ATOM ID OF SECOND ATOM DEFINING TETRAHED-
                                     RAL CHAIN FOR ORIENTATION OF =HYDROGEN=S
             21         $          BLANK
           22-27                   ATOM ID OF THIRD ATOM DEFINING TETRAHED-
                                     RAL CHAIN, AND TO WHICH THE =HYDROGENS=
                                     ARE ATTACHED.  THE FIRST =HYDROGEN= IS
                                     GENERATED FROM THE SAME VECTOR SENSE AS
                                     ATOMS 1 (COL 8-13) - 2 (COL 15-20).
                                     CHAIN, AND TO WHICH THE =HYDROGENS= ARE
                                     ATTACHED. THE FIRST =HYDROGEN= GENERATED
                                     FROM THE SAME VECTOR SENSE AS ATOMS
                                     1 (COL 8-13) AND 2 (COL 15-20).
             28         $          BLANK
           29-34        XX.XXX     BONDING DISTANCE. ZERO OR BLANK WILL USE
                                     1.075 ANGSTROM UNITS.
             35         $          BLANK
           36-41                   ATOM ID FOR FIRST GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
             42         $          BLANK
           43-48                   ATOM ID FOR SECOND GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
             49         $          BLANK
           50-55                   ATOM ID FOR THIRD GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
           56-72                   BLANKS.

END     - END CARD.
          FORMAT (A6)
            1- 6        END$$$
              7         $          BLANK
            8-72        ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR =BONDLA= PROGRAM.

LINK 6000 BOND LENGTHS AND ANGLES PROGRAM

BONDLA	PROGRAM FOR CALCULATION OF BOND LENGTHS AND ANGLES (LINK 6000)
LSACS	ARCCOSINE ROUTINE.
BANGL	COMPUTE BOND ANGLES.
BDIST	COMPUTE BOND DISTANCES.
BDDIS	COMPUTE THE STANDARD DEVIATIONS OF THE BOND DISTANCES.
BONSEK	BOND SEEKING PROGRAM.
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
SYMTR3	INTERPRET SYMMETRY CARD (GENERAL EXPRESSION)

A. CARD ORDER SUMMARY FOR SYSTEM =ORFFE=

ORFFE	CALLING CARD FOR BUSING-MARTIN-LEVY FUNCTION AND ERROR
*GRID	FOURIER GRID CARD. REQUIRED ONLY IF =ATOMG= CARDS ARE USED.
*CELL	REQUIRED IF TAPE IS NOT READ.
*CELLSD	STANDARD DEVIATIONS OF CELL DIMENSIONS. INCLUDED IN ERRORS IF THIS CARD IS READ.
*CELLMX	CELL DIMENSION ERROR MATRIX.
*SYMTRY	SYMMETRY OPERATIONS NOT READ FROM TAPE.
*ATOM	ATOM PARAMETER CARD IN FRACTIONAL COORDINATES.
*ATOMG	ATOM PARAMETER CARD IN FOURIER GRID COORDINATES. THIS CARD REQUIRES A =GRID= CARD (ABOVE).
*B	ISOTROPIC TEMPERATURE FACTOR CARD.
*BIJ	ANISOTROPIC TEMPERATURE FACTOR CARD.
*UIJ	ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRATION IN CRUICKSHANK NOTATION.
*BETA	ANISOTROPIC TEMPERATURE FACTOR FACTOR CARD.
FUNCTN	SPECIFICATIONS OF FUNCTION TO BE EVALUATED. ANY NUMBER OF THESE CARDS MAY BE INCLUDED.
END	RETURNS CONTROL TO NEXT PROGRAM SEGMENT.

* THESE CARDS ARE NOT ALWAYS REQUIRED

***** READS =NTAPE8= *****

B. CARD FORMATS FOR SYSTEM =ORFFE=

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
ORFFE  - CALLING CARD FOR BUSING-MARTIN-LEVY FUNCTION AND ERROR
         FORMAT(A6,1X,A6,3I3)
           1- 6      ORFFE$
             7       $          BLANK
           8-13                 COMPID - COMPOUND IDENTIFICATION CODE
          14-16      $$X          0 = ALL INFORMATION TO BE READ FROM
                                      CARDS.
                                    1 = REFLECTION TAPE TO BE READ.
                                    2 = ERRORS TO BE ESTIMATED FROM MATRIX
                                      ON =ORFLS= OUTPUT REFLECTION TAPE.
          17-19      $$X        (BLANK)/(1) FOR (USE)/(IGNORE) ATOM
                                  PARAMETERS ON REFLECTION TAPE.
          20-22      $$X        (BLANK)/(1) FOR (USE)/(IGNORE) SYMMETRY
                                  OPERATIONS ON REFLECTION TAPE (IDENTITY
                                  MATRIX IS ALWAYS IGNORED)
          23-72                 IGNORED

CELL   - CELL CONSTANT CARD.
         FORMAT (A6,1X,A6,3F8.3,3F9.5,F7.0)
           1- 6      CELL$$
             7       $          BLANK
           8-13                 SIX COLUMNS OF HOLLERITH PUNCHING OR
                                  BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                  (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                  NOT ALLOWED. THIS IDENTIFICATION IS
                                  CHECKED BY VARIOUS PROGRAMS FOR
                                  CONSTANCY, SO CHOOSE CAREFULLY AND
                                  REMEMBER YOUR CHOICE.      (A6)
          14-21      $AAA.AAA   A CELL DIMENSION  (F8.3)
          22-29      $AAA.AAA   B CELL DIMENSION  (F8.3)
          30-37      $AAA.AAA   C CELL DIMENSION  (F8.3)
          38-46      $+A.AAAAA  COS ALPHA  (F9.5)
          47-55      $+A.AAAAA  COS BETA  (F9.5)
          56-64      $+A.AAAAA  COS GAMMA  (F9.5)
          65-71      $AAAAA.    F(0,0,0)  (F7.0)

CELLSD - STANDARD DEVIATIONS OF CELL DIMENSIONS.
         FORMAT (A6,1X,A6,3F8.3,3F9.5)
           1- 6      CELLSD
             7       $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-21      $AAA.AAA   STANDARD DEVIATION OF =A= AXIAL LENGTH.
          22-29      $AAA.AAA   STANDARD DEVIATION OF =B= AXIAL LENGTH.
          30-37      $AAA.AAA   STANDARD DEVIATION OF =C= AXIAL LENGTH.
          38-46      $+A.AAAAA  STANDARD DEVIATION OF COS ALPHA.
          47-55      $+A.AAAAA  STANDARD DEVIATION OF COS BETA.
          56-64      $+A.AAAAA  STANDARD DEVIATION OF COS GAMMA.
          65-72                 BLANKS

CELLMX - VARIANCE-COVARIANCE MATRIX OF CELL DIMENSION ERRORS - THE 21
         UNIQUE ELEMENTS OF THE 6X6 MATRIX ARE READ FROM 3 CARDS.
         FORMAT(A6,1X,A6,I2,7F8.0)
           1- 6      CELLMX
             7       $          BLANK
           8-13                 COMPID - COMPOUND IDENTIFICATION CODE
          14-15      $X         CARD NUMBER - 1, 2 OR 3

                                 CARD 1        CARD 2        CARD 3
          16-23      XXXXXXXX    AM(A,A)       AM(B,C)       AM(C,COS G)
          24-31      XXXXXXXX    AM(A,B)       AM(B,COS A)   AM(COS A,COS A)
          32-39      XXXXXXXX    AM(A,C)       AM(B,COS B)   AM(COS A,COS B)
          40-47      XXXXXXXX    AM(A,COS A)   AM(B,COS G)   AM(COS A,COS G)
          48-55      XXXXXXXX    AM(A,COS B)   AM(C,C)       AM(COS B,COS B)
          56-63      XXXXXXXX    AM(A,COS G)   AM(C,COS A)   AM(COS B,COS G)
          64-71      XXXXXXXX    AM(B,B)       AM(C,COS B)   AM(COS G,COS G)
             72                 IGNORED
```

```
ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
              7      $            BLANK
            8-13                  ATOM NAME - CONSISTS OF TWO PARTS. THE
                                    FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                    THE ATOM-TYPE NAME (SEE FORMFX). THE
                                    REST OF THE WORD, UP TO A TOTAL OF SIX
                                    COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                    OF THE PARTICULAR ATOM. THIS SECOND PART
                                    MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX   X    FRACTIONAL COORDINATE    (F8.4)
                                    DECIMAL POINT MUST BE PUNCHED IN ORDER
                                    TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX   Y
           30-37     $XX.XXXX   Z
           38-43     $X.XXX       INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                    MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                    ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                    TEMPERATURE FACTOR CARD IS USED, SINCE
                                    THIS WORD IS THEN IGNORED.
           44-48     $X.XX        INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                    BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX     STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                    REQUIRED BY PROGRAM BEING USED.)
           57-64     $X.XXXXX     STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX     STANDARD DEVIATION IN Z.

ATOMG   - ATOMIC PARAMETER CARD BASED ON GRID POINTS.
          FORMAT (A6,1X,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOMG$
            7-72                  SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                    EXPRESSED AS GRID VALUES FROM FOURIER
                                    MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                    CARDS MUST BE PRECEDED BY A LEADING
                                    GRID CARD.

B       - ISOTROPIC TEMPERATURE FACTOR CARD.
          FORMAT (A6,1X,A6,F8.4)
            1- 6     B$$$$$
              7      $            BLANK
            8-13                  COMPID IF OVERALL TEMPERATURE FACTOR.
            8-13                  NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
           14-21     $XX.XXXX   B
           22-61                  MUST BE BLANK.
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BIJ     - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                     8*(PI**2)*U(I,J)=B(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BIJ$$$
              7      $            BLANK
            8-13                    NAMEAT.
           14-21     $XX.XXXX   B11   (F8.4)
           22-29     $XX.XXXX   B22
           30-37     $XX.XXXX   B33
           38-45     $XX.XXXX   B12
           46-53     $XX.XXXX   B13
           54-61     $XX.XXXX   B23
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

UIJ     - ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRAT.
          SEE D.W.J.CRUICKSHANK, ACTA CRYST., VOL 9, 747-758 (1956).
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     UIJ$$$
            7-61     FORMAT IDENTICAL WITH BIJ CARD.
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BETA    - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                     2*(PI**2)*ASTAR(I)*ASTAR(J)*U(I,J)=BETA(I,J)
          FORMAT (A6,1X,A6,6F8.4)
            1- 6     BETA$$
            7-61     FORMAT IDENTICAL WITH BIJ CARD
           62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
FUNCTN - FUNCTION SPECIFICATION CARD (SEE FOLLOWING SECTIONS FOR
           SPECIFIC FUNCTIONS)

         FORMAT(A6,1X,21I3,I2)
           1- 6      FUNCTN
             7       $          BLANK
           8-10      XXX        FUNCTION NUMBER
          11-70                 FUNCTION SPECIFICATION INTEGERS IN THREE
                                  COLUMN FIELDS  (20 FIELDS)
          74-72      $X         (BLANK)/(1) FOR (FUNCTION SPECIFICATION
                                  COMPLETE)/(CONTINUATION CARD FOLLOWS)

FUNCTN - FUNCTION CONTINUATION CARD - UP TO 10 ALLOWED PER FUNCTION
         FORMAT(A6,1X,21I3,I2)
           1- 6      FUNCTN
             7       $          BLANK
           8-70                 FUNCTION SPECIFICATION INTEGERS IN THREE
                                  COLUMN FIELDS  (21 FIELDS)
          71-72      $X         (BLANK)/(1) FOR (FUNCTION SPECIFICATION
                                  COMPLETE)/(ANOTHER CONTINUATION CARD
                                  FOLLOWS)

END    - END CARD
         FORMAT(A6)
           1- 6      END$$$
             7       $          BLANK
           8-72                 IGNORED
```

ATOM DESIGNATION AND SYMMETRY TRANSFORMATIONS

IN THE COURSE OF PREPARING AN INSTRUCTION CARD TO SPECIFY A FUNCTION TO BE COMPUTED IT WILL BE NECESSARY TO DEFINE THE ONE OR MORE ATOMS INVOLVED IN THIS FUNCTION. THIS IS DONE BY MEANS OF AN ATOM DESIGNATION CONSISTING OF THE TWO INTEGERS A AND 100C+S. HERE A = 1,2,3,... IS THE NUMBER OF THE ATOM IN THE PARAMETER LIST, S = 0, 1, 2, ... IS THE NUMBER OF THE SYMMETRY TRANSFORMATION TO BE APPLIED, AND C = 0, 1, ... 7 DEFINES THE UNIT CELL TRANSLATIONS AS DESCRIBED BELOW.

THE PROGRAM OBTAINS THE COORDINATES OF AN ATOM IN THE FOLLOWING WAY.
1. THE INTEGER A IS USED TO COMPUTE THE LOCATION OF THE COORDINATES IN THE PARAMETER LIST AND X, Y, Z ARE PICKED UP. IF A = 0 THE PROGRAM SETS X = Y = Z = 0.
2. THESE COORDINATES ARE THEN TRANSFORMED TO X', Y', Z' ACCORDING TO THE SYMMETRY INFORMATION S. IF S = 0 NO TRANSFORMATION IS MADE.
3. THE CELL TRANSLATIONS ARE THEN MADE ACCORDING TO THE FOLLOWING TABLE.

C	Z''	Y''	X''
0	Z'	Y'	X'
1	Z'	Y'	X' - 1
2	Z'	Y' - 1	X'
3	Z'	Y' - 1	X' - 1
4	Z' - 1	Y'	X'
5	Z' - 1	Y'	X' - 1
6	Z' - 1	Y' - 1	X'
7	Z' - 1	Y' - 1	Z' - 1

(AS A MEMORY AID, NOTE THAT THE 1'S IN THIS TABLE CORRESPOND TO THE BINARY REPRESENTATION OF C.)

FOR EXAMPLE, ATOM (3,208) IS ATOM 3 IN THE PARAMETER LIST TRANSFORMED TO SYMMETRY POSITION 8 OF CELL 2, WHILE ATOM (5,0) IS ATOM 5 JUST AS IT APPEARS IN THE LIST OF PARAMETERS. IN THE SUBSEQUENT SECTION WE WILL USE THE TERM ''MOLECULE'' IN A NON-RIGOROUS WAY, REFERRING TO ATOM 3 IN MOLECULE 208 OR ATO 5 IN THE BASIC MOLECULE (MOLECULE 0).

NOTE THAT TRANSFORMATIONS SUCH AS X' =-X AND X' = 1-X ARE NOT EQUAVALENT FOR PURPOSES OF THIS PROGRAM.

THE PROGRAM OBTAINS THE MATRIX OF THE ANISOTROPIC TEMPERATURE FACTOR COEFFICIENTS OF AN ATOM IN A SIMILAR WAY EXCEPT THAT THE ELEMENTS OF THIS MATRI ARE TRANSFORMED AS THE CORRESPONDING PRODUCTS OF THE COORDINATES. THIS PROCEDURE IS VALID FOR AN ATOM IN EITHER A SPECIAL OR GENERAL POSITION PROVIDED THAT THE SYMMETRY TRANSFORMATION S IS WRITTEN FOR A GENERAL POSITION. (SEE H. A. LEVY, ACTA CRYST. 9,679 (1956). THE TRANSLATIONAL PART OF THE SYMMETRY TRANSFORMATION IS IRRELEVANT IN THIS CASE AS IS THE CELL TRANSLATION C. SETTING A AT ZERO CAUSES A NULL MATRIX TO BE GENERATED.

DETAILS OF INSTRUCTION INPUT

EACH FUNCTION TO BE COMPUTED BY THE PROGRAM IS SPECIFIED BY A SEQUENCE INTEGERS, IN, WHICH ARE READ FROM ONE OR MORE INSTRUCTION CARDS. THE FIRST INTEGER IN THIS SEQUENCE, IN(1), DEFINES THE TYPE OF FUNCTION TO BE COMPUTED, AND THE INTREPRETATION OF THE REMAINING INSTRUCTION INTEGERS WILL IN GENERAL BE DIFFERENT FOR DIFFERENT TYPES OF FUNCTIONS. DETAILS OF THE INSTRUCTION INTEGERS FOR EACH TYPE OF FUNCTION ARE GIVEN BELOW.

EACH INSTRUCTION CARD IS READ WITH FORMAT (A6,1X, 21I3, I2). OF THE 22 INTEGERS ON THIS CARD ONLY THE FIRST 21 ARE CONSIDERED TO BE PART OF THE INSTRUCTION, IN. USUALLY ONE CARD WILL SUFFICE TO SPECIFY A FUNCTION, BUT IF A FUNCTION REQUIRES MORE THAN 21 INTEGERS TO DEFINE IT THEN UP TO TEN CARDS MAY BE USED WITH 21 INTEGERS ON EACH CARD. PUNCHING A ONE (OR ANY NON-ZERO INTEGE IN FIELD 22 OF AN INSTRUCTION CARD INDICATES THAT THE INSTRUCTION IS CONTINUED ON THE NEXT CARD.

FUNCTION 1
ONE INTERATOMIC DISTANCE.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       1
11-13       A(1)
14-16       100 C(1) + S(1)    ATOM DESIGNATION 1.
17-19       A(2)
20-22       100 C(2) + S(2)    ATOM DESIGNATION 2.
```

FUNCTION 101
ALL DISTANCES (LESS THEN D(MAX)) BETWEEN ATOMS IN TWO MOLECULES.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       101
11-13       A(MAX),  THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16       100 C(1) + S(1)    MOLECULE DESIGNATION 1.
17-19       $$$
20-22       100 C(2) + S(2)    MOLECULE DESIGNATION 2.  (MAY BE THE SAME AS 1.)
23-25       THE INTEGER 10 D(MAX).  IF THIS IS LEFT BLANK, THEN  D(MAX) = 5
23-25       THE INTEGER 10 D(MAX).  IF THIS IS LEFT BLANK, D(MAX) = 4.0 ANGSTR
```

FUNCTION 201
ALL DISTANCES (LESS THAN D(MAX)) BETWEEN ATOMS IN THE BASIC MOLECULE AND ALL MOLECULES (I.E., ALL COMBINATIONS OF C AND S). NOTE THAT THIS DOES NOT NECESSARILY COMPUTE ALL DISTANCES IN THE CRYSTAL WHICH ARE LESS THAN D(MAX).

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       201
11-13       A(MAX),  THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-22       $$$$$$$$$
23-25       THE INTEGER 10 D(MAX).  IF THIS IS LEFT BLANK, D(MAX) = 4.0 ANGSTR
```

```
FUNCTION 2
      ANGLE DEFINED BY THREE ATOMS.
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$2
11-16        ATOM DESIGNATION 1.
17-22        ATOM DESIGNATION 2 (VERTEX).
23-28        ATOM DESIGNATION 3.
FUNCTION 3
      ANGLE BETWEEN NORMALS TO PLANES EACH DEFINED BY THREE ATOMS. THE DIRECTI
OF THE NORMALS IS THAT OF (1,2)X(1,3) AND (4,5)X(4,6) WHERE (1,2)
IS THE VECTOR DEFINED BY ATOM DESIGNATIONS 1 AND 2, ETC.
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$3
11-16        ATOM DESIGNATION 1. **
17-22        ATOM DESIGNATION 2.  **    PLANE 1
23-28        ATOM DESIGNATION 3. **
29-34        ATOM DESIGNATION 4. **
35-40        ATOM DESIGNATION 5.  **    PLANE 2
41-46        ATOM DESIGNATION 6. **

FUNCTION 4
      DIFFERENCE BETWEEN TWO INTERATOMIC DISTANCES.
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$4
11-16        ATOM DESIGNATION 1. **
17-22        ATOM DESIGNATION 2. ***    DISTANCE 1
23-28        ATOM DESIGNATION 3. **
29-34        ATOM DESIGNATION 4. ***    DISTANCE 2

FUNCTION 5
      DIFFERENCE BETWEEN TWO ANGLES EACH DEFINED BY THREE ATOMS.
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$5
11-16        ATOM DESIGNATION 1.          **
17-22        ATOM DESIGNATION 2 (VERTEX).  **    ANGLE 1
23-28        ATOM DESIGNATION 3.          **
29-34        ATOM DESIGNATION 4.          **
35-40        ATOM DESIGNATION 5 (VERTEX).  **    ANGLE 2
41-46        ATOM DESIGNATION 6.          **

FUNCTION 6
      THE SUM OF SEVERAL ANGLES EACH DEFINED BY THREE ATOMS.
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$6
11-13        N, THE NUMBER OF ATOMS TO BE SUMMED.
14-19        ATOM DESIGNATION 1.          **
20-25        ATOM DESIGNATION 2 (VERTEX).  **    ANGLE 1
26-31        ATOM DESIGNATION 3.          **
32-37        ATOM DESIGNATION 4.          **
38-43        ATOM DESIGNATION 5 (VERTEX).  **    ANGLE 2
44-49        ATOM DESIGNATION 6.          **
             ETC.
```

FUNCTION 7
THE RMS COMPONENT OF THERMAL DISPLACEMENT OF ONE ATOM ALONG PRINCIPAL AXIS R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$7
11-16        ATOM DESIGNATION
17-19        R (= 1, 2 OR 3)
```

FUNCTION 107
SAME AS FUNCTION 7 COMPUTED FOR EACH OF THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        107
11-16        ATOM DESIGNATION
```

FUNCTION 207
SAME AS FUNCTION 7 COMPUTED FOR EACH ATOM OF A GIVEN MOLECULE, EACH WITH THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        207
11-13        A(MAX), THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16        MOLECULE DESIGNATION
```

FUNCTION 8
ANGLE BETWEEN PRINCIPAL AXIS R OF ATOM 1 AND A VECTOR DEFINED BY ATOMS 2 AND 3.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$8
11-16        ATOM DESIGNATION 1.
17-19        R (= 1, 2 OR 3)
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. ***    VECTOR
```

FUNCTION 108
SAME AS FUNCTION 8 COMPUTED FOR EACH OF THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        108
11-16        ATOM DESIGNATION 1.
17-19        $$$
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. **    VECTOR
```

FUNCTION 208
SAME AS FUNCTION 8 COMPUTED FOR EACH ATOM IN A GIVEN MOLECULE, EACH WITH THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        208
11-13        A(MAX), THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16        MOLECULE DESIGNATION
17-19        $$$
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. ***    VECTOR
```

FUNCTION 9
THE RMS COMPONENT OF THREMAL DISPLACEMENT OF ATOM 1 ALONG PRINCIPAL AXIS R, PROJECTED ON A VECTOR DEFINED BY ATOMS 2 AND 3.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $$9
11-16        ATOM DESIGNATION 1.
17-19        R (= 1, 2 OR 3)
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. *** VECTOR
```

FUNCTION 109
SAME AS FUNCTION 9 COMPUTED FOR THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        109
11-16        ATOM DESIGNATION 1.
17-19        $$$
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. ***   VECTOR
```

FUNCTION 209
SAME AS FUNCTION 9 COMPUTED FOR EACH ATOM IN A GIVEN MOLECULE, EACH WITH THE THREE VALUES OF R.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        209
11-13        A(MAX), THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16        MOLECULE DESIGNATION
17-19        $$$
20-25        ATOM DESIGNATION 2. **
26-31        ATOM DESIGNATION 3. ***   VECTOR
```

FUNCTION 10
ANGLE BETWEEN PRINCIPAL AXIS R OF ATOM 1 AND AXIS I OF A CARTESIAN CO-ORDINATE SYSTEM. THE LATTER IS DEFINED BY ATOMS 2, 3, 4, AND 5 AS FOLLOWS - AXIS 1 IS VECTOR (2,3). AXIS 2 IS (AXIS 1)X(4,5). AXIS 3 IS (AXIS 1)X(AXIS 2)

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        $10
11-16        ATOM DESIGNATION 1.
17-19        R (= 1, 2 OR 3)
20-22        I (= 1, 2 OR 3)
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***   VECTOR **
35-40        ATOM DESIGNATION **                 ***   AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***   VECTOR **
```

FUNCTION 110
SAME AS FUNCTION 10 COMPUTED FOR THE NINE COMBINATIONS OF R AND I.

```
COLUMNS
 1- 6        FUNCTN
    7        $
 8-10        110
11-16        ATOM DESIGNATION 1.
17-22        $$$$$$
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***   VECTOR **
35-40        ATOM DESIGNATION 4. **              **   AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***   VECTOR **
```

FUNCTION 210

SAME AS FUNCTION 10 COMPUTED FOR ALL ATOMS IN A GIVEN MOLECULE, EACH WITH THE NINE COMBINATIONS OF R AND I.

COLUMNS

```
 1- 6        FUNCTN
   7         $
 8-10        210
11-13        A(MAX),  THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16        MOLECULE DESIGNATION
17-22        $$$$$$
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***    VECTOR **
35-40        ATOM DESIGNATION 4. **            **    AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***    VECTOR **
```

FUNCTION 11

THE RMS COMPONENT OF THERMAL DISPLACEMENT OF ATOM 1 ALONG PRINCIPAL AXIS R, PROJECTED ON AXIS I OF A CARTESIAN COORDINATE SYSTEM DEFINED BY ATOMS 2, 3, 4, AND 5 AS DESCRIBED UNDER FUNCTION 10.

COLUMNS

```
 1- 6        FUNCTN
   7         $
 8-10        $11
11-16        ATOM DESIGNATION 1.
17-19        R (= 1, 2 OR 3)
20-22        I (= 1, 2 OR 3)
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***    VECTOR **
35-40        ATOM DESIGNATION 4. **            **    AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***    VECTOR **
```

FUNCTION 111

SAME AS FUNCTION 11 COMPUTED FOR THE NINE COMBINATIONS OF R AND I.

COLUMNS

```
 1- 6        FUNCTN
   7         $
 8-10        111
11-16        ATOM DESIGNATION 1.
17-22        $$$$$$
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***    VECTOR **
35-40        ATOM DESIGNATION 4. **            **    AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***    VECTOR **
```

FUNCTION 211

SAME AS FUNCTION 11 COMPUTED FOR ALL ATOMS IN A GIVEN MOLECULE, EACH WITH THE NINE COMBINATIONS OF R AND I.

COLUMNS

```
 1- 6        FUNCTN
   7         $
 8-10        211
11-13        A(MAX),  THE NUMBER OF ATOMS IN THE PARAMETER LIST.
14-16        MOLECULE DESIGNATION
17-22        $$$$$$
23-28        ATOM DESIGNATION 2. **
29-34        ATOM DESIGNATION 3. ***    VECTOR **
35-40        ATOM DESIGNATION 4. **            **    AXIS DEFINING VECTORS
41-46        ATOM DESIGNATION 5. ***    VECTOR **
```

FUNCTION 12
THE RMS COMPONENT OF THERMAL DISPLACEMENT OF ATOM 1 IN THE DIRECTION OF A VECTOR DEFINED BY ATOMS 2 AND 3.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       $12
11-16       ATOM DESIGNATION 1.
17-22       ATOM DESIGNATION 2. **
23-28       ATOM DESIGNATION 3. ***    VECTOR
```

FUNCTION 13
THE RMS RADIAL THERMAL DISPLACEMENT OF AN ATOM.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       $13
11-16       ATOM DESIGNATION
```

FUNCTION 14
INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. SECOND ATOM IS ASSUM TO RIDE ON THE FIRST. THE FUNCTION IS

```
     R = R(0) + (R(2)**2-D(2)**2-R(1)**2+D(1)**2)/2 R(0)
```

WRERE R(0) IS THE FIRST UNCORRECTED INTERATOMIC DISTANCE, R(I)**2 IS THE MEAN SQUARE RADIAL THERMAL DISPLACEMENT OF ATOM I, AND D(I)**2 IS THE MEAN SQUARE COMPONENT OF DISPLACEMENT OF ATOM I IN THE DIRECTION DEFINED BY THE INTERATOMIC VECTOR.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       $14
11-16       ATOM DESIGNATION 1.
17-22       ATOM DESIGNATION 2.
```

FUNCTION 15
INTERATOMIC DISTANCE AVERAGED OVER THERMAL MOTION. ATOMS ASSUMED TO MOVE INDEPENDENTLY. THE FUNCTION IS

```
     R = R(0) + (R(2)**2-D(2)**2+R(1)**2-D(1)**2)/2 R(0)
```

WHERE THE SYMBOLS ARE DEFINED AS IN FUNCTION 14 ABOVE.

```
COLUMNS
 1- 6       FUNCTN
    7       $
 8-10       $15
11-16       ATOM DESIGNATION 1.
17-22       ATOM DESIGNATION 2.
```

A. CARD ORDER SUMMARY FOR LEAST-SQUARES LINES AND PLANES.

LSQPL PROGRAM CALLING CARD FOR LINK 6500.

CELL UNIT CELL PARAMETERS (SEE NOTE 1)

ATOM ATOMIC PARAMETERS (SEE NOTES 2 AND 3)

END INITIATES CALCULATION.

***** READS =NTAPE8= IF NO CELL CARD IS USED *****

NOTE 1 - THE CELL CARD HAS A VERY IMPORTANT FUNCTION OTHER THAN PROVIDING CELL PARAMETERS. IF THE CELL CARD IS OMITTED, THE PROGRAM WILL AUTOMATICALLY EXPECT AN X-RAY SYSTEM REFLECTION TAPE ON =NTAPE8= FROM WHICH CELL DATA WILL BE OBTAINED. IF A CELL CARD IS GIVEN, NO TAPE WILL BE USED AS INPUT.

NOTE 2 - IF A CELL CARD IS PROVIDED TO =LSQPL= IN THE DATA, ATOM PARAMETERS ARE TO BE SUPPLIED ON THE ATOM CARDS. IF NO CELL CARD IS PROVIDED, THE MINIMAL FUNCTION OF ATOM CARDS IS TO GIVE ATOMIC IDENTIFICATION CODES FOR ATOMS INVOLVED IN THE CALCULATION. IF AN ATOM CARD IS BLANK (EXCEPT FOR CARD I.D. (ATOM) AND AN ATOM I.D. (E.G.- C3)) THE ATOMIC PARAMETERS WILL BE PICKED UP FROM SYSTEM DATA TAPE. IF THE PARAMETERS FOR AN ATOM ARE GIVEN ON THE =ATOM= CARD THEY WILL TAKE PRECEDENCE OVER TAPE PARAMETERS. IF AN =X= COORDINATE IS GIVEN ON THE =ATOM= CARD, THEN THE =Y= AND =Z= COORDINATES MUST ALSO BE GIVEN ON THE =ATOM= CARD. IF AN ATOM I.D. ON AN =ATOM= CARD CANNOT BE MATCHED WITH AN ATOM I.D. ON THE SYSTEM REFLECTION TAPE, THE PROGRAM WILL USE THE ATOM I.D. AND THE ATOMIC PARAMETERS ON THE =ATOM= CARD (USED, FOR EXAMPLE, WITH ATOMS NOT IN THE ASYMMETRIC UNIT).

NOTE 3 - THERE MUST BE AT LEAST (N) =ATOM= CARDS SUPPLIED, WHERE (N) IS THE NUMBER OF ATOMS DEFINING THE PLANE OR LINE (AS SPECIFIED IN COLS 16-19 OF THE =LSQPL= CARD). IF MORE THAN (N) =ATOM= CARDS ARE PROVIDED, THE FIRST (N) WILL BE USED IN THE LEAST-SQUARES LINE OR PLANE CALCULATION AND FOR THE REMAINING ATOMS THEIR DISTANCE FROM THE LINE OR PLANE WILL BE CALCULATED. THE PROGRAM LIMITS CALCULATIONS TO A MAXIMUM OF 200 ATOMS DEFINING THE LINE OR PLANE, AND TO A MAXIMUM OF 200 =ATOM= CARDS SUPPLIED AFTER THE FIRST (N) =ATOM= CARDS.

B. CARD FORMATS FOR =LSCPL= PROGRAM.

```
LSCPL   - CALLING CARD FOR LEAST-SQUARES LINES AND PLANES.
          FORMAT (A6,1X,A6,1X,I1,1X,I3,2(1X,I1))
            1- 6        LSCPL$
                7       $           BLANK
            8-13                    COMPID. COMPOUND IDENTIFICATION CODE.
           14-15        $X          (1)/(2) FOR L.S. (LINE)/(PLANE)  (LORP)
           16-19        $XXX        NUMBER OF ATOM CARDS OF ATOMS TO DEFINE
                                      (OR MAKE-UP) THE L.S. LINE OR PLANE (N1)
           20-21        $X          IGNORED IF = ZERO. IF NON-ZERO INTEGER
                                      CAUSES CALC. OF ANGLES BETWEEN THIS LINE
                                      OR PLANE AND ANY PRECEEDING LINES AND/OR
                                      PLANES CODED NON-ZERO.  (IANGLE)
           22-23        $X          IGNORED IF = ZERO. IF NON-ZERO INTEGER,
                                      CAUSES CALC. OF L.S. LINE OR PLANE WITH
                                      ATOMS PROVIDED AS INPUT PLUS THE ATOMS
                                      RELATED TO THE GIVEN ATOMS BUT GENERATED
                                      THRU THE ORIGIN AS A CENTER OF SYMMETRY.
           24-72                    (IGNORED)


CELL    - CELL CONSTANT CARD.
          FORMAT (A6,1X,A6,3F8.3,3F9.5,F7.0)
            1- 6      CELL$$
                7     $             BLANK
            8-13                    SIX COLUMNS OF HOLLERITH PUNCHING OR
                                      BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                      (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                      NOT ALLOWED. THIS IDENTIFICATION IS
                                      CHECKED BY VARIOUS PROGRAMS FOR
                                      CONSTANCY, SO CHOOSE CAREFULLY AND
                                      REMEMBER YOUR CHOICE.     (A6)
           14-21      $AAA.AAA    A CELL DIMENSION  (F8.3)
           22-29      $AAA.AAA    B CELL DIMENSION  (F8.3)
           30-37      $AAA.AAA    C CELL DIMENSION  (F8.3)
           38-46      $+A.AAAAA   COS ALPHA  (F9.5)
           47-55      $+A.AAAAA   COS BETA (F9.5)
           56-64      $+A.AAAAA   COS GAMMA (F9.5)
           65-71      $AAAAA.     F(0,0,0)  (F7.0)
```

```
ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
               7     $              BLANK
            8-13                    ATOM NAME - CONSISTS OF TWO PARTS. THE
                                      FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                      THE ATOM-TYPE NAME (SEE FORMFX). THE
                                      REST OF THE WORD, UP TO A TOTAL OF SIX
                                      COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                      OF THE PARTICULAR ATOM. THIS SECOND PART
                                      MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX    X     FRACTIONAL COORDINATE    (F8.4)
                                      DECIMAL POINT MUST BE PUNCHED IN ORDER
                                      TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX    Y
           30-37     $XX.XXXX    Z
           38-43     $X.XXX      INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                      MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                      ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                      TEMPERATURE FACTOR CARD IS USED, SINCE
                                      THIS WORD IS THEN IGNORED.
           44-48     $X.XX       INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                      BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX    STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                      REQUIRED BY PROGRAM BEING USED.)
           57-64     $X.XXXXX    STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX    STANDARD DEVIATION IN Z.


END     - END CARD.
          FORMAT (A6)
            1- 6     END$$$
               7     $              BLANK
            8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR =LSQPL=.

LINK 6500 COMPUTATION OF LEAST-SQUARES LINES AND PLANES.

LSQPL	PROGRAM FOR LEAST-SQUARES LINES AND PLANES.
LSHEQ	SOLUTIONS OF THREE HOMOGENEOUS EQUATIONS.
LSCRT	ROOTS OF A CUBIC EQUATION.
LSMIV	INVERSION OF A 3X3 MATRIX.
LSMMPY	MATRIX-MATRIX OR MATRIX-VECTOR MULTIPLY.
LSACS	ARCCOSINE ROUTINE.
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)

A. CARD ORDER SUMMARY FOR =DELSIG= PROGRAM.

DELSIG PROGRAM CALLING CARD.

*SCALE FC SCALE CARD. USE IS OPTIONAL. USED ONLY FOR A GROUP WHOSE SCALE IS TO BE MODIFIED FROM THE SCALING REQUESTED ON THE =DELSIG= CALLING CARD.

*GRAFTL GRAPH TITLE CARD. OPTIONAL. LABELS THE GRAPH IF A GRAPH WAS CODED IN THE =DELSIG= CALLING CARD.

END END CARD SIGNALS END OF DATA AND TO INITIATE CALCULATION.

* INDICATES OPTIONAL CARDS.

***** READS REFLECTION TAPE ON =NTAPEB= *****

B. CARD FORMATS FOR =DELSIG= PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
DELSIG - CALLING CARD FOR =DELSIG= PROGRAM (LINK 8000).
         FORMAT (A6,1X,A6,1X,A1,1X,A3,2(1X,I1),7X,2F10.4,(F10.4 OR I3))
           1- 6        DELSIG
             7         $            BLANK
           8-13                     COMPID, COMPOUND IDENTIFICATION CODE.
          14-15        $X           (A)/(B) FOR GROUPING F-OBSERVEDS BY EQUAL
                                      (NUMBERS)/(INTERVALS OF MAGNITUDE)(CIND)
          16-19        $XXX         (ORD)/(RMS) FOR (ARITHMETIC)/(ROOT-MEAN-
                                      SQUARE) AVERAGED DELTA-F  (RMSORD)
          20-21        $X           1=USE REFLECT. TAPE SCALE FACTORS  (ISCAL)
                                    2=MAKE ALL SCALE FACTORS = 1.0.
                                    3=USE RESCALE FACTORS ON REFLECT. TAPE.
          22-23        $X           1=NO GRAPH      (IGRAF)
                                    2=FOR GRAPH PLOTTED MODULO 100.
                                    3=FOR SCALED DELTA-F SO MAXIMUM = 100.
                                    4=BOTH GRAPHS 2 AND 3.
          31-40        XXXXX.XXXX MINIMUM FO TO BE CONSIDERED IN CALC.
          41-50        XXXXX.XXXX MAXIMUM FO TO BE CONSIDERED IN CALC.
          51-53        XXX        FOR COL 15 = A, NUMBER OF REFLECTIONS
                                      PER GROUP.
          51-60        XXXXX.XXXX FOR COL 15 = B, RANGE OF FO PER GROUP.

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6       SCALE$
           7-16       $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20       $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                   A GROUP IDENTITY OF ZERO WILL APPLY
                                   OVERALL F-RELATIVE SCALE TO STORED
                                   VALUES OF SCALE FACTORS. SCALE CARDS
                                   LOADED AFTER GROUP=ZERO WILL NOT BE
                                   AFFECTED.
          21-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.

GRAFTL - PUTS A TITLE ON =DELSIG= GRAPHS.
         FORMAT (12A6)
           1- 6         GRAFTL
           7-72                     ANY DESIRED TITLE FOR GRAPH.

END    - END CARD.
         FORMAT (A6)
           1- 6       END$$$
             7        $            BLANK
           8-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR =DELSIG=.

LINK 8000 PROGRAM FOR DELTA-F VS FO PLOT

DELSIG PROGRAM TO GIVE DELTA-F VS FO PLOT (LINK 8000)

DELGRF PROGRAM TO PLOT A GRAPH

DELPLT PROGRAM TO ASSIST PLOTTING OF A GRAPH

NFIXER SUBROUTINE FOR FIXING A FLOATING POINT NUMBER

SLIUW FORTRAN SHORT LIST INPUT (9SLI)

SLOUW FORTRAN SHORT LIST OUTPUT (9SLO)

SQRUW FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)

A. CARD ORDER SUMMARY FOR DATA REDUCTION PROGRAM.

CATRON	PROGRAM CALLING CARD
*LABEL	TAPE HEADING. TAPE IDENTIFICATION INFORMATION.
CELL	UNIT CELL PARAMETERS.
FORMFX	ATOMIC SCATTERING FACTORS FOR X-RAYS. GROUPED BY ATOM TYPE BY INCREASING (SIN THETA)/LAMBDA.
(OR)	
FORMFN	ATOMIC SCATTERING FACTORS FOR NEUTRONS.
LATICE	SPECIFIES CENTROSYMMETRY AND LATTICE TYPE. FOR THE MENTAL EASE OF THE GRAMMARIANS, THIS CARD MAY BE SPELLED =LATTICE=
SYMTRY	SYMMETRY OPERATIONS FOR THE SPACE GROUP. UP TO 48 ALLOWED. MUST HAVE AT LEAST ONE =SYMTRY= CARD (I.E. X,Y,Z).
*DISPER	TEMPLETON DISPERSION CORRECTION (ONE PER ATOM TYPE).
CONDIT	CONDITION CARD TO KEY CALCULATIONS.

FROM THIS POINT ONWARD, THE CARD ORDER IS DETERMINED BY THE DATA UNDER CONSIDERATION (I.E. DEALERS CHOICE) AND CARDS WITH THE FOLLOWING DESIGNATIONS ARE PERMITTED...

*FILTER	SPECTROMETER FILTER CARD (MUST OCCUR BEFORE THE FIRST REFLECTION REQUIRING IT).
*ABSORB	BOND ABSORPTION CORRECTIONS (MUST BE GROUPED FOR EACH DIFFERENT CRYSTAL).
*SCALE	SCALE CARD SUPPLIES ERROR, WEIGHTING, AND SCALING DATA.
*CONDIT	CONDITIONS CARD SETS-UP CODES BASED ON CAMERA TYPE AND CALCULATIONS TO BE PERFORMED.
*FORMAT	ACTUAL FORMAT FOR UNUSUAL BCD REFLECTION INPUT
*REFIN	INSTRUCTION CARD FOR UNUSUAL REFLECTION INPUT
*ENDOBS	SIGNALS THAT REFLECTIONS WHICH FOLLOW ARE SYSTEMATICALLY ABSENT. ONLY REQUIRED WHEN A SHARPENED ORIGIN-REMOVED PATTERSON (VECTOR MAP) IS TO BE CALCULATED.

IF REFLECTIONS AFTER =ENDOBS= CARD ARE IN A DIFFERENT FORMAT THAN THE ONES PRECEEDING, THEN =CONDIT= AND/OR =FORMAT= CARDS WILL BE NECESSARY.

*REFIN CAREFUL USE OF =REFIN= CARDS CAUSES DESIRED REFLECTIONS TO BE SKIPPED. USE THE =REFIN= CARD WITH CARE.

*TAPFUL ONLY NEEDED WHEN MORE THAN 13,000 REFLECTIONS ARE IN DATA DECK (TO BE STORED ON LOW DENSITY TAPE)

$$$$$$ REFLECTION CARDS (IDENTIFIED BY BLANKS IN COLS 1-6).

*STARTT STARTT CARD USED TO SET-UP CODES IDENTIFYING CONTINUATION TAPE(S) AFTER THE USE OF A =TAPFUL= CARD.

AFTER AN APPROPRIATE COMBINATION OF THESE CARDS, AN =END= CARD CAUSES THE PROGRAM TO SUMMARIZE AND RETURN CONTROL TO THE MONITOR OR THE NEXT PROGRAM SEGMENT.

* THESE CARDS ARE OPTIONAL.

THE FACT THAT THE VARIOUS CARDS CAN BE OPTIONALLY USED AT ANY TIME PERMITS CHANGES IN SCALE, FILTER FACTORS, ABSORPTION CORRECTIONS, OR EVEN CONDITIONS (E.G. WEISSENBERG, PRECESSION, ETC.) DURING THE COURSE OF THE PROCESSING OF REFLECTION CARDS.

***** READS =NTAPEB= IF REFLECTION DATA IS TO BE TAKEN FROM TAPE. ***
***** WRITES REFLECTION DATA ON =NTAPEA= *****

B. CARD FORMATS FOR DATA REDUCTION.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
DATRDN - CALLING CARD FOR DATA REDUCTION PROGRAM (LINK 10000)
         FORMAT (A6,1X,A6,6X)
           1- 6     DATRDN
             7                    BLANK
           8-13                   SIX COLUMNS OF HOLLERITH PUNCHING OR
                                    BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                    (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                    NOT ALLOWED. THIS IDENTIFICATION IS
                                    CHECKED BY VARIOUS PROGRAMS FOR
                                    CONSTANCY, SO CHOOSE CAREFULLY AND
                                    REMEMBER YOUR CHOICE.     (A6)
          14-18                     BLANK
          19-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

LABEL  - TAPE LABELING CARD. USED TO IDENTIFY BINARY TAPE.
         FORMAT (12A6)
           1- 6    LABEL$
           7-72     ALPHANUMERIC INFORMATION TO BE USED AS TAPE LABEL

CELL   - CELL CONSTANT CARD.
         FORMAT (A6,1X,A6,3F8.3,3F9.5,F7.0)
           1- 6     CELL$$
             7      $            BLANK
           8-13                   SIX COLUMNS OF HOLLERITH PUNCHING OR
                                    BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                    (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                    NOT ALLOWED. THIS IDENTIFICATION IS
                                    CHECKED BY VARIOUS PROGRAMS FOR
                                    CONSTANCY, SO CHOOSE CAREFULLY AND
                                    REMEMBER YOUR CHOICE.     (A6)
          14-21     $AAA.AAA    A CELL DIMENSION  (F8.3)
          22-29     $AAA.AAA    B CELL DIMENSION  (F8.3)
          30-37     $AAA.AAA    C CELL DIMENSION  (F8.3)
          38-46     $+A.AAAAA   COS ALPHA  (F9.5)
          47-55     $+A.AAAAA   COS BETA (F9.5)
          56-64     $+A.AAAAA   COS GAMMA (F9.5)
          65-71     $AAAAA.     F(0,0,0)  (F7.0)

FORMFX - ATOMIC FORM FACTORS FOR X-RAYS.
         FORMAT (A6,1X,A6,F7.5,F8.3,6A6,A4)
           1- 6     FORMFX
             7      $            BLANK
           8-13                   UP TO SIX CHARACTERS, THE LAST OF WHICH
                                    MUST NOT BE A DIGIT, TO IDENTIFY THE
                                    ATOM-TYPE. BLANKS ARE IGNORED.
          14-20     $.XXXXX     SIN(THETA)/LAMBDA  (F7.5)
          21-28     $FFF.FFF    ATOMIC SCATTERING FACTOR  (F8.3)
             29     $           BLANK
          30-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

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FORMFN - ATOMIC FORM FACTORS FOR NEUTRONS.
         FORMAT (A6,1X,A6,F8.3,8A6,A1)
           1- 6     FORMFN
             7      $            BLANK
           8-13                  ATOM TYPE NAME (SEE COLS. 8-13 OF FORMFX).
          14-21     $FFF.FFF     COHERENT ATOMIC SCATTERING FACTOR (F8.3)
          22-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

LATICE - CENTRICITY IDENTIFICATION CARD.
         FORMAT (A6,2X,A1,2X,A1)
           1- 6     LATICE       =LATTICE= SPELLING ALSO ACCEPTED
           7- 9     $$X          C = CENTRIC CELL,  A = ACENTRIC CELL.
          10-12     $$X          DESIGNATION OF LATTICE TYPE
                                   P,A,B,C,R,I,F   ONE OF THE
                                   FOREGOING MUST BE PUNCHED.
          13-72                  ANY LEGAL PUNCHING DESIRED OR BLANKS.

SYMTRY - SYMMETRY OPERATION CARD.
         THE SYMMETRY OF THE SPACE GROUP IS INDICATED BY SUPPLYING THE
         SET OF GENERAL EQUIVALENT POSITIONS. EACH EQUIVALENT POSITION
         IS SPECIFIED ON A SEPARATE SYMTRY CARD.
                A SIMPLE RULE IS THAT ANY GENERAL EQUIVALENT POSITION
         IN THE INTERNATIONAL TABLES MAY BE WRITTEN VERBATIM WITH THE
         FOLLOWING CONVENTIONS, (1) MINUS SIGNS PRECEDE THE NEGATIVE
         QUANTITY, E.G. -X FOR X-BAR,  (2) FRACTIONS ARE WRITTEN WITH
         THE SLASH, E.G. 1/2 FOR ONE-HALF,  (3) BLANKS ARE IGNORED.
         NOTE-  1/2-X  OR  -X+1/2  ARE BOTH ACCEPTABLE FORMATS.
                AS AN EXAMPLE SPACE GROUP C2/M COULD HAVE THE
         FOLLOWING FOUR CARDS.
         SYMTRY    X,    Y,    Z
         SYMTRY    X,    -Y,   Z
         FORMAT (12A6)
         1 - 6     SYMTRY
         7 - 72    GENERAL EQUIVALENT POSITION

DISPER - TEMPLETON DISPERSION CORRECTION CARD.
         FORMAT (A6,1X,A3,3X,2F10.3)
           1- 6     DISPER
             7      $            BLANK
           8-13                  ATOM TYPE NAME (SEE COLS. 8-13 OF FORMFX).
          14-21     $XXX.XXX     DELTA FJ PRIME  (F8.3)
          22-29     $XXX.XXX     DELTA FJ DOUBLE PRIME  (F8.3)
          30-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

CONDIT - CONDITION CARD.  SETS-UP CALCULATIONS CODES.
         FORMAT (A6,1X,A6,3F8.5,7I3,F8.5)
           1- 6     CONDIT
             7      $            BLANK
           8-13                  COMPOUND IDENTIFICATION (SEE COLS. 8-13
                                   OF THE CELL CARD).
          14-21     $X.XXXXX     WAVELENGTH  (F8.5)
          22-29     $X.XXXXX     SIN THETA (MAX).  (F8.5)
          30-37     $X.XXXXX     MINIMUM OBSERVED INTENSITY  (F8.5)
                                   (THE VALUE PUNCHED INTO THE SCALE CARD
                                   WILL SUPERCEDE THIS VALUE WHEN USING
                                   MULTIPLE LEVEL DATA.)
                    (THE NEXT SEVEN FIELDS ARE READ I3.)
          38-40     $$X          RADIATION TYPE (SWITCH LLL)
                                   (1)/(2) FOR (X-RAY)/(NEUTRON)
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CONDIT - CONDITION CARD (CONTINUED)
          41-43     $$X          CAMERA TYPE (SWITCH LL)
                                   (1)/(2)/(3)/(4)  FOR  (POWDER)/
                                   (SPECTROMETER)/EQUI-INCLINATION
                                   WEISSENBERG)/(PRECESSION)
          44-46     $$X          (1)/(2)  FOR  (APPLY I/LP)/(BYPASS THE
                                 APPLICATION OF 1/LP)
          47-49     $$X          (1)/(2)  FOR  (CALCULATION OF THE SQUARE
                                 ROOT OF INTENSITY, FREL**2, ETC)/(BYPASS
                                 CALCULATION OF SQUARE ROOT)
          50-52     $$X          REFLECTION CARD FORMAT (SWITCH LLL8)
                                   (1)/(2)/(3) FOR (STANDARD FORMAT)/
                                   (MARK-SENSE FORMAT)/(FORMAT SPECIFIED
                                   IN =REFIN= AND =FORMAT= CARDS)
          53-55     $$X          JAX.  AXIS OF ROTATION FOR WEISSENBERG,
                                 AXIS CLOSEST TO HORIZONTAL FOR PRECESSION.
                                 (1)/(2)/(3) FOR (A)/(B)/(C) AXIS
          56-58     $$X          KAX.  AXIS PARALLEL TO THE BEAM FOR THE
                                 PRECESSION METHOD.
          59-66     $X.XXXXX     COS TAU 0.  ANGLE BETWEEN KAX AND THE
                                 HORIZONTAL FOR PRECESSION METHOD   (F8.5)
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

CONDIT - CONDITION CARD FOR CHANGE OF DATA.
         FORMAT (A6,1X,A6,3F8.5,7I3,F8.5)
           1- 6     CONDIT
             7      $            BLANK
           8-13                  COMPOUND IDENTIFICATION (SEE COLS. 8-13
                                   OF THE CELL CARD).
          14-66     PUNCH ONLY THOSE APPLICABLE COLUMNS FOR WHICH THERE
                                 IS A CHANGE OF DATA. LEAVE ALL OTHER
                                 COLUMNS BLANK UNLESS CAMERA TYPE CHANGES
                                 THEN PUNCH IN FULL.
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

FILTER - FILTER CARD. FOR USE WITH SPECTROMETER DATA.
         FORMAT (A6,1X,I2,F10.8)
           1- 6     FILTER
           7- 9     $NN          ID NUMBER OF FILTER-- 1 TO 99     (I3)
          10-19     $.FFFFFFFF     TRANSMITTANCY OF FILTER  (F10.8)
          20-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

ABSORB - ABSORPTION CORRECTION CARD - TYPE 1. (REQUIRES ONE CARD FOR
         EACH ENTRY IN TABLE.  TOTAL = 19 CARDS.)
         FORMAT (A6,1X,I1,I4,F4.0,2X,F10.3)
           1- 6     ABSORB
             7      $            BLANK
             8        X          ABSORPTION TYPE.    (1)/(2)  FOR (NO
                                     CORRECTION)/(SPHERE OR CYLINDER)  (I1)
                                   TYPE (1) IS USED TO CANCEL PREVIOUS
                                   TYPE CODES IF NO CORRECTIONS ARE DESIRED
                                   FOR FOLLOWING SET OF DATA.
           9-12     $$$I         GROUP NUMBER OF DATA ALONG THE AXIS OF
                                   ROTATION.    (I4)
          13-16       $XX.       TYRTA.    THETA, OR UPSILON/2 (BUERGERS
                                     NOTATION).    (F4.0)
                                   SEE W.L.BOND IN INTERNATIONAL TABLES,
                                   VOL 2, PP 291-306. USE TABLE 5.3.50 FOR
                                   CYLINDER (P 295-298) AND TABLE 5.3.6B
                                   FOR SPHERE (P 302-305).
          17-18       $$         BLANK.
          19-28     $XXXXX.XXX ABSORBTION CORRECTION AS LISTED IN TABLE
                                   (F10.3)
          29-72     ANY DESIRED LEGAL PUNCHING OR BLANKS.
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ABSORB - ABSORPTION CORRECTION CARD - TYPE II.
         FORMAT (A6,1X,I1, **********)  (FINAL FORMAT NOT SET)
           1- 6     ABSORB
              7     $                 BLANK
              8       X               ABSORPTION TYPE.   (1)/(3)/(4)  FOR (NO
                                        CORRECTION)/(ELLIPSOIDAL)/(BUSING
                                        GENERAL CASE)     (I2)
                                        TYPE (1) USED TO CANCEL ANY PREVIOUS
                                        TYPE CODES IF NO CORRECTIONS ARE DESIRED
                                        FOR FOLLOWING SET OF DATA.
                                          NOTE= PRESENTLY (3) AND (4) CALCULATE
           9-72                           LIKE (1) PENDING PROGRAMMING OF TYPE.
                                        NO DETAILS OF CARD FORMAT SET PENDING
                                        COMPLETION OF PROGRAMMING OF THESE CASES

SCALE  - SCALE CARD FOR INTENSITY DATA.
         FORMAT (A6,F10.4,I4,F10.4,I2,5F5.3)
           1- 6     SCALE$
           7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO INPUT INTENSITY,
                               FREL, OR FREL**2   (F10.4)
          17-20       $$XX       GROUP IDENTIFICATION  (ONE NUMBER PER
                                   GROUP FROM 01 TO MAX OF 64).    (I4)
          21-30     $XXXX.XXXX MINIMUM OBSERVED INTENSITY  (F10.4)
          31-32     $W         WEIGHT ROUTINE SWITCH  (1)/(2)/(3)
                                  FOR (COPY FREL MIN INTO WEIGHT BAND)/
                                (APPLY U. OF W. WEIGHTING SCHEME)/(APPLY
                                USER SUPPLIED WEIGHT SCHEME)     (I2)
                                U.W. SCHEME IS  (WEIGHT = Q1/MAX1F
                                  (SIGMA,Q2*FREL+Q3,Q4*FRELM+Q5)
                     (REFER TO SECTION 1.100 FOR EXPLANATION OF NEXT
                       FIVE FIELDS, F5.3)
          33-37       X.XXX     Q1
          38-42       X.XXX     Q2
          43-47       X.XXX     Q3
          48-52       X.XXX     Q4
          53-57       X.XXX     Q5
          58-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.

FORMAT - DEFINES BCD REFLECTION DATA.
         FORMAT (12A6)
           1- 6     FORMAT
           7-72                THE FORMAT OF THE BCD REFLECTION DATA, AS
                                IF A STANDARD FORTRAN CARD (E.G.-
                                =USUAL= FORMAT IS (7X,A6,4I4,F10.2))

REFIN  - INSTRUCTION CARD FOR UNUSUAL REFLECTION INPUT.
         FORMAT (A6,I3,2I6,3I3,14(1X,A2))
           1- 6     REFIN$
           7- 9     $$X        (1)/(2)/(3) FOR (BIN TAPE)/(BCD TAPE)/
                                 (BCD CARD)
          10-15     XXXXXX     NUMBER OF REFLECTIONS TO SKIP BEFORE
                                 PROCESSING FIRST REFLECTION RECORD
          16-21     XXXXXX     MAXIMUM NUMBER OF REFLECTIONS TO PROCESS
                                 USING INFORMATION FROM THE LAST
                               PRECEEDING =SCALE= CARD
          22-24     XXX        VALUE OF H FOR LAST REFLECTION TO BE
                                 PROCESSED USING INFORMATION FROM LAST
                                 PRECEEDING =SCALE= CARD
          25-27     XXX        VALUE OF K FOR LAST REFLECTION
          28-30     XXX        VALUE OF L FOR LAST REFLECTION

                    NOTE - THERE ARE TWO WAYS TO TERMINATE USE OF INFOR-
                    MATION FROM THE PRECEEDING =SCALE= CARD- THE NUMBER
                    OF REFLECTIONS OR THE VALUES OF H, K, L FOR THE LAST
                    REFLECTION. EITHER MAY BE USED OR BOTH. IF BOTH ARE
                    SPECIFIED THE FIRST TO BE SATISFIED WILL TERMINATE
                    TREATMENT OF THAT REFLECTION  GROUP.
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REFIN  - INSTRUCTION CARD (CONTINUED)
          31-72     $XX            FOURTEEN FIELDS FOR SPECIFICATIONS OF
                                   REFLECTION DATA
                    THIS SERVES TO SPECIFY THE ORDER AND MODE (WHETHER
                    FIXED OR FLOATING) OF THE ITEMS TO BE READ AS REFLEC-
                    TION DATA. IT ALSO INDICATES WHICH WORDS OF A RECORD
                    ARE TO BE IGNORED. TREAT EACH FIELD AS REPRESENTING
                    FROM 1 TO 9 WORDS IN A REFLECTION RECORD. IF A WORD
                    OR GROUP OF WORDS IS TO BE SKIPPED, PUNCH =X8= WHERE
                    X IS AN INTEGER FROM 1 TO 9 DEPENDING ON HOW MANY
                    CONSECUTIVE WORDS ARE TO BE SKIPPED. IF X IS ZERO ONE
                    WORD WILL BE SKIPPED.

                    IN FIELDS CORRESPONDING TO USEFUL INFORMATION PUNCH-
                      FH OR IH FOR FLOATING OR FIXED H
                      FK OR IK FOR FLOATING OR FIXED K
                      FL OR IL FOR FLOATING OR FIXED L
                      FR OR IR FOR FLOAT. OR FIXED FUNCTION OF INTENSITY
                      FW OR IW FOR FLOATING OR FIXED WEIGHT
                      FD OR ID FOR FLOAT. OR FIXED LESS-THAN INDICATOR
                      FI OR II FOR FLOAT. OR FIXED LEVEL INDICATOR
                    THESE FIELDS MUST BE PUNCHED IN THE SAME ORDER AS
                    THEY APPEAR IN YOUR REFLECTION DATA RECORDS. A BLANK
                    IN ANY OF THESE FIELDS CAUSES IMMEDIATE TERMINATION
                    OF READING THIS CARD.

ENDCBS - SIGNALS THAT FOLLOWING REFLECTIONS ARE SYSTEMATICALLY ABSENT.
         FORMAT (A6)
           1- 6     ENDCBS
           7-72                    (IGNORED)

REFLECTION CARD - FOR INPUT INTENSITY DATA FROM FILMS OR COUNTER.
         FORMAT (A6,1X,A6,I2,3I4,F10.2,F10.4)
           1- 6     $$$$$$       BLANKS  (A6)
             7      $            BLANK
           8-13                  COMPOUND IDENTIFICATION, OPTIONAL OR BLANK
          14-15     $X           LESS-THAN INDICATOR--   1, OR 9 MEANS THAT
                                   REFLECTION OBSERVED, ANY OTHER NUMBER
                                   MEANS REFLECTION WAS LESS-THAN MINIMUM
                                   OBSERVABLE. A BLANK OR ZERO COMPARES
                                   PUNCHED INTENSITY WITH MINIMUM OBSERVED
                                   INTENSITY.   (I2).
          16-19     $XXX         H INDEX  (I4)
          20-23     $XXX         K INDEX  (I4)
          24-27     $XXX         L INDEX  (I4)
          28-37     $XXXXXX.XX     INTENSITY/FREL/FREL**2   (F10.2)
                                   OR PEAK DEKACOUNTS FOR SPECTROMETER.
          38-47     XXXXX.XXXX SIGMA. STANDARD DEVIATION OF MEASUREMENT
                                   (F10.4.  (OPTIONAL OR BLANK)
          48-72     ANY LEGAL PUNCHING DESIRED OR BLANKS (FOR FILM ONLY).
         FOLLOWING FOR SPECTROMETER DATA ONLY- FORMAT FOR ENTIRE CARD
         FORMAT (A6,1X,A6,I2,3I4,F10.2,F10.4,I3,F6.1,F10.2,I3,F6.1)
          48-50     XXX          PEAK FILTER CODE (I3)
          51-56     XXXX.X       PEAK SCAN TIME (DECISECONDS). (F6.1)
          57-66     XXXXXXX.XX BACKGROUND DECACOUNTS.  (F10.2)
          67-69     XXX          BACKGROUND FILTER CODE (I3).
          70-75     XXXX.X       BACKGROUND SCAN TIME (DECISECONDS).
                                   MAY NOT BE LESS THAN 0.1.
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REFLECTION CARD - MARK SENSE CARD FOR COUNTER DATA (650 CARD FORMAT).
          FORMAT (A6,2A1,A5,A4,A1,A5,A4,3A3)
            1- 6                BLANK.
              11                MEASUREMENT TYPE (A1)
              12                PEAK FILTER CODE (A1)
           13-17                PEAK DEKACOUNTS (A5)
           18-21                PEAK SCAN TIME (DECISECONDS) (A4)
              22                BACKGROUND FILTER CODE (A1)
           23-27                BACKGROUND DEKACOUNTS (A5)
           28-31                BACKGROUND SCAN TIME (DECISECONDS). MUST
                                  NOT BE LESS THAN ONE SECOND. (A4)
           72-74                H INDEX (A3)
           75-77                K INDEX (A3)
           78-80                L INDEX (A3)
           NOTE - ALL FIELDS ARE READ ALPHANUMERIC, THEN CONSIDERED AS
                  DECIMAL INTEGERS WITH LEADING ZEROS REQUIRED. SIGNS
                  PUNCHED OVER UNITS POSITION.

TAPFUL - CARD TO INDICATE FILLED REFLECTION TAPE.
         USED IF THE BCD TAPE TO DATA REDUCTION MUST BE SPLIT.
         FORMAT (A6)
           1- 6     TAPFUL
              7     $           BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

STARTT - CARD TO START CONTINUATION REFLECTION TAPE.
         USED IF THE BCD TAPE TO DATA REDUCTION MUST BE SPLIT.
         FORMAT (A6)
           1- 6     STARTT
              7     $           BLANK
           8-72                 (IGNORED)

END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
              7     $           BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR DATA REDUCTION PROGRAM.

LINK 10000 DATA REDUCTION PROGRAM.

DATRDN	PROGRAM FOR DATA REDUCTION.
ABSORB	BOND ABSORPTION CORRECTION FOR EACH REFLECTION.
ATNAME	LEFT JUSTIFY AND DISCARD BLANKS IN ATOM SYMBOLS.
BSTUW	FORTRAN BACK SPACE TAPE (9BST)
BTSNU	TRANSLATE UW IBM 650 SIGN-OVER-UNITS MARK-SENSE INTENSITY CARDS
CELFAC	CALCULATES NECESSARY CELL CONSTANTS AND WRITES RESULTS ON BINARY TAPE.
ERASE	WRITES BLANK TAPE AFTER RECORDS TO BE RE-WRITTEN BY SUBSEQUENT PROGRAMS.
GEN	DEVELOPS FOURIER DIRECTING CODES FOR EACH REFLECTION.
GENCHK	ARRANGES AND CHECKS THE SYMMETRY OPERATIONS FOR GEN.
INABS	INITIALIZES ABSORPTION CORRECTION SUB-ROUTINE ABSORB.
INPUT	FOR READING REFLECTION CARD DATA= H,K,L,I, ETC. THIS SUB-ROUTINE MAY BE MODIFIED BY USER FOR HANDLING DIFFERENT CARD FORMATS.
OUTPUT	FOR WRITING OUT ANY SPECIAL RESULTS. THIS SUB-ROUTINE IS USUALLY A DUMMY FOR USER MODIFICATIONS.
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
SYMTRY	SCANS SYMMETRY OPERATION CARDS AND STORES IN FORTRAN MATRIX ARRAY IN PROPER LOCATIONS.
TSHUW	FORTRAN TAPE-TO-STORAGE HOLLERITH (9TSH)
WTFN	FOR CALCULATION OF SPECIAL LEAST SQUARES WEIGHTING FACTORS. USUALLY A DUMMY FOR USER MODIFICATIONS.
XMODTW	CONVERTS A FIXED POINT FRACTION INTO INTEGER TWELFTHS FOR SYMTRY.
XNOD	MAKES INTEGER TWELFTHS FROM 0/12 TO 11/12 EXPRESSED AS 1 TO 12 FOR SYMTRY.

A. CARD ORDER SUMMARY FOR DATA MANIPULATION PROGRAM.

DATFIX	PROGRAM CALLING CARD
*EPSILON	ZONE WEIGHTING FACTORS
CELCON	UNIT CELL CONTENTS (ONE PER ATOM TYPE)
*BLIMIT	FOR SPECIAL CONTROL OF TEMPERATURE FACTOR AND SCALE FACTOR ESTIMATION.
*XLIMIT	(SEE NOTE 1)
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

* THESE CARDS ARE OPTIONAL.

***** READS =NTAPEA= AND WRITES =NTAPEB= *****

NOTE 1 = EVEN IF AN =XLIMIT= CARD IS USED, THE TEMPERATURE AND SCALE FACTORS ESTIMATED FOR X=2 ARE THE ONES PLACED AS OUTPUT ON THE BINARY TAPE. IF THERE IS NO =XLIMIT= CARD, X IS NOT ADJUSTED.

B. CARD FORMATS FOR DATA MANIPULATION PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DATFIX - CALLING CARD FOR DATA MANIPULATION PROGRAM.
FORMAT (A6,1XA6,1XI1,4F8.4)

1- 6	DATFIX	
7	$	BLANK
8-13		COMPID - COMPOUND IDENTIFICATION CODE
14	$	BLANK
15	X	(0 OR BLANK)/(1) FOR (DO NOT)/(DO) LIST INDIVIDUAL REFLECTION INFORMATION H, K, L, F, AND E.
16-23	XXX.XXXX	INITIAL VALUE OF B (0 OR BLANK = 3.0)
24-31	XXX.XXXX	E(0,0,0) TO OVERRIDE CALCULATED VALUE (USUALLY LEFT BLANK)
32-39	XXX.XXXX	F(0,0,0) TO OVERRIDE VALUE ON TAPE (USUALLY LEFT BLANK)
40-47	XXX.XXXX	MINIMUM VALUE OF F FOR WHICH AN E IS TO BE CALCULATED (BLANK = 0.0)
48-72		(IGNORED)

EPSILON - ZONE WEIGHTS CARD
FORMAT (A6,1X,6F3.0)

1- 7	EPSILON	
8-10	XXX	EPSILON FOR H00 (BLANK = 1)
11-13	XXX	0K0
14-16	XXX	00L
17-19	XXX	0KL
20-22	XXX	H0L
23-25	XXX	HK0
26-72		(IGNORED)

CELCON - CELL CONTENTS CARD
FORMAT (A6,1XF3.0,A6)

1- 6	CELCON	
7	$	BLANK
8-10	XXX	NUMBER OF ATOMS OF SPECIFIED TYPE IN THE WHOLE UNIT CELL
11-16		BCD ATOM TYPE NAME (SYMBOL)
17-72		(IGNORED)

BLINIT - CARD TO CONTROL ESTIMATION OF OVERALL ISOTROPIC TEMPERATURE FACTOR AND LEVEL SCALE FACTORS.
FORMAT (A6,1X3F6.3)

1- 6	BLINIT	
7	$	BLANK
8-13	XX.XXX	MAXIMUM PERMISSIBLE ERROR IN ESTIMATED B (BLANK = 0.1)
14-19	XX.XXX	MINIMUM PERMISSIBLE RATIO FOR AN ESTIMATED LEVEL SCALE FACTOR TO THE OVERALL ESTIMATED SCALE FACTOR (BLANK = 1.0, I.E. NO VARIATION)
20-25	XX.XXX	MAXIMUM PERMISSIBLE RATIO FOR A LEVEL SCALE FACTOR TO THE OVERALL SCALE FACTOR (BLANK = 1.0)
26-72		(IGNORED)

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XLIMIT - LIMITS X VALUE TO GIVE BETTER FIT IN E
         FORMAT (A6,1X3F6.3)
           1- 6       XLIMIT
             7        $          BLANK
           8-13       XX.XXX     PERMISSIBLE MAXIMUM ERROR IN ESTIMATED X
                                   (BLANK = 0.2) WHERE X IS POWER OF
                                   (SIN THETA)/LAMBDA. USED TO GIVE BETTER
                                   EMPIRICAL FIT OF E,S.
          14-19       XX.XXX     MINIMUM PERMISSIBLE RATIO FOR AN ESTIMATED
                                   LEVEL SCALE FACTOR TO THE OVERALL
                                   ESTIMATED SCALE FACTOR (BLANK = 1.0, I.E
                                   NO VARIATION)
          20-25       XX.XXX     MAXIMUM PERMISSIBLE RATIO FOR A LEVEL
                                   SCALE FACTOR TO THE OVERALL SCALE FACTOR
                                   (BLANK = 1.0)
          26-72                  (IGNORED)


END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $          BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR PROGRAM TO MANIPULATE DATA.

LINK 10500 CALCULATION OF UNITARY STRUCTURE FACTORS, SCALE AND OVERALL TEMPERATURE FACTORS

DATFX	PROGRAM TO CALCULATE UNITARY STRUCTURE FACTORS (LINK 10500)
CRAM	SUBROUTINE TO STORE INTEGERS IN LEAST SIGNIFICANT DIGITS OF A FLOATING POINT NUMBER
SCRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
XPFUW	FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)
XP3UW	FORTRAN EXPONENTIAL ROUTINE - FLOAT.PT. BASE AND EXPONENT (9XP3)

A. CARD ORDER SUMMARY FOR =MODIFY= PROGRAM.

MODIFY CALLING CARD FOR MODIFY PROGRAM (LINK 10600)

*MODREF REFLECTIONS TO BE MODIFIED BY CARDS (IF ANY).

END INITIATES CALCULATION.

* INDICATES OPTIONAL CARDS.

***** READS =NTAPEA= AND WRITES =NTAPEB= *****

8. CARD FORMATS FOR =MODIFY= PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
MODIFY - CALLING CARD FOR =MODIFY= PROGRAM.
         FORMAT (A6,1X,A6,3I3,I6,4F5.3,12I2)
           1- 6       MODIFY
             7        $          BLANK
           8-13                  COMPID, COMPOUND IDENTIFICATION CODE.
          14-16       $$X        1=REPLACE SPECIFIED WORD OF REFLECTION
                                   RECORD WITH QUANTITIES FROM CARDS
                                   SUPPLIED AND COPY REST OF TAPE.
                                 2=PLACE SPECIFIED PHASE ON REFLECTION
                                   (CENTROSYMMETRIC ONLY)
                                 3=REPLACE F-RELATIVE BY F-CALCULATED WITH
                                   A SPECIFIED GAUSSIAN ERROR FOR ALL
                                   REFLECTIONS.
                                 4=PLACE PHASE OF FC IN E FOR ALL REFLECT.
                                 5=RESCALE F-RELATIVE FOR ALL REFLECTIONS.
                                 6=TRANSFORM INDICES        (MODE3)
          17-19       XXX        NUMBER BETWEEN 1-263 TO INDICATE WORD OF
                                   REFLECTION RECORD TO BE CHANGED (BLANK
                                   IF COL 16 GREATER THAN 2)     (MODE1)
          20-22       $$X        (1)/(2) FOR (FLOATING)/(FIXED) POINT DATA
                                   IN COLS 28-37 OF =MODREF= INPUT REFLEC-
                                   TION CARDS (BLANK IF COL 16 IS GREATER
                                   THAN 2)            (MODE1)
          23-28       XXXXXX     NUMBER OF REFLECTIONS TO LIST (BLANK OR
                                   ZERO = 100)    (ILIST)
          29-33       X.XXX      MEAN RANDOM ERROR EXPRESSED AS A FRACTION
                                   BETWEEN 1 AND 0 (CODE 3 ONLY)  (ERROR)
          34-38       X.XXX      THRESHOLD VALUE OF INTENSITY FOR MANUFAC-
                                   TURED DATA (CODE 3 ONLY)    (FIMIN)
          39-43       X.XXX      MULTIPLICATIVE PARAMETER FOR ESTABLISHING
                                   WEIGHTS (CODE 3 ONLY)    (SLOP)
          44-48       X.XXX      ADDITIVE PARAMETER FOR ESTABLISHING
                                   WEIGHTS (CODE 3 ONLY)     (SEPT)
          49-72       XX         ROW-BY-ROW TRANSFORMATION MATRIX AND
                                   TRANSLATION VECTOR FOR PERMUTING THE
                                   INDICES (CODE 6 ONLY)     (MSYM)

MODREF - CARD TO MODIFY A REFLECTION RECORD.
         FORMAT (A6,1X,A6,2X,3I4,F10.2)
           1- 6       MODREF
             7        $          BLANK
           8-15                  COMPID (OPTIONAL OR BLANK)
          16-19       XXXX       H INDEX
          20-23       XXXX       K INDEX
          24-27       XXXX       L INDEX
          28-37       XXXXXXX.XX QUANTITY TO BE INSERTED IN REFLECTION
                                   TAPE AS SPECIFIED ON =MODIFY= CARD.
          38-72                  (IGNORED)

END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $          BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR =MODIFY= PROGRAM.

LINK 10600 PROGRAM TO SEARCH AND MODIFY REFLECTION TAPE

MDIF	PROGRAM FOR UPDATING A REFLECTION TAPE (LINK 10600)
ATNUW	FORTRAN FLOATING POINT ARCTANGENT ROUTINE (9ATN)
RANDY	FUNCTION SUBROUTINE TO GENERATE RANDOM ERRORS
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
XPFUW	FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)

A. CARD ORDER SUMMARY FOR PROGRAM TO SORT FOR KARLE-HAUPTMAN PHASES.

ESORT PROGRAM CALLING CARD

END TERMINATES PROGRAM, PUBLISHES FINAL SUMMARY, AND RETURNS CONTROL TO THE SYSTEM.

THE CARD ORDER IS NOT OPTIONAL AND MUST BE FOLLOWED EXPLICITLY.

READS =NTAPEB= AND DOES NOT WRITE A BINARY TAPE.

B. CARD FORMATS FOR PROGRAM TO SORT FOR KARLE-HAUPTMAN PHASES.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

ESORT - CALL THE UNITARY STRUCTURE FACTOR SORTING PROGRAM.
FORMAT (A6,1X,A6,I1,F7.3)

1- 6	ESORT$	
7	$	BLANK
8-13		COMPID, COMPOUND IDENTIFICATION CODE.
14	X	(BLANK)/(1) FOR (YES)/(NO) LIST THREE-DIMENSIONAL E VALUES IN ORDER ON TAPE.
15-21	XXX.XXX	MINIMUM VALUE OF E ON WHICH TO SORT.
22-72		(IGNORED)

END - END CARD.
FORMAT (A6)

1- 6	END$$$	
7	$	BLANK
8-72		ANY LEGAL PUNCHING DESIRED OR BLANKS.

C. SUBROUTINES FOR PROGRAM TO SORT FOR KARLE-HAUPTMAN PHASES.

LINK 10800 PROGRAM TO SORT FOR KARLE-HAUPTMAN PHASES

ESORT	PROGRAM TO SORT UNITARY STRUCTURE FACTORS (LINK 10800)
CRAM	PACKS FIXED POINT NUMBERS INTO STORAGE LOCATIONS, INCLUDES =UNCRAM= WHICH UNPACKS THEM.
DIM	DETERMINES DIMENSION OF REFLECTION.
GU	DETERMINES SYMMETRY CLASS OF REFLECTION.
MIXUP	SORTS EVEN OR ODD INDICES OF REFLECTIONS.
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SOR	SORTS REFLECTIONS ON THEIR INDICES.
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)

A. CARD ORDER SUMMARY FOR =LISTFC=.

LISTFC	PROGRAM CALLING CARD.
=650	INDICATES INPUT BY 650-FORMAT CARDS.
=	650-FORMAT FC DECK IN PROPER SORT WITH X-40 CARD REMOVED.
END	END CARD TO INITIATE CALCULATION.

***** BINARY INPUT ON =NTAPE8= *****
***** WHEN 650 CARDS ARE SPECIFIED, =NTAPE8= IS NOT USED *****

NOTE 1 - THE 650 DATA DECK ABSOLUTELY MUST NOT HAVE X-50 AND OTHER RELATED SUMMARY CARDS. MOREOVER, THE X-40 CARD MUST BE REPLACED BY AN =END= CARD.

NOTE 2 - A 650 FC DECK MAY BE OBTAINED THROUGH THE USE OF THE =BYEBYE= PROGRAM. IF ORIGINAL DATA OF THE BINARY REFLECTION TAPE IS NOT SORTED THIS PROCEDURE WILL GIVE A SIGNS-OVER-UNITS DECK WHICH MAY BE EASILY SORTED ON AN IBM SORTER INTO THE APPROPRIATE ORDER.

NOTE 3 - WHEN INPUT IS FROM THE SYSTEM =REFLECTION TAPE= SCALING IS AUTOMATICALLY TAKEN FROM =SCALE=. THE VALUES OF =RESCALE= CAN BE TRANSFERRED TO THE =SCALE= BAND DURING THE LAST =FC= CALCULATION IF SCALING OF F-REL BY =RESCALE= IS DESIRED.

8. CARD FORMATS FOR =LISTFC= PROGRAM.

```
LISTFC - CALLING CARD FOR =LISTFC= PROGRAM (LINK 11000).
         FORMAT (A6,1X,A6,3I1,I4,A1,I3,5I2,2A2,5I2)
           1- 6       LISTFC
             7        $          BLANK
           8-13                  COMPID, COMPOUND IDENTIFICATION CODE.
            14        X          (1)/(2)/(3) FOR EACH INDEX DEPENDING UPON
                                   THE SORT, FOR (MINOR SORT INDEX THAT
                                   CHANGES MOST FREQUENTLY)/(INTERMEDIATE
                                   SORT)/(MAJOR SORT CHANGES LEAST IN
                                   FREQUENCY)  FOR H INDEX.
            15        X          SORTING FREQUENCY FOR  K  INDEX.
            16        X          SORTING FREQUENCY FOR  L  INDEX.
         17-20        XXXX       EITHER THE NUMBER OF LINES/PAGE, OR ELSE
                                   THE TOTAL NUMBER OF PAGES TO BE LISTED.
            21        X          (L)/(P) IF COLS 17-20 IS (LINES)/(PAGES).
         22-24        XXX        NUMBER OF COLUMNS/PAGE
         25-26        XX         NUMBER OF BLANK SPACES BETWEEN COLUMNS.
         27-28        XX         NUMBER OF PRINT COLUMNS PER INDEX,
                                   (USUALLY 3)
         29-30        XX         NUMBER OF COLUMNS FOR F-OBSERVED.
         31-32        XX         NUMBER OF COLUMNS FOR F-CALCULATED
         33-34        XX         NUMBER OF COLUMNS FOR PHASE (IN CYCLES).
         35-36        XX         SPECIAL =LESS-THAN= FLAG (E.G.-  * ).
         37-38        XX         SPECIAL =EXTINCT= FLAG (E.G.-  E  ).
         39-40        $X         (BLANK)/(1) FOR (DO)/(DO NOT) PLACE MINUS
                                   SIGN IN FRONT OF THE F-OBSERVED THAT ARE
                                   LESS-THANS (THIS MAY THEN BE CONVERTED
                                   TO A LESS-THAN SIGN WITH PEN-AND-INK).
         41-42        $X         (BLANK)/(1) IF DESIRED TO (NOT PRINT)/
                                   (PRINT) THE PHASE ON FC IN THE CENTRIC
                                   CASE (LEAVE ZERO OR BLANK FOR ACENTRIC).
         43-44        $X         (BLANK)/(1) FOR (SINGLE)/(DOUBLE) SPACE.
         45-46        $X         (BLANK)/(1) FOR (DO NOT)/(DO) RESTORE
                                   PAGES AUTOMATICALLY.
         47-48        $X         (BLANK)/(1) FOR (PRINT)/(SUPRESS) PAGE
                                   TITLING.
         49-72                   BLANK.

650    - CARD TO SIGNAL INPUT 650-FORMAT CARDS FOR =LISTFC=.
         FORMAT (A6)
           1- 6       650$$$
           7-72                  BLANKS.

END    - END CARD.
         FORMAT (A6)
           1- 6       END$$$
             7        $          BLANK
           8-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

NOTE - FOR THE FORMAT OF THE IBM 650 SYSTEM FC-DECK FORMAT, REFER TO WRITE-UP FOR =BYEBYE= PROGRAM, SECTION 1.310.

C. SUBROUTINES FOR =LISTFC= PROGRAM.

LINK 11000 PROGRAM FOR FINAL STRUCTURE FACTOR LISTING

LISTFC	PROGRAM FOR FINAL STRUCTURE FACTOR LISTING (LINK 11000)
ARCTN	FIXED POINT ARCTANGENT ROUTINE.
BTSNU	CONVERT SIGN-OVER-UNITS BCD INTEGER TO BINARY.
LISTIN	READ THE BINARY REFLECTION RECORDS.
LISTK	READ AND CHECK FIRST SEVEN RECORDS OF BINARY TAPE.
ORDNL	MAKES PROPER SUFFIX FOR ORDINAL NUMBERS.
SLIUW	FORTRAN SHORT LIST INPUT (9SLI)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)

A. CARD ORDER SUMMARY FOR =CRYSET= PROGRAM.

CRYSET	PROGRAM CALLING CARD.
	BLANK CARD
	BLANK CARD
M	MONOCLINIC SYSTEM DATA CARD.
	BLANK CARD
A	TRICLINIC SYSTEM DATA CARD.
END	END CARD TO INITIATE CALCULATION.

NOTE 1 - THIS PROGRAM, ALTHOUGH ON THE SYSTEM TAPE, HAS NOT YET BEEN CONVERTED FULLY TO THE SYSTEM FORMAT. HENCE THIS DESCRIPTION MUST BE CONSIDERED INTERIM. ONLY THE MONOCLINIC AND TRICLINIC SYSTEMS ARE AVAILABLE AT PRESENT.

NOTE 2 - ANY NUMBER OF SETS OF DATA CAN BE CALCULATED AT A TIME. IT IS NECESSARY THAT ALL MONOCLINIC DATA CARDS BE GROUPED TOGETHER AND ALL TRICLINIC DATA CARDS BE GROUPED TOGETHER. IT IS ESSENTIAL THAT THERE BE THREE BLANK CARDS BETWEEN THE =CRYSET= CARD AND THE =END= CARD, WHETHER OR NOT THERE ARE ANY =M= OR =A= CARDS IN THE DATA DECK.

8. CARD FORMATS FOR =CRYSET= PROGRAM.

```
CRYSET - CALLING CARD FOR DONNAY-TAKEDA TRANSFORMATION PROGRAM.
         FORMAT (A6)
           1- 6     CRYSET
           7-72                    (IGNORED)

TITLE - TITLE CARD.  OPERATION CARD.  PRINTS TITLE ON EACH PAGE OF
        OFF-LINE OUTPUT.
        FORMAT (12A6)
           1- 6     TITLE$      (A6)
           7-72     ALPHANUMERIC INFORMATION FOR PAGE TITLE.

A       - =CRYSET= DATA CARD FOR TRICLINIC SYSTEM.
M       - =CRYSET= DATA CARD FOR MONOCLINIC SYSTEM.
        (THESE CARDS ARE NON-STANDARD FORMAT AND ARE NOT INCLUDED
         IN THE ALPHABETIC LISTING OF APPENDIX II, SECTION 3.2).
              1        M          (MONOCLINIC SYSTEM)
              1        A          (TRICLINIC SYSTEM)
           2- 9        THE DIMENSION OF THE CELL EDGE (A) WITH DECIMAL
                         POINT FOLLOWED BY ONLY THOSE FIGURES WHICH ARE
                         SIGNIFICANT.
          10-17        CELL EDGE (B).
          18-25        CELL EDGE (C).
          26-29        DEGREE PART OF CELL ANGLE ALPHA, RIGHT ADJUSTED.
             30        BLANK OR * INDICATING DEGREE AND DECIMAL POINT
                         OF HUNDREDTHS OF DEGREE.
          31-32        MINUTES PART OF CELL ANGLE ALPHA, RIGHT ADJUSTED,
                         OR HUNDREDTHS OF DEGREE, LEFT ADJUSTED.
          33-36        SAME FOR ANGLE BETA.
             37        SAME FOR ANGLE BETA.
          38-39        SAME FOR ANGLE BETA.
          40-43        SAME FOR ANGLE GAMMA, OR FIRST SETTING OF
                         MONOCLINIC.
             44        SAME FOR ANGLE GAMMA.
          45-46        SAME FOR ANGLE GAMMA.
             47        BLANK
             48        LATTICE LETTER OF THE SPACE-GROUP SYMBOL (ALPHABET)
          49-54        SYMBOL OF THE REMAINING SYMMETRY ELEMENTS OF THE
                         SPACE-GROUP SYMBOL BY NUMBER AND CAPITAL ALPHABET
                         (2SUB1 SCREW AS 21, 1-BAR AS -1).  TO INDICATE A
                         DIFFRACTION ASPECT * IS PUNCHED IN PLACE OF M,
                         21, ETC.
          55-57        NUMBER, Z, OF FORMULA UNITS PER CELL AS AN INTEGER.
             58        A          KX TO A FOR PRE-1948 POST-1900 DATA HAVE
                                    BEEN CHANGED.
                       K          STILL IN KX FOR POST-1948 DATA.
                       S          SUPPLEMENT OF BETA MUST BE TAKEN (FOR
                                    ACUTE BETA).
                       T          A TRANSFORMATION IS NEEDED FOR ACUTE BETA
                                    DATA.
          59-60        XX         YEAR OF PUBLICATION AS TWO-DIGIT NUMBER
                                    (E.G.-  63).
          61-72                   ENTRY IDENTIFICATION, ANY CHARACTERS.

END     - END CARD.
          FORMAT (A6)
           1- 6     END$$$
              7     $           BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR DONNAY-TAKEDA CRYSTAL TRANSFORMATION PROGRAM.

LINK 11100 PROGRAM FOR CRYSTAL TRANSFORMATION

TRXLS	TRANSFORMATION OF CRYSTAL SETTING AND SPACE-GROUP SYMBOL
AINPT	CONVERT A,B,C BY 24A1 TO FLOAT.PT. NUMBER (A(I),I=1,3)
AOUTP	PRINT OUT A/B,C/B,A,B,C IN ACCORDANCE WITH ACCURACY
ARCOS	ARCCOSINE ROUTINE
ARR	ARRANGE SCALAR PRODUCTS IN DECREASING ORDER
ATNUW	FORTRAN FLOATING POINT ARCTANGENT ROUTINE (9ATN)
ATOFL	BCD INTEGERS TO FLOATING POINT NUMBERS
BLANK	INSERT A BLANK CHARACTER IN AN =A= FORMAT WORD
CHAC	INTERCHANGE A AND C AXES
CHEK	CHECK TRANSFORMED CELL DIMENSIONS AND ANGLES
COMNT	PRINT COMMENTS ACCORDING TO NUMBER OF GROUP AND ENTRY
CONVM	REWRITE THE SPACE-GROUP SYMBOL TO OBEY CONVENTION
CONVO	REWRITE THE SPACE-GROUP SYMBOL TO OBEY PRIORITY RULES
DEGR	CONVERT RADIANS TO DEGREES
DPSUW	FORTRAN DOUBLE PRECISION ARITHMATIC ROUTINE (9DPS)
DSQRT	FORTRAN DOUBLE PRECISION FLOAT.PT. SQUARE ROOT ROUTINE (9DSQ)
EX221	EXAMINE SPACE-GROUP SYMBOL WITH ONE 2-FOLD AXIS EXCEPT F,I
HOLLER	TO MAKE BCD CHARACTER FOR CRYSET
MCL	DEAL WITH MONOCLINIC SYSTEM
NWAX	CALCULATE NEW CELL DIMENSIONS AND ANGLES
ORT	DEAL WITH ORTHORHOMBIC SYSTEM
RANGL	IF 90-ANGLE WERE ACUTE, GIVES GAMMA AND TRANSFORM. MATRIX FOLLOW
REDUC	REDUCE TRICLINIC CELL
RHOTP	PRINT C/A,A HEX,C HEX, IN ACCORDANCE WITH ACCURACY
RHH	DEALS WITH RHOMBOHEDRAL SYSTEM

SAME	PRINT OUT ANOTHER TRANSFORM. MATRIX IF CELL HAS SOME EDGES
SCAL	CALCULATES SCALAR PRODUCTS A.A, A.B, A.C, B.B, B.C, C.C
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SHORT	FIND THE SHORTEST TRANSLATION IN A PLANE
SLASH	CHANGES BLANK TO SLASH IN FRONT OF M,A,B,C,N, OR *
SLOUW	FORTRAN SHORT LIST OUTPUT (9SLO)
SMINP	CONVERT INPUT FORM OF SPACE-GROUP SYMBOL TO INTERNAL FORM
SMTR	INTERCHANGE SYMMETRY SYMBOL
SPREO	REORIENT SPACE-GROUP SYMBOL OF MONOCLINIC SYSTEM
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
TCL	DEALS WITH TRICLINIC SYSTEM
TRANS	CALCULATE PRODUCTS OF TRANSFORMATION MATRIX
UKEEP	KEEP U(I,J)
VOL	CALCULATE THE CELL VOLUME
XP2UW	FORTRAN EXPONENTIAL ROUTINE - FLOAT.PT. BASE AND FIXED EXPONENT

A. CARD ORDER SUMMARY FOR R PLANE PROGRAM.

RPLANE	CALLING CARD FOR R PLANE PROGRAM.
*SCALE	AS FOR FC PROGRAM (LINK 1000)
*GRID	AS FOR FC PROGRAM
*B	ONLY AS OVERALL ISOTROPIC TEMPERATURE FACTOR
*ATOM	AS FOR FOUREF PROGRAM (LINK 5000)
*ATOMG	AS FOR FOUREF PROGRAM
*MAXHKL	USED TO LIMIT REFLECTIONS USED
PLANE	USED TO DESIGNATE THE TWO DIMENTIONAL PLANE, ITS LIMITS, AND THE FINENESS OF GRID DESIRED. THIS CARD MAY BE REPEATED AS OFTEN AS DESIRED, BUT ONE SUCH CARD IS MANDATORY.
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

* THESE CARDS ARE OPTIONAL.

***** READS *NTAPEA* *****

```
ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOM$$
              7      $            BLANK
            8-13                   ATOM NAME - CONSISTS OF TWO PARTS. THE
                                     FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                     THE ATOM-TYPE NAME (SEE FORMFX). THE
                                     REST OF THE WORD, UP TO A TOTAL OF SIX
                                     COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                     OF THE PARTICULAR ATOM. THIS SECOND PART
                                     MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21     $XX.XXXX     X    FRACTIONAL COORDINATE    (F8.4)
                                     DECIMAL POINT MUST BE PUNCHED IN ORDER
                                     TO SUPERCEDE FORMAT.
           22-29     $XX.XXXX     Y
           30-37     $XX.XXXX     Z
           38-43     $X.XXX       INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                     MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                     ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                     TEMPERATURE FACTOR CARD IS USED, SINCE
                                     THIS WORD IS THEN IGNORED.
           44-48     $X.XX        INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                     BE ZEROS OR BLANK TO BE IGNORED.
           49-56     $X.XXXXX     STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                     REQUIRED BY PROGRAM BEING USED.)
           57-64     $X.XXXXX     STANDARD DEVIATION IN Y.
           65-72     $X.XXXXX     STANDARD DEVIATION IN Z.

ATOMG   - ATOMIC PARAMETER CARD BASED ON GRID POINTS.
          FORMAT (A6,1X,A6,3F8.4,F6.3,F5.2,3F8.5)
            1- 6     ATOMG$
            7-72                   SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                     EXPRESSED AS GRID VALUES FROM FOURIER
                                     MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                     CARDS MUST BE PRECEDED BY A LEADING
                                     GRID CARD.

MAXHKL  - LIMITS FOR FOURIER SUMMATION.
          FORMAT (A6,1X,A6,3I4,2F8.4)
            1- 6     MAXHKL
              7      $            BLANK
            8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
           14-17     $XXX         MAXIMUM H TO BE USED    (I4)
           18-21     $XXX         MAXIMUM K TO BE USED
           22-25     $XXX         MAXIMUM L TO BE USED
           26-33     $X.XXXXX     MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                     NO LIMIT)    (F8.4)
           34-41     $X.XXXXX     MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                     NO LIMIT)    (F8.4)
           42-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

B. CARD FORMATS FOR R PLANE PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
RPLANE - CALLING CARD FOR PROJECTION OF MOLECULE ON PLANE
         FORMAT (A6,1XA6,2I2)
           1- 6        RPLANE
             7         $          BLANK
           8-13                   COMPID - COMPOUND IDENTIFICATION CODE
          14-15        $X         (0)/(1)/(2) FOR SCALES BY (1.0)/(SCALE)/
                                    (RESCALE) FACTOR
          16-17        $X         (0)/(1) FOR (DO NOT)/(DO) READ THE ATOMS
                                    FROM TAPE. SOME OR ALL MAY BE SUPERCEDED
                                    BY =ATOM= CARDS.
          18-72                   (IGNORED)

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6      SCALE$
           7-16      $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20      $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                  A GROUP IDENTITY OF ZERO WILL APPLY
                                  OVERALL F-RELATIVE SCALE TO STORED
                                  VALUES OF SCALE FACTORS. SCALE CARDS
                                  LOADED AFTER GROUP=ZERO WILL NOT BE
                                  AFFECTED.
          21-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.

GRID   - FOURIER GRID CARD.
         FORMAT (A6,1X,A6,3I4)
           1- 6      GRID$$
             7       $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-17      $XXX       NUMBER OF GRID INTERVALS ALONG THE X
                                  AXIAL DIRECTION.
          18-21      $XXX       GRID INTERVALS ALONG Y AXIAL DIRECTION
          22-25      $XXX       GRID INTERVALS ALONG Z AXIAL DIRECTION
          26-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.

B      - ISOTROPIC TEMPERATURE FACTOR CARD.
         FORMAT (A6,1X,A6,F8.4)
           1- 6      B$$$$$
             7       $          BLANK
           8-13                 COMPID IF OVERALL TEMPERATURE FACTOR.
           8-13                 NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
          14-21      $XX.XXXX   B
          22-61                 MUST BE BLANK.
          62-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
PLANE  - DESIGNATES PLANE TO BE TREATED
         FORMAT (A6,1XA4,I2,6F8.4)
           1- 6       PLANE$
              7       $          BLANK
           8-11       A$A$       X$Y$, Y$X$, X$Z$, Z$X$, Y$Z$, OR Z$Y$
                                   TO DESIGNATE THE PLANE DESIRED
          12-13       $X         (0)/(1) TO (SEARCH WHOLE TAPE)/(QUIT WHEN
                                   FIRST NON-ZONE REFLECTION IS FOUND)
          14-21       XXX.XXXX BEGINNING POINT OF FIRST COORDINATE DIRECT
                                   (IN FRACTIONAL COORDINATES)
          22-29       XXX.XXXX FINAL POINT OF FIRST COORDINATE DIRECTION
          30-37       XXX.XXXX INTERVAL IN FIRST DIRECTION
          38-45       XXX.XXXX BEGINNING POINT OF SECOND COORDINATE
                                   DIRECTION (IN FRACTIONAL COORDINATES)
          46-51       XXX.XXXX FINAL POINT OF SECOND COORDINATE DIRECTION
          52-59       XXX.XXXX INTERVAL IN SECOND DIRECTION
          60-72                (IGNORED)


END    - END CARD.
         FORMAT (A6.
           1- 6     END$$$
              7     $          BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR R-PLANE PROGRAM.

LINK 12000 PROGRAM TO CALCULATE R OVER A PROJECTION

RPLANE	PROGRAM TO CALCULATE R OVER A PROJECTION
ATNUM	GET ATOM TYPE NUMBER FROM ATOM AND DICTIONARY NAME
RCAL	CALCULATION OF R
RCOR	MOVES MOLECULE
RTABL	GENERATES TABLE OF IRIG FUNCTIONS
SCNUW	FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)
SQRUW	FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)
XPFUW	FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)

A. CARD ORDER SUMMARY FOR RLIST PROGRAM.

RLIST	CALLING CARD FOR R LISTING PROGRAM
*SCALE	F RELATIVE SCALE FACTOR CARD(S)
END	END CARD

INPUT FROM = NTAPEB =

* THESE CARDS ARE OPTIONAL

B. CARD FORMATS FOR RLIST PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
RLIST - CALLING CARD FOR RLIST PROGRAM(LINK 12200)
        FORMAT (7XAL,2XA1,I3,2F3.3)
          1 - 6      RLIST$
            7        $          BLANK
          8 - 13                COMPID - COMPOUND IDENTIFICATION CODE
          14 - 15    $          BLANK
          16         X          (H)/(K)/(L)/(A) FOR LIST LEVEL BY LEVELS
                                OF H, K, L, OR A = ALL LEVELS.
          17-19      $$X        (0 OR BLANK)/(1)/(2)/ FOR (USE SCALE
                                FACTORS)/(USE RESCALE FACTORS)/(SET SCALES
                                =1).SCALES WILL BE SUPERCEEDED BY ANY
                                SCALE CARDS WHICH MAY BE SUPPLIED.
          20-24      .XXX       EQUAL DIVISIONS OF SIN THETA /LAMBDA FOR
                                GROUPING REFLECTIONS. BLANK OR ZERO = 0.09
                                PER ANGSTROM.
          25-28      .XXX       FRACTION OF TOTAL REFLECTIONS TO BE
                                INCLUDED IN APPROXIMATELY EQUAL GROUPS OF
                                INCREASING SIN THETA /LAMBDA (BLANK OR
                                ZERO , OR LESS THAN 0.01) = 0.1.
          29-72                 ANY LEGAL PUNCHING DESIRED OR BLANKS

SCALE   - SCALE CARD FOR F RELATIVE DATA.
        FORMAT (A6,F10.4,I4)
          1- 6     SCALE$
          7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
         17-20     $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                A GROUP IDENTITY OF ZERO WILL APPLY
                                OVERALL F-RELATIVE SCALE TO STORED
                                VALUES OF SCALE FACTORS. SCALE CARDS
                                LOADED AFTER GROUP=ZERO WILL NOT BE
                                AFFECTED.
         21-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

END     - END CARD.
        FORMAT (A6)
          1- 6     END$$$
            7      $          BLANK
          8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. PROGRAM DECK AND SUBROUTINES FOR RLIST PROGRAM.

LINK 12200 RLIST PROGRAM

RRIS	MAIN PROGRAM FOR PREPARING LIST OF R' VALUES.
RREA	READS BINARY REFECTION TAPE
RRLS	CLASSIFIES REFLECTIONS INTO CORRECT GROUPS
RSUM	CALCULATES AND STORES SUMS FOR R CALCULATIONS
RRHE	CALCULATES R VALUES FOR PRINT OUT

A. CARD ORDER SUMMARY FOR PROGRAM TO SEARCH FOURIER MAPS.

PEKPIK	PROGRAM CALLING CARD
END	SIGNALS PROGRAM TO BEGIN CALCULATION

THE CARD ORDER HAS NO OPTIONS AND MUST BE FOLLOWED EXPLICITLY.

THIS PROGRAM READS =NTAPEB=, WHICH MUST BE A COMPOUND REFLECTION TAPE, AND ALSO READ =NTAPED=, WHICH MUST BE THE BINARY OUTPUT OF THE =FOURR= PROGRAM. (SEE =MAP= CARD, FUNCTION 3 PAGE 2.408X TO SEE HOW THIS LATTER TAPE IS PREPARED.)

WRITES =NTAPEC= WHEN =ATOM= CARD PUNCHING IS SPECIFIED IN PEKPIK CARD.

8. CARD FORMATS FOR PEAK SEARCHING PROGRAM.

```
PEKPIK - CALLING CARD FOR PEAK SEARCHING PROGRAM(LINK 30600)
         FORMAT(13X2F10.5,4I5,F10.5)
           1- 6     PEKPIK
             7      $            BLANK
           8-13                  COMPID, THE COMPOUND IDENTIFICATION CODE.
          14-23     XXXX.XXXXX   UPPER AND LOWER LIMITS BETWEEN WHICH SEARCH IS
          24-33     XXXX.XXXXX   BE SUPRESSED (TO AVOID RIPPELS) THIS IS THE
                                 SAME FUNCTION AS THE =MAP= CARD OF =FOURR= SO
                                 THAT IF THESE FEILDS ARE LEFT BLANK VALUES FROM
                                 THE =MAP= CARD WILL BE USED (FROM =NTAPE0=)
         34-38      XXXXX        NUMBER OF PEAKS OF HIGHEST DENSITY EXPECTED
                                 TO BE LOCATED IN THE ASSYMETRIC UNIT
          39-43     XXXXX        MAXIMUM NUMBER OF PEAKS TO BE SOUGHT
                                 BLANK OR 0 = 100
          44-48     XXXXX        (BLANK)/(1) - (DO NOT)/(DO)  PUNCH =ATOM= CARDS
                                 FOR PEAKS LOCATED DURING SEARCH.
          49-53     XXXXX        (BLANK)/(1) - (DO NOT)/(DO) SEARCH FOR HOLES AS
                                 WELL AS PEAKS
          54-63     XXXX.XXXXX   DESIRED RESOLUTION IN TERMS OF GRID COORDINATES
                                 SQUARED  (BLANK OR 0 = 3.0)
          64-72                  MUST BE BLANK

END      - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $            BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

A. CARD ORDER SUMMARY FOR =BYEBYE= PROGRAM.

BYEBYE PROGRAM CALLING CARD.

*SCALE FC SCALE CARD. USE IS OPTIONAL, USED ONLY FOR A GROUP WHOSE SCALE IS TO BE MODIFIED.

END END CARD. TO INITIATE CALCULATION.

***** READS =NTAPEB= *****
***** PUNCHES CARDS ON =NTAPCC= *****
***** WRITES BINARY OUTPUT ON =NTAPEE= *****

B. CARD FORMATS FOR =BYEBYE= PROGRAM.

OPERATION CARDS (DESCRIBED IN SECT 1.0-A, AND CARD FORMATS ARE GIVEN IN SECT 2.0-C) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

```
BYEBYE - CALLING CARD FOR NON-SYSTEM INPUT FORMATS.
         FORMAT (A6,1X,A6,I5,I3,2I2)
           1- 6     BYEBYE
             7                  BLANK
           8-13                 SIX COLUMNS OF HOLLERITH PUNCHING OR
                                  BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                  (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                  NOT ALLOWED. THIS IDENTIFICATION IS
                                  CHECKED BY VARIOUS PROGRAMS FOR
                                  CONSTANCY, SO CHOOSE CAREFULLY AND
                                  REMEMBER YOUR CHOICE.     (A6)
          14-18     $XXXX        650 REFLECTION DECK ID NUMBER.
          19-21     $XX          650 FC DECK TRIAL NUMBER.
          22-23     $X           OUTPUT TYPE.
                                  1 = 650 REFLECTION CARD
                                  2 = 650 FC CARD
                                  3 = BUSING TAPE
          24-25     $X           OUTPUT SCALING OF FREL DATA FROM TAPE.
                                  1 = USES FREL SCALE FACTOR ON TAPE
                                  2 = ALL SCALES SET EQUAL TO 1.0
                                  3 = USES FREL RESCALE FACTOR ON TAPE
                                  AN FC SCALE CARD MODIFIES THE SCALE
                                 FOR THE INDICATED GROUP ONLY.
          26-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6     SCALE$
           7-16     $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20     $$XX       GROUP IDENTIFICATION (1-64)     (I4)
                                  A GROUP IDENTITY OF ZERO WILL APPLY
                                  OVERALL F-RELATIVE SCALE TO STORED
                                  VALUES OF SCALE FACTORS. SCALE CARDS
                                  LOADED AFTER GROUP=ZERO WILL NOT BE
                                  AFFECTED.
          21-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $          BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

C. SUBROUTINES FOR =BYEBYE= PROGRAM.

LINK 31000 CONVERT SYSTEM TAPE TO NON-SYSTEM FORMATS

BYEBYE PROGRAM TO CONVERT X-RAY SYSTEM REFLECTION TAPE TO NON-SYSTEM INPUT FORMATS.

BDZ BINARY TO ZONED DECIMAL.

SLIUW FORTRAN SHORT LIST INPUT (9SLI).

SQRUW FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR).

XLSOUT WRITE BUSING ORXLS-TYPE BINARY REFLECTION RECORD.

A. SUBROUTINES FOR =ERLINK= PROGRAM.

LINK 32700 EXECUTION ERROR DIAGNOSTICS PROGRAM.

ERLINK	PROGRAM TO CALL DIAGNOSTIC SUBROUTINE.
CALLER	CONTROL SUBROUTINE FOR X-RAY SYSTEM.
ERREC	EXECUTION ERROR DIAGNOSTICS SUBROUTINE.
IOHUW	FORTRAN INPUT-OUTPUT HOLLERITH (9IOH).
IOSW	MODIFIED FORTRAN INPUT-OUTPUT SUPERVISOR (9IOS).
SPHW	MODIFIED FORTRAN STORAGE TO PRINTER HOLLERITH (9SPH).
STHW	MODIFIED FORTRAN STORAGE TO TAPE HOLLERITH (9STH).
TESUW	FORTRAN TEST LAST WRITE (9TES).
WERW	MODIFIED FORTRAN TAPE WRITE ERROR (9WER).

8. ERROR STOPS RECOGNIZED BY =ERREC=.

THE FOLLOWING CODES ARE UTILIZED BY =LINK 32700= IN WRITING OUT EXECUTION ERROR DIAGNOSTICS.

HPR	
0,1	BAD FORMAT CHARACTER.
1,1	BAD CHARACTER IN INPUT DATA.
2,1	BAD CHARACTER IN INPUT DATA.
3,1	BAD CHARACTER IN INPUT DATA.
4,1	BAD CHARACTER IN INPUT DATA.
0,3	I/O CHECK READING TAPE.
1,3	REDUNDENCY FAILURE READING TAPE (PERSISTANT).
2,3	END-OF-FILE ON TAPE NOT HANDLED BY =CALLER=.
0,5	I/O CHECK WRITING TAPE.
1,5	REDUNDENCY CHECK WRITING TAPE.
2,5	ERASE FAILURE CHECK WRITING TAPE.
3,5	END-OF-TAPE CHECK WRITING TAPE.
0,6	LOGICAL UNIT NOT IN IOU.

APPENDIX I. LIST OF ENTRY POINTS AND FIRST CARDS OF SYMBOLIC PROGRAM DECKS

```
*       LABEL                                                           11110
$EXECUTE        FORTRAN                                                 11110
*       LABEL                                                           185BE
*        ROW                                                            185BE
*        FAP                                                            185BE
*185BEL - ON-LINE START CARD FOR X-RAY SYSTEM ON 85 UNDER BELL MONITOR  185BE
* THIS CARD WILL INITIATE THE XRAY SYSTEM ON 85.  PUT CARD IN ON-LINE   185BE
* CARD READER, PUT PROGRAM TAPE ON 85, CLEAR, LOAD CARDS.               185BE
* STUFF+1, RESPECTIVELY.                                                185BE
*   $$$REQUIRES IOUBE VERSION OF IO TABLES$$$                           185BE
*                                                                       185BE
*       LABEL                                                           185CO
*        ROW                                                            185CO
*        FAP                                                            185CO
*185CARD - ON-LINE START CARD FOR X-RAY SYSTEM ON 85))                  185CO
* THIS CARD WILL INITIATE THE XRAY SYSTEM ON 85.  PUT CARD IN ON-LINE   185CO
* CARD READER, PUT PROGRAM TAPE ON 85, CLEAR, LOAD CARDS.               185CO
* PROVISION IS MADE FOR REDEFINING NTINM AND NTOUTM AT STUFF+2 AND      185CO
* STUFF+1, RESPECTIVELY.                                                185CO
*                                                                       185CO
*       LABEL                                                           ABSOO
CABSORB- BOND ABSORBTION CORRECTION FOR EACH REFLECTION.                ABSOO
        SUBROUTINE ABSORB                                               ABSOO
C       VERSION OF NOV 62                                               ABSOO
C       BLOCK 1500 APPLICATION OF ABSORBTION CORRECTIONS                ABSOO
C         VERSION WHICH APPLIES BOND CORRECTIONS --- B. MOROSIN         ABSOO
C                          MAY BE ADVISABLE TO TEST JCODE (2 = LESS-THAN,ABSOO
C       1 = OBSERVED). FREL IS NOW STORED. LPSQRT = 1 IF SQUARE ROOT MUST ABSOO
C       BE TAKEN BEFORE APPLICATION TO FREL OR LPSQRT = 2 IF FREL IS I OR ABSOO
C       I/LP. ANY DATA SPECIFIC FOR ABSORBTION REQUIRED BY THE PROGRAM  ABSOO
C       SHOULD HAVE BEEN READ IN BLOCK  900. JAX TELLS THE AXIS OF      ABSOO
C       ROTATION 1=A,2=B,3=C. NOTE THAT THERE ARE OTHER ORIENTATION CODES ABSOO
C       IN THE PROGRAM AS WELLAS ALL THE DATA USUALLY CALCULATED BY A   ABSOO
C       REDUCTION OF DATA PROGRAM, SIN THETA, SIN(THETA)/LAMBDA( THEIR  ABSOO
C       SQUARES, SCATTERING FACTORS, ETC., ETC.                         ABSOO
C       PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO    ABSOO
C       CHANGE COMMON IN SUBROUTINES.                                   ABSOO
C       SYSTEM COMMON ASSIGNMENTS                                       ABSOO
*       LABEL                                                           ABSIN
CINABS - INITIALIZES ABSORBTION CORRECTION SUB-ROUTINE  ABSORB.         ABSIN
        SUBROUTINE INABS                                                ABSIN
C       VERSION OF NOV 62                                               ABSIN
C         VERSION WHICH APPLIES BOND CORRECTIONS --- B. MOROSIN         ABSIN
C       THIS BLOCK IS DESIGNED TO READ IN THE CONSTANTS AND SWITCH SETT- ABSIN
C       INGS REQUIRED IN ORDER TO CALCULATE VARIOUS KINDS OF ABSORBTION ABSIN
C       CORRECTIONS. IT MUST ALSO SWITCH IN BLOCK 1500 (IABSW) WHICH IS ABSIN
C       THE ONCE PER REFLECTION BLOCK. THIS ABSORB CARD WILL BE RECOGNIZEDABSIN
C       AT ANY TIME AFTER A CONDITION CARD IS READ. THEREFORE THIS BLOCK ABSIN
C       SHOULD BE INITIALIZED AND CANCEL BLOCK 1500 BY MEANS OF IABSW.  ABSIN
C       STUDY BLOCKS  660 TO  800 FOR PHILOSOPHY REGARDING BLANK FIELDS ABSIN
C       AND SWITCH SETTINGS. UNTIL THIS BLOCK IS PROGRAMMED IABSW IS SET ABSIN
C       TO ONE (1) AT THE BEGINNING OF THE PROGRAM.                     ABSIN
C       PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO    ABSIN
C       CHANGE COMMON IN SUBROUTINES.                                   ABSIN
C       SYSTEM COMMON ASSIGNMENTS                                       ABSIN
*       LABEL                                                           AINPO
CAINPT     CONVERT A,B,C BY 24A1 TO FLOATING POINT NUMBER (A(I),I=1,3)  AINPO
C          DETECT  DECIMAL PLACES AFTE DECIMAL POINT (IDEC)             AINPO
        SUBROUTINE AINPT (AA,A,IDEC)                                    AINPO
*       LABEL                                                           AINPO
CAINPT     PREPARE A(I), DETECT DECIMAL PLACES AFTER DEC. POINT         AINPO
        SUBROUTINE AINPT (AA,A,IDEC)                                    AINPO
*       LABEL                                                           AOUTO
CAOUTP     PRINT OUT A/B,C/B,A,B,C IN ACCORDANCE WITH THE ACCURACY      AOUTO
        SUBROUTINE AOUTP (SYST,ACB,CCB,T,IDEC,INFO)                     AOUTO
C       SYSTEM COMMON ASSIGNMENTS                                       AOUTO
*       LABEL                                                           ARCOS
*ARCOS                          ARCCOSINE ROUTINE                       ARCOS
        ENTRY   ARCOS                                                   ARCOS
*       LABEL                                                           ARROO
CARR       ARRANGE SCALAR PRODUCTS IN DECREASING ORDER                  ARROO
        SUBROUTINE ARR  (S1,S2)                                         ARROO
C       SYSTEM COMMON ASSIGNMENTS                                       ARROO
*       LABEL                                                           ATNOO
*ATN    - LOOK UP ATOM NAME IN ATOM-TYPE DICTIONARY.                    ATNOO
*                        18 SEPT 61                                     ATNOO
        ENTRY   ATN                                                     ATNOO
```

```
* A FORTRAN CLOSED-SUBROUTINE FUNCTION TO GET INDEX OF SCATTERING      ATNOOC
* FACTOR WHOSE BCD NAME IS SUPPLIED.  INDEX IS NEGATIVE IF DISPERSION ISATNOOC
```

```
* TO BE APPLIED. INDEX IS ZERO IF FJ NOT IN TABLE.                    ATNOO
*       NOTE - THIS SUBROUTINE USES ERASEABLE STORAGE IN UPPER MEMORY.  ATNOO
* UNPACK CHARACTERS INTO 6 WORDS                                       ATNOO
*       LABEL                                                          ATNAM
*ATNAME- PREPARE ATOM-TYPE NAME FOR DICTIONARY.                        ATNAM
*ATNAMEF - NORMALIZE ATOM-TYPE NAME FOR DATA-REDUCTION     DARRELL HIGH ATNAM
*                        18 SEPT 61                                    ATNAM
*       ENTRY   ATNAME                                                 ATNAM
* A FORTRAN CLOSED-SUBROUTINE FUNCTION TO LEFT-JUSTIFY ALL NON-BLANK   ATNAM
* CHARACTERS IN A BCD ATOM-TYPE NAME.  THE NORMALIZED RESULT IS RETURNEDATNAM
* IN THE AC.  ZERO WILL BE RETURNED IF AND ONLY IF THE NAME ENDED IN A ATNAM
* DIGIT, WHICH IS ILLEGAL.                                             ATNAM
*       NOTE - THIS SUBROUTINE USES ERASEABLE STORAGE IN UPPER MEMORY. ATNAM
* UNPACK CHARACTERS INTO 6 WORDS                                       ATNAM
*       LABEL                                                          ATNUO
*ATNUM   GET ATOM TYPE NUMBER FROM ATOM NAME AND DICTIONARY NAME.      ATNUO
*       ENTRY   ATNUM                                                  ATNUO
*  A FORTRAN SUBROUTINE WITH THREE ARGUMENTS.  USED BY                 ATNUO
*      CALL ATNUM(N,ATNAM,ATTBL)                                       ATNUO
*         WHERE N IS THE ATOM TYPE NUMBER TO BE FOUND BY THE SUBROUTINE ATNUO
*         ATNAME IS THE BCD ARGUMENT. ALL BLANKS ARE ELIMINATED,       ATNUO
*         ALL NUMBERS TO THE RIGHT OF THE RIGHT-MOST ALPHABETIC        ATNUO
*         CHARACTER ARE IGNORED.  C 1 = C123 =   C 01 = C     6        ATNUO
*         TBL IS THE NAME OF THE 16 PLACE ARRAY OF ATOM TYPES.         ATNUO
*         THESE MUST EITHER HAVE BEEN WRITTEN BY DATA REDUCTION OR     ATNUO
*         LEFT JUSTIFIED BY ATNAME FUNCTION.                           ATNUO
*                                                                      ATNUO
*         THE INDEX N IS RETURNED AS ZERO IF THERE IS NO ATOM OF       ATNUO
*         SUCH AND SUCH TYPE IN THE DICTIONARY.                        ATNUO
*       NOTE - THIS SUBROUTINE USES ERASEABLE STORAGE IN UPPER MEMORY. ATNUO
*                                                                      ATNUO
*       LABEL                                                          ATNUO
*ATNUW - FORTRAN FLOATING POINT ARCTANGENT ROUTINE  (9ATN)             ATNUW
*       ENTRY   ATAN                                                   ATNUW
*       LABEL                                                          ATNUW
*ATOFL CONVERT BCD INTEGERS TO FLOATING POINT NUMBERS                  ATOFO
*       ENTRY   ATOFL                                                  ATOFO
* A FAP     SUBROUTINE TO EXAMINE A ALPHANUMERICAL NUMBER BY A1 FORMAT ATOFO
* AND RETURN A FLOATING NUMBER FROM 0. 1. .... TO 9.                   ATOFO
* CALLING SEQUENCE ... CALL ATOFL (AA1,AFL)                            ATOFO
*       LABEL                                                          ATOFO
*B58ELL    PROGRAM TO USE X-RAY SYSTEM UNDER THE BELL MONITOR          B58EO
*                                                                      B58EO
*       LABEL                                                          B58EO
*B5FOR    PROGRAM TO CALL X-RAY SYSTEM FROM B5                         B5FOR
*                                                                      B5FOR
*                                                                      B5FOR
*       LABEL                                                          B5FOR
*B5IBSY     PROGRAM TO USE X-RAY SYSTEM UNDER THE IBSYS MONITOR....   B5IBO
*       LABEL                                                          B5IBO
*BDZ    -    BINARY TO ZONED DECIMAL                                   BDZOO
*       ENTRY   BDZIN              INTEGER INPUT (B35)                 BDZOO
*       ENTRY   BDZFX              FIXED-POINT INPUT                   BDZOO
*       ENTRY   BDZFL              FLOATING-POINT INPUT                BDZOO
* A FORTRAN SUBROUTINE SUBPROGRAM TO CONVERT BINARY TO SIGN-OVER-UNITS BDZOO
* (ZONED) BCD, WITH LEADING ZEROS, AS FOR 650 INPUT.                   BDZOO
* DEFINITIONS -                                                        BDZOO
*       X OR I  FLOATING- OR FIXED-POINT ARGUMENT                      BDZOO
*       NB      BINARY SCALE OF FIXED-POINT INPUT (INTEGER=35)         BDZOO
*       ND      DECIMAL SCALE OF OUTPUT (INTEGER=0)                    BDZOO
*       NW      WIDTH OF DECIMAL FIELD (LIMIT 6 CHARACTERS)            BDZOO
*       A       ALPHANUMERIC OUTPUT - NW CHARACTERS LEFT-JUSTIFIED     BDZOO
* OVERFLOW OR CALLING-SEQUENCE ERROR RESULT IN A WORD OF BLANKS.       BDZOO
* NORMALLY THE AC IS ZERO UPON EXIT, BEING NON-ZERO ONLY IF AN ERROR   BDZOO
* OCCURRED.  THUS THE FORTRAN FUNCTION SUBPROGRAM CALLING METHOD MAY   BDZOO
* BE USED, WITH THE FUNCTIONAL VALUE BEING AN ERROR INDICATOR.         BDZOO
* INTEGER CONVERSION - CALL BDZIN(I,NW,A)                              BDZOO
*       LABEL                                                          BDZOO
*BEGIN - SYSTEM BEGIN ROUTINE AND BSS LOADER (PROGRAM TAPE GENERATOR)  BEGOO
*                                                                      BEGOO
*       LABEL                                                          BEGOO
*BLANK INSERT A BLANK CHARACTER IN AN =A= FORMAT WORD                  BLANO
*       ENTRY   BLANK                                                  BLANO
* A SUBROUTINE TO ADD ONE BLANK SPACE IN FRONT OF ALPHANUMERICAL LETTER BLANO
* CALLING SEQUENCE ... CALL BLANK (OSM1,SM2)                           BLANO
* THE ARGUMENT OSM1 BY A1 FORMAT ,SM2 BECOMES A2 BY ADDITION OF BLANK  BLANO
*       LABEL                                                          BLANO
CBOANG  - ANGLE FUNCTION                                               BOANO
   MAIN PROGRAM                                                        BOANO
*       LABEL
CBODIS   - DIST FUNCTION                                               BODIS
   MAIN PROGRAM                                                        BODIS
```

```
*       LABEL                                                           BODDO
CBODDIS  - DDIST SUBROUTINE                                             BODDO
        SUBROUTINE DDIST                                                BODDO
C                                                                       BODDO
C       SYSTEM COMMON STORAGE                                           BODDO
*       LABEL                                                           BONDO
CBONDLA     GEOMETRICAL FUNCTIONS, MARK III  8/8/63                     BONDO
C                                                                       BONDO
C       SYSTEM COMMON STORAGE                                           BONDO
   MAIN PROGRAM
*       LABEL                                                           BONSK
CBONSEK - ATOM I.D. LOOK-UP                                             BONSK
        SUBROUTINE BONSEK (NATOM,IMX,IERR)                              BONSK
C                                                                       BONSK
C       SYSTEM COMMON STORAGE                                           BONSK
*       LABEL                                                           BOSIG
CBOSIGD    - STANDARD DEVIATION OF DISTANCE                             BOSIG
   MAIN PROGRAM
*       LABEL                                                           BSTUW
*BSTUW - FORTRAN BACKSPACE TAPE  (9BST)                                 BSTUW
*             BACKSPACE N                LINKAGE COMPILED BY I/O TRANSLATOR.BSTUW
*                                                                       BSTUW
*A      CAL  N                          UNIT DESIGNATION.               BSTUW
*       TSX  (BST),4                    BACKSPACE TAPE.                 BSTUW
*                                                                       BSTUW
        ENTRY   (BST)                                                   BSTUW
*       LABEL                                                           BTSUO
*BTSNU - CONVERT SIGN-OVER-UNITS BCD INTEGERS TO BINARY.                BTSUO
*BTSNU AND XBTSNU ENABLE FORTRAN TO READ SIGN-OVER-UNITS                BTSUO
        ENTRY   BTSNU                                                   BTSUO
        ENTRY   XBTSNU                                                  BTSUO
        ENTRY   BTCBZ1                                                  BTSUO
*THIS SUBROUTINE IS A JACKET AROUND BTCBZ1 WHICH ALLOWS                 BTSUO
* FORTRAN PROGRAMS TO READ NUMBERS PUNCHED WITH                         BTSUO
* SIGN-OVER-UNITS.                                                      BTSUO
*IT IS A LIBRARY FUNCTION-TYPE SUBROUTINE                               BTSUO
*       LABEL                                                           BYEOO
CBYEBYE - PREPARE 650 CARDS OR BUSING TAPE FROM SYSTEM REFLECTION TAPE. BYEOO
C       VERSION OF 2 JAN 63                                             BYEOO
C                                                                       BYEOO
   MAIN PROGRAM
*       LABEL                                                           CALLO
*CALLER - CONTROL SUBROUTINE FOR X-RAY SYSTEM                           CALLO
        ENTRY   CALLER                                                  CALLO
        ENTRY   EXIT                                                    CALLO
        ENTRY   LINK                                                    CALLO
        ENTRY   IFFW                                                    CALLO
        ENTRY   IFFI                                                    CALLO
        ENTRY   IFFC                                                    CALLO
        ENTRY   IFFY                                                    CALLO
        ENTRY   (BSH)                                                   CALLO
        ENTRY   (CSH)                                                   CALLO
        ENTRY   LINES                                                   CALLO
        ENTRY   NPS                                                     CALLO
* THE SET OF SUBROUTINES IN THIS PACKAGE PERFORM MANY CONTROL FUNCTIONS.CALLO
* ALL INPUT-CARD RECORDS ARE READ BY CALLER, IFFI, OR EXIT.  A *DATA    CALLO
* CARD IS RECOGNIZED AT ANY TIME AND CAUSES IMMEDIATE INITIALIZATION OF CALLO
* THE SYSTEM.  CERTAIN CARDS WILL BE RECOGNIZED AT ANY TIME BY CALLER   CALLO
* AND IFFI, WHICH WILL PERFORM THE REQUIRED OPERATION AND CONTINUE      CALLO
* READING.  (SEE TABLE BELOW.)  SEE INDIVIDUAL ENTRY LOCATIONS FOR      CALLO
* FURTHER INFORMATION.                                                  CALLO
*                                                                       CALLO
*       LABEL                                                           CHACO
CCHAC   INTERCHANGE A AND C AXES                                        CHACO
        SUBROUTINE CHAC (AT1,AT3)                                       CHACO
C       SYSTEM COMMON ASSIGNMENTS                                       CHACO
*       LABEL                                                           CHEKO
CCHEK   CHECK TRANSFORMED CELL DIMENSIONS AND ANGLES                    CHEKO
        SUBROUTINE CHEK (TS,TNS)                                        CHEKO
C       SYSTEM COMMON ASSIGNMENTS                                       CHEKO
*       LABEL                                                           CELOO
CCELFAC- CALCULATES CELL CONSTANTS AND WRITES ON BINARY TAPE.           CELOO
        SUBROUTINE CELFAC                                               CELOO
C       VERSION OF NOV 62                                               CELOO
C       PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO    CELOO
C       CHANGE COMMON IN SUBROUTINES.                                   CELOO
C       SYSTEM COMMON ASSIGNMENTS                                       CELOO
*       LABEL                                                           COMNO
CCOMNT     PRINT MANY COMMENTS IN ACCORDANCE WITH NO OF GROUP AND ENTRY COMNO
        SUBROUTINE COMNT (NGRP,NENT,PT,ITP,MTP,U)                       COMNO
C       SYSTEM COMMON ASSIGNMENTS                                       COMNO
*       LABEL                                                           CONVO
CCONVO    REWRITE THE SPACE-GROUP SYMBOL TO OBEY THE PRIORITY RULE      CONVO
```

```
C          M,A,B,C,N,D   EXCEPT   I BCA  FOR ORTHORHOMBIC SYSTEM          CONVO
      SUBROUTINE CONVO                                                     CONVO
C     SYSTEM COMMON ASSIGNMENTS                                            CONVO
```

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*       LABEL                                                           CONVM
CCONVM    REWRITE THE SPACE GROUP SYMBOL TO OBEY THE CONVENTION         CONVM
C         (2) TRANSFORM B AND F LATTICE TO P  FOR MONOCLINIC SYSTEM     CONVM
C         (1) TO OBEY THE PRIORITY RULE  M,A,B,C,N,D. EXCEPT  I BCA     CONVM
        SUBROUTINE CONVM (VOO,Z,AT1,AT3,BE)                             CONVM
C       SYSTEM COMMON ASSIGNMENTS                                       CONVM
*       LABEL                                                           COORO
CCOOR                                                                   COORO
        SUBROUTINE COOR                                                 COORO
C       SYSTEM COMMON ASSIGNMENTS                                       COORO
*       LABEL                                                           CRAMO
*CRAM    A SUBROUTINE TO STORE INTEGERS IN LEAST SIGDIG OF F.P. NUM.    CRAMO
         ENTRY   CRAM                                                   CRAMO
         ENTRY   UNCRAM                                                 CRAMO
*                                                                       CRAMO
* THE CALLING SEQUENCES FOR THIS SUBROUTINE ARE                         CRAMO
*          CALL CRAM  (ARG,I1,IPOS,IFLOW)                               CRAMO
*          CALL UNCRAM(ARG,I1,IPOS,IFLOW)                               CRAMO
*                                                                       CRAMO
* WHEN CRAM IS CALLED, ARG IS MODIFIED, STARTING WITH ITS LEAST         CRAMO
* SIGNIFICANT DIGITS WITH FIXED POINT VARIABLE I1 HAVING A              CRAMO
* FIELD WIDTH OF IFLOW BINARY PLACES.  THE ARGUMENT I1 IS PLACED IN A   CRAMO
* FIELD, THE POSITION OF WHICH IS SPECIFIED, STARTING WITH THE LEAST SIGCRAMO
* DIG OF ARG AND FILLING IN TO THE LEFT.  UNCRAM EXTRICATES THE I1      CRAMO
* SPECIFIED LEAVING ARG UNTRAMMLED.  FOR EXAMPLE......                  CRAMO
*       CALL CRAM(ARG,I1,2,8)                                           CRAMO
* PLACES I1 IN ARG AS 8 BINARY PLACES WIDE (7 NUMBERS + SIGN) IN BIT    CRAMO
* POSITIONS 20 TO 27 OF ARGH                                            CRAMO
* RESTRICTIONS    (A) THE FIELD WIDTH MUST BE ONE GREATER THAN THE      CRAMO
*                     MAGNITUDE OF I INDICATES IN ORDER TO SAVE THE SIGN CRAMO
*                 (B) A MAXIMUM OF 17 2-BIT INTEGERS MAY BE SPECIFIED... CRAMO
*              OR(C) A MAXIMUM FIELD WIDTH OF 35                        CRAMO
*                                                                       CRAMO
* NEEDLESS TO SAY THIS PROGRAM USED IMPROPERLY WILL GIVE VERY           CRAMO
* STRANGE RESULTS -------- EXERCISE CARE IN CHECK OUT - A CORE          CRAMO
* DUMP OF THE CRAMMED NUMBERS MAY BE WORTHWHILE                         CRAMO
*                                                                       CRAMO
*       LABEL                                                           DEGRO
CDEGR   CONVERT RADIAN INTO DEGREE                                      DEGRO
        SUBROUTINE DEGR                                                 DEGRO
C       SYSTEM COMMON ASSIGNMENTS                                       DEGRO
*       LABEL                                                           DELSO
CDELSIG - A PROGRAM TO GIVE DELTA F VS FO.                              DELSO
   MAIN PROGRAM
*       LABEL                                                           DFAOO
CDFA     MAIN PROGRAM OF DFSYNA  (QUKDYF)                               DFAOO
C       VERSION OF 9 NOVEMBER 1963                                      DFAOO
C       BLOCK DO  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    DFAOO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL DFAOO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY  DFAOO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....DFAOO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        DFAOO
C       CONTROL-PROGRAM COMMUNICATION REGION                            DFAOO
   MAIN PROGRAM
*       LABEL                                                           DFFCO
CDFFC      STRUCTURE FACTORS AND GENERATOR FOR DIFSYN                   DFFCO
C                                                                       DFFCO
        SUBROUTINE DIFTWO(IF2SW)                                        DFFCO
C       UPDATED ON DECEMBER 62                                          DFFCO
C       FC IS IN FORTRAN RATHER THAN AS A SUBROUTINE                    DFFCO
C       GENERATION OF SYMMETRIC PARAMETERS AND CALC OF STRUCTURE FACTORS. DFFCO
C         GENERATION OF PARAMETERS FOR ALL ASYMMETRIC UNITS, CALCULATION  DFFCO
C         OF FC, AND OPERATIONS WITH SUMMARY DATA.                      DFFCO
C       VERSION OF 9 NOVEMBER 1963                                      DFFCO
C       BLOCK DO  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    DFFCO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL DFFCO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY  DFFCO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....DFFCO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        DFFCO
C       CONTROL-PROGRAM COMMUNICATION REGION                            DFFCO
*       LABEL                                                           DFGNO
CDFGN      GENRAT OF DIFSYN                                             DFGNO
C                                                                       DFGNO
        SUBROUTINE GENRAT    (MINI, MAXI,KILO)                          DFGNO
C                                                                       DFGNO
C       VERSION OF 9 NOVEMBER 1963                                      DFGNO
C       BLOCK DO  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    DFGNO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL DFGNO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY  DFGNO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....DFGNO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        DFGNO
C       CONTROL-PROGRAM COMMUNICATION REGION                            DFGNO
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*     LABEL
CDFRD      REFLECTION TAPE READER FOR DIFSYN                          DFRDO
       SUBROUTINE READER                                              DFRDO
C      VERSION OF 9 NOVEMBER 1963                                     DFRDO
C      VERSION OF 9 NOVEMBER 1963                                     DFRDO
      BLOCK DO  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    DFRDO
C       INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL DFRDO
C       THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY  DFRDO
C       OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....DFRDO
C     DIMENSION STATEMENTS AND COMMON STORAGE.                        DFRDO
C     CONTROL-PROGRAM COMMUNICATION REGION                            DFRDO
*     LABEL                                                           DFSDO
CDFSO      SOLVE PARAMETER SHIFTS FOR DIFSYN                          DFSDO
C                                                                     DFSDO
C                                                                     DFSDO
      SUBROUTINE SOLVPM( A,PB,ITAPE,NAME,IERR,PS)                     DFSDO
C                                                                     DFSDO
C                                                                     DFSDO
      THIS SUBROUTINE SOLVES PARAMETER MATRIX RETURNING ERROR         DFSDO
C     IF CHANGEA ARE GREATER THAN 0.01 AND 0.02 UNIT CELL.            DFSDO
C     REFLECT FOR A MINUTE ATE THE FACT OF DIFFERENT CELL LENGTHS     DFSDO
C                                                                     DFSDO
C                                                MORDSIN-JAN 62       DFSDO
      THE REASONABLE ASSUMPTION THAT PEAK HEIGHT AT ATOM              DFSDO
C     CITE DOES NOT EQUAL ZERO IS MADE                                DFSDO
C                                                                     DFSDO
*     LABEL                                                           DFTSO
CDFTS      SOLVE TEMPERATURE FACTOR SHIFTS FOR DIFSYN                 DFTSO
C                                                                     DFTSO
C                                                                     DFTSO
      SUBROUTINE SOLVTM( Z,TB,ITAPE,NAME,IERR)                        DFTSO
C                                                                     DFTSO
C     THIS SUBROUTINE SOLVES TEMP. FACTOR MATRIX RETURNING ERROR      DFTSO
C     IF CHANGE ARE GREATER THAN 0.02 FOR BETAS                       DFTSO
C                                                MORDSIN-JAN 62       DFTSO
C                                                                     DFTSO
*     LABEL                                                           DFXPO
CDFXP      EXPAND ATOM BAND FOR DIFSYN                                DFXPO
C                                                                     DFXPO
C                                                                     DFXPO
      SUBROUTINE EXPAND(ILOF,INDXCN )                                 DFXPO
C                                                                     DFXPO
C     CALL EXPAND ( ILOF, INDXN)                                      DFXPO
C     THIS IS TO EXPAND 200 ATOMS FROM INDXC= 7 TO                    DFXPO
C     13 OR 6 TO 7 OR 13                          MORDSIN JAN 62      DFXPO
C      VERSION OF 9 NOVEMBER 1963                                     DFXPO
C     BLOCK DO  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    DFXPO
C       INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL DFXPO
C       THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY  DFXPO
C       OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....DFXPO
C     DIMENSION STATEMENTS AND COMMON STORAGE.                        DFXPO
C     CONTROL-PROGRAM COMMUNICATION REGION                            DFXPO
*     LABEL                                                           DIMOO
*DIM   SUBROUTINE DIMEN TO DETERMINE DIMENSION OF A REFLECTION        DIMOO
       ENTRY   DIMEN                                                  DIMOO
*   THIS IS A SUBROUTINE TO DETERMINE THE DIMENSION OF A REFLECTION   DIMOO
*   STORED IN THE SECOND MEMBER OF THE CALLING SEQUENCE IS A          DIMOO
*        0 IF THE REFLECTION IS OOO                                   DIMOO
*        1 IF THE REFLECTION IS OOL                                   DIMOO
*        2 IF THE REFLECTION IS OKO                                   DIMOO
*        3 IF THE REFLECTION IS HOO                                   DIMOO
*        4 IF THE REFLECTION IS OKL                                   DIMOO
*        5 IF THE REFLECTION IS HOL                                   DIMOO
*        6 IF THE REFLECTION IS HKO                                   DIMOO
*        7 IF THE REFLECTION IS HKL                                   DIMOO
*   THE FIRST MEMBER OF THE CALLING SEQUENCE IS THE CRAMMED WORD      DIMOO
*   CONTAINING THE THREE INDICES IN THE ORDER L,K,H IN FIELDS 10 WIDE DIMOO
*     LABEL                                                           DMPOO
*DMPUW - FORTRAN DUMP ROUTINE (9DMP).                                 DMPOO
       ENTRY   DUMP                                                   DMPOO
       ENTRY  PDUMP                                                   DMPOO
*                                                                     DMPOO
*     LABEL                                                           DOTOO
CDOT   - DOT PRODUCT BETWEEN TWO VECTORS.                             DOTOO
   MAIN PROGRAM
*     LABEL                                                           DPSUO
*DSQUW - FORTRAN DOUBLE PRECISION SQUARE ROOT FUNCTION  (9DSQ)        DPSUO
*     LABEL                                                           DSQUW
*DSQUW - FORTRAN DOUBLE PRECISION SQUARE ROOT FUNCTION (9DSQ)          DSQUW
*               THIS PROGRAM IS A MODIFICATION OF                     DSQUW
*               IBSQD,A SHARE DISTRIBUTION.                           DSQUW
       ENTRY   DSQRT                                                  DSQUW
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*       LABEL
CDTCR            TEMPORARY FILM DATA TREATMENT PROGRAM                  DTCRO
C       VERSION OF 11/10/63                                             DTCRO
C       NF - NUMBER OF FILMS PER EXPOSURE                               DTCRO
C       IR - ROTATION AXIS, 1 FOR H, 2 FOR K, 3 FOR L                   DTCRO
C       TMN - MINIMUM VALUE TO BE USED IN DETN. OF INTERFILM SCALING    DTCRO
C             RATIOS                                                    DTCRO
C       TMX - MAXIMUM VALUE TO BE USED                                  DTCRO
C       TAM - ABSOLUTE MINIMUM VALUE - USED FOR LESS-THANS              DTCRO
C       FFS - INTENSITY MULTIPLICATION FACTOR                           DTCRO
C          NFMT = 0  -  FORMAT FOR OCTB CARDS                           DTCRO
C         NFMT = 1  -  FORMAT FOR DATB-I CARDS                          DTCRO
   MAIN PROGRAM
*       LABEL
CDATFX    PROGRAM TO CALCULATE UNITARY STRUCT. FACTORS (LINK 10500)     DTFXO
C       MARK II VERSION - 27 MAY 1963                                   DTFXO
C       SYSTEM COMMON ASSIGNMENTS                                       DTFXO
   MAIN PROGRAM
*       LABEL                                                           EDITO
*EDIT   - EDITS SELECTED REFLECTIONS AT FC TIME.                        EDITO
        ENTRY   EDIT                                                    EDITO
*                                                                       EDITO
* THIS PROGRAM IS CALLED BY THE PARAMETER LOADER (PASS ONE)             EDITO
*  BY A STATEMENT THAT LOOKS LIKE THIS.........                         EDITO
*       CALL EDIT(NEDIT,NHC,NKC,NLC,NJCODE,NLEVEL)                      EDITO
*        NEDIT IS THE RUNNING COUNT OF REFLECTIONS TO BE EDITED         EDITO
*        ONLY 25 AT A PASS MAY BE TOUCHED ALL OTHERS WILL BE IGNORED.   EDITO
*       LABEL                                                           EFTOO
*EFTUW - FORTRAN ENDFILE TAPE (9EFT).                                   EFTOO
*             ENDFILE N                LINKAGE COMPILED BY I/O TRANSLATOR.EFTOO
*                                                                       EFTOO
*A      CAL  N                          UNIT DESIGNATION.               EFTOO
*       TSX  (EFT),4                    END OF FILE ON TAPE.            EFTOO
*                                                                       EFTOO
        ENTRY   (EFT)                                                   EFTOO
*       LABEL                                                           ERASE
*ERASE - WRITES BLANK TAPE FOR RECORDS TO BE RE-WRITTEN.                ERASE
        ENTRY   ERASE                                                   ERASE
* A FORTRAN SUBROUTINE SUBPROGRAM TO WRITE BLANK TAPE.                  ERASE
*     CALL ERASE(N,K) TO WRITE K*3.75 INCHES OF BLANK TAPE ON  LOGICAL  ERASE
*       TAPE N.                                                         ERASE
*       LABEL                                                           ERLIN
*ERLINK - ERROR LINK MAIN PROGRAM (LINK 32700)                          ERLIN
*     CALL ERASE(N,K) TO WRITE K*3.75 INCHES OF BLANK TAPE ON  LOGICAL  ERASE
*       TAPE N.                                                         ERASE
*       LABEL                                                           ERROO
*ERREC - ERROR RECORD SUBROUTINE                                        ERROO
        ENTRY   ERREC                                                   ERROO
        ENTRY   (EXE)                                                   ERROO
        ENTRY   (EXEN)                                                  ERROO
* THIS PROGRAM PERFORMS FOR XEMW THE SERVICES THAT THE MONITOR SOURCE   ERROO
* AND MACHINE ERROR RECORDS PERFORM FOR 9XEM.  ANY EXECUTION ERROR NOT  ERROO
* REQUIRING ACTION ON THE SPOT COMES TO THIS LINK.                      ERROO
* THOUGH DESIGNED TO BE IN A SEPARATE LINK, THIS SUBROUTINE MAY BE USED ERROO
* AS AN EXEM.                                                           ERROO
* THE ROUTINE USES THE FORTRAN I/O SUBROUTINES TO DO ITS DIRTY WORK,    ERROO
* AND ACTS AS ITS OWN EXEM.  THE IDEA IS THAT MACHINE ERRORS ARE TREATEDERROO
* WITH ON-LINE COMMENTS, WHICH CANNOT MAKE ANY ERROR.  =SOURCE= ERRORS  ERROO
* WRITE ON-LINE AND OFF-LINE, AND SO ARE SUBJECT TO ERROR.  THE ON-LINE ERROO
* MESSAGE IS WRITTEN FIRST, SO SOMETHING WILL BE SEEN.  THEN IF ANOTHER ERROO
* ERROR SHOWS UP, THE FIRST ONE IS FORGOTTEN.  ELABORATE PRECAUTIONS    ERROO
* ARE TAKEN WITH RESPECT TO ILLEGAL LOGICAL TAPE NUMERS, TO PREVENT ANY ERROO
* NASTY LOOPS FORMING WHEN THE SYSTEM TRIES TO USE AN UNDEFINED TAPE.   ERROO
* SOURCE ERRORS CALL EXIT.  MACHINE ERRORS STOP AND GIVE THE OPERATOR   ERROO
* AN OPTION.  HE CAN MAKE IT CALL EXIT, OR IT WILL TRY ITS BEST TO      ERROO
* RESTART THE LAST DATA DECK.                                           ERROO
*       LABEL                                                           ESOOO
CESORT PROGRAM TO SORT UNITARY STRUCTURE VALUES FROM TAPE (LINK 10800)  ESOOO
C       VERSION OF 9 MAY 1963                                           ESOOO
C        VERSION OF MAY 2 1963                                          ESOOO
C       NECESSARY CARD FORMATS                                          ESOOO
C             COL  1- 6    ESORT                                        ESOOO
C             COL      7    BLANK                                        ESOOO
C             COL  8-13    COMPOUND ID                                  ESOOO
C       SYSTEM COMMON                                                   ESOOO
   MAIN PROGRAM
*       LABEL                                                           EX220
CEX221    EXAMINE THE SPACE-GROUP SYMBOL WITH ONE 2-FOLD AXIS EXCEPT F,IEX220
C         IF 21 IS WRITEN INSTEAD OF 2, MAKE IT TO 21                   EX220
        SUBROUTINE EX221                                                EX220
C       SYSTEM COMMON ASSIGNMENTS                                       EX220
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*       LABEL                                                           EXEMO
*EXEMW - EXECUTION ERROR MONITOR FOR X-RAY SYSTEM                       EXEMO
        ENTRY   (EXEM)                                                  EXEMO
        ENTRY   (EXE)                                                   EXEMO
* THIS SUBROUTINE HANDLES ANY CONTINGENCIES ENCOUNTERED BY THE I/O      EXEMO
* SUBROUTINES.  THOSE PERMITTING CONTINUATION ARE HANDLED HERE, THOSE   EXEMO
* WHICH NECESSITATE TERMINATION OF THE CALCULATION ARE REFERRED TO A    EXEMO
* SEPARATE LINK (ERREC, LINK NO. 32700) WHERE THERE IS MORE ROOM TO     EXEMO
* WAX LOQUACIOUS.                                                       EXEMO
*       LABEL                                                           FCAOO
*FCALC - CALCULATION OF STRUCTURE FACTORS.                              FCAOO
        ENTRY   FCALC                                                   FCAOO
        ENTRY   SEMION          FOR MULTIPLE TAPES.                     FCAOO
* CALLING SEQUENCE FCALC(K) WHERE FCALC(K) AND K BECOME NON ZERO IF     FCAOO
* AND ONLY IF THE FC PROGRAM DETECTS AN INCURABLE ERROR.                FCAOO
*       LABEL                                                           FCOOO
C       22 MARCH 63                                                     FCOOO
CFCONE - FC PROGRAM (LINK 1000). PARAMETER LOADING AND STORING.         FCOOO
C                                                                       FCOOO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL FCOOO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY FCOOO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....FCOOO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        FCOOO
C       CONTROL-PROGRAM COMMUNICATION REGION                            FCOOO
   MAIN PROGRAM
*       LABEL                                                           FCPAT
*FCPACH- (DUMMY) ALLOWS PATCHING OF FC.                                 FCPAT
        ENTRY   FCPACH                                                  FCPAT
        ENTRY   SETFCP                                                  FCPAT
*    SUBROUTINE (FCPACH). THE SUBROUTINE IS INSERTED JUST AFTER FC IS   FCPAT
*    CALCULATED AND JUST BEFORE THE BINARY OUTPUT TAPE IS WRITTEN.      FCPAT
* PERMITS USER TO OPERATE ON A REFLECTION BY WRITING A FORTRAN OR FAP   FCPAT
*       LABEL                                                           FCSMO
CFCSUMS- ACCUMULATES SUMS FOR R AND RESCALE IN FC PROGRAM.              FCSMO
        SUBROUTINE FCSUMS(FO,DF)                                        FCSMO
C       VERSION OF NOV 62                                               FCSMO
C                                                                       FCSMO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL FCSMO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY FCSMO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....FCSMO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        FCSMO
C       CONTROL-PROGRAM COMMUNICATION REGION                            FCSMO
*       LABEL                                                           FCTOO
CFCTWO - FC PROGRAM (LINK 1001). CALLS GENRAT, FCALC, GIVES STATISTICS. FCTOO
C         GENERATION OF PARAMETERS FOR ALL ASYMMETRIC UNITS, CALCULATION FCTOO
C         OF FC, AND OPERATIONS WITH SUMMARY DATA.                      FCTOO
C       VERSION OF NOV 62                                               FCTOO
C                                                                       FCTOO
C       BLOCK 00  INTER-PROGRAM STORAGE ALLOCATION.  THIS IS PROGRAM    FCTOO
C         INTER-COMMUNICATION AND INTERLOCUTION.  CHANGES HERE AFFECT ALL FCTOO
C         THE PROGRAMS AND SUBPROGRAMS OF THE FC FAMILY, AS WELL AS MANY FCTOO
C         OTHER PROGRAMS WHICH SHARE THE BINARY TAPE.  CAVEAT TWIDDLER....FCTOO
C       DIMENSION STATEMENTS AND COMMON STORAGE.                        FCTOO
C       CONTROL-PROGRAM COMMUNICATION REGION                            FCTOO
   MAIN PROGRAM
*       LABEL                                                           FOFNO
CFOFUN - FOURIER REFLECTION READING, GENERATOR, AND FOSUM FEEDER.       FOFNO
        SUBROUTINE FOFUN                                                FOFNO
C       VERSION OF 15 FEB 1963                                          FOFNO
C       A SUBROUTINE FOR READING THE REFLECTION TAPE AND PREPARING THE  FOFNO
C       CORRECT SET OF REFLECTIONS FOR FOSUM THE FOURIER SUMMATION      FOFNO
C       PROGRAM. ALL QUANTITIES COMMON TO THE PROGRAMS ARE HELD IN COMMON FOFNO
C       STORAGE. CALLING SEQUENCE CALL FOFUN.                           FOFNO
C       COMMON AND DIMENSION STATEMENTS FOR FOURIER ROUTINES            FOFNO
C                                                                       FOFNO
C       SYSTEM COMMON ASSIGNMENTS                                       FOFNO
*       LABEL                                                           FOMPO
CMAP      SUBROUTINE FOR SPECIAL FOURIER PRINT FEATURES.                FOMPO
        SUBROUTINE MAP                                                  FOMPO
C       VERSION OF 7 MAY 1963                                           FOMPO
C       COMMON AND DIMENSION STATEMENTS FOR FOURIER ROUTINES            FOMPO
C                                                                       FOMPO
C       SYSTEM COMMON ASSIGNMENTS                                       FOMPO
*       LABEL                                                           FOOBO
CFOOB       A SUBROUTINE TO TAKE CARE OF BELL MONITOR ON LINE CARDS     FOOBO
        SUBROUTINE FOOLBE                                               FOOBO
C       VERSION OF 15 FEB. 1963                                         FOOBO
C       X-RAY 62 CARD READER UNDER BELL SYSTEM.                         FOOBO
*       LABEL                                                           FOSMO
CFOSUM - FOURIER SUMMATION SUBROUTINE.                                  FOSMO
        SUBROUTINE FOSUM                                                FOSMO
C       VERSION OF FEB 20, 1964                                         FOSMO
C       COMMON AND DIMENSION STATEMENTS FOR FOURIER ROUTINES            FOSMO
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*       LABEL                                                           FOU0000
CFOURR - CONTROL PROGRAM FOR FOURIER SYNTHESIS (LINK 4000).             FOU0001
C        VERSION OF 18 FEB 1963                                         FOU0002
C       INNER LOOPS BASED ON U. W. METHOD.                              FOU0003
C       REFLECTIONS NEED NOT BE ORDERED EXCEPT FOR SPEED.               FOU0004
C       SEE FOSUM FOR STORAGE LIMITATIONS-ANY UNIQUE SET OF REFL. ACCEPT. FOU0005
C       SEE GEN AND GENCHK OF DATA REDUCTION AND COMMENTS IN FOFUN FOR  FOU0006
C       MORE DETAILED DESCRIPTION                                       FOU0007
C                                                                       FOU0008
C       COMMON AND DIMENSION STATEMENTS FOR FOURIER ROUTINES            FOU0009
C                                                                       FOU0010
C       SYSTEM COMMON ASSIGNMENTS                                       FOU0011
   MAIN PROGRAM
*       LABEL                                                           FPT0000
*FPTUW - FORTRAN FLOATING POINT TRAP ROUTINE (9FPT).                    FPT0002
         ENTRY   (FPT)                                                  FPT0004
*       LABEL                                                           FRE0000
CEOCAL   FOURIER BLOCK CLACULATOR FOR *FOUREF*                          FRE0001
        SUBROUTINE EOCAL(LL)                                            FRE0002
C       SYSTEM COMMON ASSIGNMENTS                                       FRE0003
*       LABEL                                                           FREF000
CFOREF       FOURIER REFINEMENT PROGRAM  -  MARK III  (LINK 5000)       FREF001
C       9 APRIL 1963                                                    FREF002
C       SYSTEM COMMON ASSIGNMENTS                                       FREF003
   MAIN PROGRAM
*       LABEL                                                           FRFC000
CSFCAL    STRUCTURE FACTOR CALCULATION OF *FOUREF*                      FRFC001
        SUBROUTINE SFCAL                                                FRFC002
C       SYSTEM COMMON ASSIGNMENTS                                       FRFC003
*       LABEL                                                           FRPK000
CPKCAL    PEAK CALCULATOR FOR *FOUREF*                                  FRPK001
        SUBROUTINE PKCAL(NNI,NPK,UP)                                    FRPK002
C       SYSTEM COMMON ASSIGNMENTS                                       FRPK003
*       LABEL                                                           GEF0000
        SUBROUTINE FOFH3                                                GEF0001
*       LABEL                                                           GEABS00
        SUBROUTINE ABSENT(IH,KUT)                                       GEABS01
*       LABEL                                                           GEC0000
CGECO - COMPUTE TWO THETA.                                              GEC0001
        SUBROUTINE COMPREC                                              GEC0002
*       LABEL                                                           GEE0000
        SUBROUTINE EOFH23                                               GEE0001
*       LABEL                                                           GEF0000
        SUBROUTINE FOFH3                                                GEF0001
*       LABEL                                                           GEN0000
        END                                                             GEN0001
*       LABEL                                                           GENC000
CGENCHK- ARRANGES AND CHECKS SYMMETRY OPERATIONS FOR GEN.               GENC001
        SUBROUTINE GENCHK                                               GENC002
C       VERSION OF NOV 62                                               GENC003
C       A FORTRAN SUBROUTINE TO CHECK SYMMETRY OPERATIONS SUPPLIED TO DATAGENC004
C       REDUCTION PROGRAM AND PUT THEM IN PROPER FORM FOR GEN THE       GENC005
C       FOURIER CODE GENERATOR. THE ROTATION MATRICES ARE SEARCHED FOR  GENC006
C       DUPLICATES. THE PRESENCE OF THE IDENTITY MATRIX IS ESTABLISHED. GENC007
C       THE SYMOP MATRICES ARE CHECKED FOR ROWS OR COLUMNS OF ZEROS. IF GENC008
C       THERE ARE MORE THAN ONE SET OF ROTATION MATRICES(I.E. TETRAGONAL GENC009
C       OR HIGHER SYMMETRY(HKL,-HKL,H-KL,-H-KL))A CHECK IS MADE TO MAKE GENC010
C       SURE ALL SETS HAVE EQUAL NUMBERS OF ENTRIES.                    GENC011
C       THE SUBROUTINE IS CALLED BY CALL GENCHK                         GENC012
C       ALL NECESSARY QUANTITIES ARE IN COMMON STORAGE.                 GENC013
C       UPON RETURN THE COMMON QUANTITY KTUGE SHOULD BE CHECKED 0= NO   GENC014
C       ERRORS +=NUMBER OF ERRORS DETECTED AND DESCRIBED ON ERROR TAPE. GENC015
C       PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO    GENC016
C       CHANGE COMMON IN SUBROUTINES.                                   GENC017
C       SYSTEM COMMON ASSIGNMENTS                                       GENC018
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*       LABEL                                                           GENRO0
*GENRAT- GENERATION OF SYMMETRIC ATOMS FROM SPACE-GROUP CONSIDERATIONS. GENRO0
        ENTRY   GENRAT                                                  GENRO0
* A FORTRAN SUBROUTINE SUBPROGRAM TO GENERATE ATOMIC PARAMETERS FOR THE GENRO0
* STRUCTURE-FACTOR SUBROUTINE.  INPUT ARE THE SYMOP MATRICES AND ATOMIC GENRO0
* PARAMETERS FOR AN ASYMMETRIC UNIT, LEFT IN COMMON BY THE PARAMETER    GENRO0
* LOADER (PASS 1), IN THE FORM OF RECORDS 4 AND 6 OF THE BINARY TAPE.   GENRO1
*                                                                       GENRO1
*                                                                       GENRO1
* GENRAT MAKES 2 PASSES OVER THE PARAMETERS.  FIRST, IT MOVES THEM FROM GENRO1
* THE UPPER(HIGH-ADDRESS) END OF THE PARAMETER-STORAGE ARRAY TO THE     GENRO1
* LOWER, FREEING WORK SPACE AT THE TOP.  (ATOMS ARE TAKEN OFF THE BOTTOMGENRO1
* FIRST, SO THE ARRAYS MAY OVERLAP.)  FLOATING-POINT DATA ARE FIXED AT  GENRO1
* THIS POINT, AND ANISOTROPIC TEMP FACTORS ARE EXPANDED INTO 9-WORD     GENRO1
* FORTRAN-ORDER MATRICES.                                               GENRO1
* THE FIRST ARRAY IS REFERRED TO AS THE INPUT ARRAY, THE SECOND AS THE  GENRO1
* HOLD, OR SOURCE ARRAY.                                                GENRO2
*                                                                       GENRO2
* THE ACTUAL GENERATION IS DONE IN THE 2ND PASS.  ATOMS ARE TAKEN ONE   GENRO2
* AT A TIME FROM THE TOP OF THE HOLD ARRAY, AND EACH SYMOP IS APPLIED   GENRO2
* IN TURN.  UNIQUENESS TESTS ARE APPLIED, SO ATOMS IN SPECIAL POSITIONS GENRO2
* ARE DETECTED AND TREATED APPROPRIATELY.  SYMMETRY OPERATIONS ARE AP-  GENRO2
* PLIED TO ANISOTROPIC TEMPERATURE FACTORS.  THE ATOM TYPE NUMBERS ARE  GENRO2
* COMPARED AND SET TO FLAG THE END OF GROUPS OF THE SAME TYPE OF ATOMS. GENRO2
* THE GENERATED ATOMS ARE STACKED UP AT THE TOP OF THE ATOM ARRAY,      GENRO2
* FORMING THE FINAL ARRAY, IN THE FORM REQUIRED BY THE FC SUBROUTINE.   GENRO2
* THE FINAL ARRAY MAY OVERLAP THE SOURCE ARRAY, AS BEFORE.  THE LAYOUTS GENRO3
* OF THE 3 ARRAYS ARE SHOWN IN THE COMMON-ASSIGNMENT SECTION.           GENRO3
* NOTE-- TO FACILITATE INDEXED ADDRESSING, THE COMMON COUNTER WAS DIS-  GENRO3
* PLACED BY ONE, SO THE SYMBOLIC ADDRESS IS 1 HIGHER THAN THE ACTUAL    GENRO3
* STORAGE LOCATION.  IN THE REMARKS THROUGHOUT THIS SUBROUTINE, IT IS   GENRO3
* THE SYMBOLIC ADDRESS WHICH IS REFERRED TO BY THE WORD ADDRESS.        GENRO3
*                                                                       GENRO3
*       LABEL                                                           GESCLO
        FUNCTION SCLPRD(X,Y)                                            GESCLO
*       LABEL                                                           GESCNO
        SUBROUTINE SCANTINE                                             GESCNO
*       LABEL                                                           GESTOO
CGESET - PROGRAM TO CALC. ANGLES FOR G.E. CRYSTAL ORIENTER              GESTOO
C       29 JUNE 63                                                      GESTOO
C                                                                       GESTOO
   MAIN PROGRAM
*       LABEL                                                           GESYSO
CGESYS - GET SYSTEMATIC ABSENCES FOR PCA2(1)                            GESYSO
        SUBROUTINE SYSABS(IH,IGONE)                                     GESYSO
C     -GET SYSTEMATIC ABSENCES FOR PCA2(1)                              GESYSO
*       LABEL                                                           GRAFOO
CGRAPH - A SUBPROGRAM TO PLOT A GRAPH                                   GRAFOO
C                                                                       GRAFOO
C     THE CALLING STATEMENT IS--CALL GRAPH(GRAFTL,KIND,ORDS,MAXPTS,     GRAFOO
C       NSPACE).  GRAFTL IS THE NAME OF AN 11A6 ARRAY CONTAINING THE    GRAFOO
C       GRAPH-S TITLE.  KIND HAS A VALUE OF 1, 2, OR 3.  IF KIND IS 1, THEGRAFOO
C       ORDS WILL BE USED MODULO 100.  IF KIND IS 2, ALL ORDS WILL BE   GRAFOO
C       MULTIPLIED BY A FACTOR SUCH THAT THE MAXIMUM ORD WILL BE EQUAL TO GRAFOO
C       OR LESS THAN 100.  IF KIND IS A 3, TWO GRAPHS WILL BE MADE -- ONE GRAFOO
C       CORRESPONDING TO KIND = 1, THE OTHER TO KIND = 2.  ORDS IS      GRAFOO
C       DIMENSIONED 500 AND REPRESENTS THE ORDINATES.  MAXPTS IS THE    GRAFOI
C       MAXIMUM NUMBER OF POINTS TO BE PLOTTED.  NSPACE CORRESPONDS TO  GRAFOI
C       AN ABSCISSA AXIS SCALE.  IT IS THE NUMBER OF LINES ALONG THE    GRAFOI
C       ABSCISSA AXIS PER POINT PLOTTED.                                GRAFOI
C                                                                       GRAFOI
        SUBROUTINE GRAPH(GRAFTL,KIND,ORDS,MAXPTS,NSPACE)                GRAFOI
C                                                                       GRAFOI
*       LABEL                                                           GUOOOO
*GU       IDENTIFIES EVEN-ODD CONDITION OF INDICES                      GUOOOO
        ENTRY   GEEYOU                                                  GUOOOO
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*       LABEL                                                           HOLL00
*HOLLER     A SUBROUTINE TO MAKE BCD CHARACTER   FOR CRYST. TRNSFORM PGM.HOLL00
        ENTRY    HOLLER                                                 HOLL00
* A FORTRAN SUBROUTINE TO EXAMINE A FLOATING POINT NUMBER AND RETURN AN HOLL00
* APPROPRIATE BCD CHARACTER TO BE PUT OUT IN AN A2 FORMAT               HOLL00
* CALLING SEQUENCE ... CALL HOLLER(ARGUMENT,ANSWER,ICODE)               HOLL00
*                                                                       HOLL00
* WHERE ARGUMENT IS A SIGNED FLOATING POINT VARIABLE IN NEED OF BCDIZINGHOLL01
* ANSWER WILL BE RETURNED AS A BCD LEFT JUSTIFIED A2 CHARACTER ACCORDINGHOLL01
* TO THE FOLLOWING.....                                                 HOLL01
* IF THE ARGUMENT IS AN INTEGER LESS THAN 10.0 THE INTEGER ITSELF IS    HOLL01
* PLACED IN ANSWER AND ICODE IS SET EQUAL TO 1                          HOLL01
* IF THE ARGUMENT IS GREATER THAN 9.0 BUT IS AN INTEGER, THEN  N  IS    HOLL01
* PLACED IN ANSWER AND ICODE IS SET EQUAL TO 2                          HOLL01
* IF THE ARGUMENT IS EXACTLY 1/2  H  IS RETURNED AND AN ICODE OF 3      HOLL01
* ANY OTHER NUMBER IS RETURNED AS  X  AND ICODE AS 4                    HOLL01
*                                                                       HOLL01
*   PLUS NUMBERS ARE RETURNED WITH A BLANK   MINUS WITH A MINUS SIGN....HOLL02
* THE ARGUMENT IS NOT DESTROYED IN THE PROCESS                          HOLL02
* FRACTIONS SMALLER THAN 2 TO THE MINUS 12TH ARE TREATED THE CLOSEST INTHOLL02
*       LABEL                                                           INPT00
CINPT READS REFLECTION DATA FOR DATA REDUCTION                          INPT00
      SUBROUTINE INPUT(KREAD)                                           INPT00
C      VERSION OF MAY 2 1963                                            INPT00
C      FOR STD U.W. FORMATS OR DEALERS CHOICE (INCLUDES BINARY)         INPT00
C     CALLED BY DATA REDUCTION BY CALL INPUT(KREAD).  THE FIRST TIME D.RINPT00
C     CALLS, KREAD IS ONE (1).  IF KREAD IS CHANGED TO 2, THE MAIN      INPT00
C     PROGRAM STOPS READING THE BCD INPUT TAPE UNTIL SUCH TIME THAT     INPT00
C     KREAD IS SET BACK TO 1.  BY PLACING A BLANK CARD ON THE BCD INPUT INPT00
C     TAPE AND SUPPLYING ANOTHER VERSION OF THIS SUBROUTINE REFLECTIONS INPT00
C     MAY BE PROCESSED IN ANY FORMAT DESIRED.  THE MAIN PROGRAM DEMANDS INPT01
C     THAT THE FOLLOWING QUANTITIES BE DELIVERED- H, K, L, JCODE (1/2/3,INPT01
C     OBS./LESS THAN/EXTINCT), RAY ( I, F**2, F (RELATIVE OR ABSOLUTE)).INPT01
C                                                                       INPT01
C     REQUIRES SUBROUTINE XBTSNU                                        INPT01
C     READ INTENSITY CARD. LLL8 = 1 MEANS USUAL FORMAT, LLL8 = 2 MEANS  INPT01
C     MARK SENSE FORMAT.                                                INPT01
C      3 MEANS DEALERS CHOICE                                           INPT01
C     BLOCK 1000 AND 7500 INTENSITY CARDS.                              INPT01
C     PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO      INPT01
C     CHANGE COMMON IN SUBROUTINES.                                     INPT02
C     SYSTEM COMMON ASSIGNMENTS                                         INPT02
*     LABEL                                                             INPT02
CINV33 - INVERT 3X3 MATRIX (JORDAN/DEKKER)   HIGH  SEPT 62              INV300
      SUBROUTINE INV33(A)                                               INV300
*     LABEL                                                             INV300
*IOBUW - FORTRAN INPUT-OUTPUT BINARY (9IOB).  (JAN. 1960)               IOB000
*                                                                       IOB000
*(IOB)          INPUT-OUTPUT BINARY  USED BY (STB). (TSB).              IOB000
*                                                                       IOB000
        ENTRY    (IOB)                                                  IOB000
        ENTRY    -(EXB)                                                 IOB000
*                                                                       IOB000
*                                                                       IOB001
*     LABEL                                                             IOH000
*IOHUW - FORTRAN INPUT-OUTPUT HOLLERITH (9IOH).                         IOH000
*                                                                       IOH000
*(IOH)       INPUT-OUTPUT HOLLERITH   USED BY (TSH),(STH),(CSH),(SCH),  IOH000
*                                     AND (SPH).                        IOH000
        ENTRY    (IOH)                                                  IOH000
        ENTRY    (FIL)                                                  IOH000
        ENTRY    (RTN)                                                  IOH000
*     LABEL                                                             IOH000
*IOSW   -  INPUT-OUTPUT SUPERVISOR (IOS) MODIFIED FOR IOU IN COMMON     IOSW00
* FOLLOWING IS THE IBM/APPLIED PROGRAMMING SUBROUTINE OF JANUARY 1960   IOSW00
* (MODIFIED TO USE (EXE)), WITH A FEW MINOR EMBELLISHMENTS.             IOSW00
* (1) ENTRIES HAVE BEEN PROVIDED IN THE VECTOR OF I/O COMMANDS FOR THE  IOSW00
* INSTRUCTIONS (LCH) AND (SCH).  (BOTH HAVE THE USUAL ADDRESSES 0,4.)   IOSW00
* (2) THE PROGRAM EXPECTS THE IOU TABLE TO HAVE BEEN STORED (IN THE     IOSW00
* INVERSE OF ITS USUAL ORDER) IN COMMON AT IOU.                         IOSW01
*                                                                       IOSW01
        ENTRY    (IOSW)                                                 IOSW01
        ENTRY    (IOS)                                                  IOSW01
        ENTRY    .UNIT.                                                 IOSW01
        ENTRY   -(RDS)                                                  IOSW01
        ENTRY   -(WRS)                                                  IOSW01
        ENTRY   -(BSR)                                                  IOSW01
        ENTRY   -(WEF)                                                  IOSW01
        ENTRY   -(REW)                                                  IOSW01
        ENTRY   -(ETT)                                                  IOSW02
        ENTRY   -(RCH)                                                  IOSW02
        ENTRY   -(LCH)                                                  IOSW02
        ENTRY   -(SCH.)                                                 IOSW02
        ENTRY   -(TEF)                                                  IOSW02
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ENTRY  -(TCO)                                                    IOSWO2
ENTRY  -(TRC)                                                    IOSWO2
                                                                 IOSWO2
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*       LABEL                                                           IOUBE
*IOUBEL  INPUT-OUTPUT ROUTINE -REPLACES FORTRAN (9IOU)  BELL MONITOR**  IOUBE
         ENTRY   (IOU)                                                  IOUBE
*       LABEL                                                           IOUWO
*IOUW   - INPUT-OUTPUT ROUTINE. REPLACES FORTRAN (9IOU). U OF W SPECIFIC.IOUWO
         ENTRY   (IOU)                                                  IOUWO
*       LABEL                                                           LISOO
*LISTF    FC PUBLICATION LISTING FROM SYS. TAPE OR 650 CARDS.           LISOO
*                                                                       LISOO
*        MAKE LIKE A GOOD SYSTEM PROGRAM AND CALL CALLER                LISOO
*       LABEL                                                           LISTI
CLISTIN   READ BINARY REFLECTION RECORDS FOR LISTFC PROGRAM             LISTI
        SUBROUTINE LISTIN(IGO ,IFO,IFC,IREJ,LTCOD,H,IK,IL,IA,IB)        LISTI
*       LABEL                                                           LISKO
CLISTK    READ AND CHECK FIRST SEVEN RECORDS OF BINARY TAPE FOR FCLIST  LISKO
        SUBROUTINE LISTKP(COMPIO,IRESC)                                 LISKO
C       17/7/63                                                         LISKO
*       LABEL                                                           LISUO
*LISTUP - LISTING TAPE UPDATE PROGRAM                                   LISUO
*       LABEL                                                           LOGOO
*LOGUW - FORTRAN FLOATING POINT LOG ROUTINE (9LOG).                     LOGOO
         ENTRY   LOG10                                                  LOGOO
         ENTRY   LOGE                                                   LOGOO
         ENTRY   LOGN                                                   LOGOO
         ENTRY   LOG                                                    LOGOO
*        ..............................................................LOGOO
*                                                                       LOGOO
*       LABEL                                                           LSACO
*LSACS    ARCOS AND ARCSIN SUBROUTINE                                   LSACO
         ENTRY   ARCOS                                                  LSACO
         ENTRY   ARCSIN                                                 LSACO
*       LABEL                                                           LSCRO
CLSCRT    SUBROUTINE CERUTS -- ROOTS OF A CUBIC EQUATION                LSCRO
C                                                                       LSCRO
        SUBROUTINE CERUTS (AA, BB, CC, DD, DISC, Y, KSOL)               LSCRO
*       LABEL                                                           LSHEO
CLSHEQ   SUBROUTINE LSHEQ -- SOL-NS OF THREE HOMOGENEOUS EQUATIONS      LSHEO
C                                                                       LSHEO
C     THIS IS A SUBROUTINE DESIGNED TO GIVE A SOLN FOR THREE HOMOGEN.   LSHEO
C      EQUATIONS OF THREE UNKNOWNS. THE SOLN RETURNED IS OF COURSE NOT  LSHEO
C      UNIQUE BUT IS PROPORTIONAL TO THE DESIRED SOLN.                  LSHEO
C      IN THE CALLING SEQUENCE NTOUT IS THE CURRENT BCD OUTPUT TO THE   LSHEO
C      PRINTER. C IS THE (3,3) MATRIX OF THE COEF-S OF THE EQS., X IS THELSHEO
C      (3,1) MATRIX OF THE SOL-N VALUES, AND IERR IS THE FLAG INDICATING LSHEO
C      ALL OK OR CAN-T BE DONE BY THE CORRESPONDING VALUES OF ZERO OR   LSHEO
C     ONE.                                                              LSHEO
        SUBROUTINE LSHEQ (NTOUT,C,X,IERR)                               LSHEO
*       LABEL                                                           LSMIV
CLSMIV   SUBROUTINE MATINV -- 3X3 MATRIX INVERSION                      LSMIV
C                                                                       LSMIV
        SUBROUTINE MATINV (A, B, JOETZE)                                LSMIV
C       INVERSE,B, OF THIRD ORDER DETERMINANT, A                        LSMIV
*       LABEL                                                           LSMMP
CLSMMPY  SUBROUTINE MATMPY -- MATRIX MULTIPLY                           LSMMP
C                                                                       LSMMP
        SUBROUTINE MATMPY (A,N,M,B,L,C)                                 LSMMP
C       A IS NXL, B IS LXM, SO C IS NXM                                 LSMMP
*       LABEL                                                           LSPOO
CLSQPL    LEAST SQUARES PLANE AND LINE PROGRAM                          LSPOO
C     VERSION AS OF 6 AUGUST 1963    CHASTAIN                           LSPOO
C                                                                       LSPOO
C     THE METHOD OF CALCULATION IS LARGELY THAT GIVEN BY V. SCHOMAKER,  LSPOO
C      ET AL. ACTA CRYST. 12,600 (1959).                                LSPOO
C      THE OUTPUT TERMINOLOGY IS AS FOLLOWS.  A, B, AND C ARE THE VECTORSLSPOO
C      DEFINING THE UNIT CELL.  A ZERO, B ZERO, AND C ZERO ARE THE MAG- LSPOO
C      NITUDES OF A, B, AND C.  X, Y, AND Z ARE THE FRACTIONAL COORD-   LSPOO
C      INATES OF THE ATOMS IN THE DIRECT CELL.                          LSPOO
C      THE ORTHOGONAL-ANGSTROM SPACE IS DEFINED AS THREE ORTHOGONAL     LSPOO
C      VECTORS, I, J, AND K, ONE ANGSTROM IN MAGNITUDE WITH I PARALLEL  LSPOO
C      TO A, K PERPENDICULAR TO A IN THE PLANE OF A AND C, AND J        LSPOO
C      PERPENDICULAR TO THE PLANE OF A AND C.                           LSPOO
C                                                                       LSPOO
C                                                                       LSPOO
   MAIN PROGRAM
*       LABEL                                                           MCLOO
CMCL     MONOCL DEAL WITH MONOCLINIC   SYSTEM                           MCLOO
        SUBROUTINE MONOCL (VOC,Z,JAHR,CM)                               MCLOO
C       SYSTEM COMMON ASSIGNMENTS                                       MCLOO
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*       LABEL
CMDIF     - A PROGRAM FOR UPDATING OR ALTERING A REFLECTION TAPE
C       MODIFY A REFLECTION TAPE BY REPLACING A SPECIFIED QUANTITY.
         VERSION OF MAY 2 1963
C       LINK 10600 IN CALLERS DICTIONARY
C
C       ONLY 5000 REFLECTIONS MAY BE CHANGED IN ONE PASS DOWN
C       THE TAPE
C
C       THE FORMAT OF THE MODIFY CARD IS AS FOLLOWS
C
C       THE REFLECTION CARDS ARE THE SAME GENERAL FORMAT
C       AS FOR DATA REDUCTION
C        1-15 BLANKS
C       16-19 FIXED POINT H   (I4)
C       20-23 FIXED POINT K   (I4)
C       24-27 FIXED POINT L   (I4)
C       28-37 FIXED OR FLOATING NUMBER TO REPLACE QUANTITY SPECIFIED
C             IN MODIFY CARD (I10 OR F10.2)
C
C       REFERENCE TO THE TAPE FORMAT IN THE WRITE-UP APPENDIX
C       WILL SHOW THE CORRECT  VALUE TO USE TO REPLACE A GIVEN QUANTITY
C       0/BLANK/OR MINUS NUMBER IS TREATED AS AN ERROR
C       HERE IS A CONDENSED LIST OF EXAMPLES
C       1/2/3 REPLACE H/K/L   (GOOD LUCK)
C         4    REPLACE F RELATIVE
C         8    REPLACE LEAST SQUARES WEIGHT
C         9    REPLACE UNITARY STRUCTURE FACTOR
C        10    REPLACE STATISTICAL PHASE (SEE ABOVE FOR SPECIAL OPTION)
C        20    REPLACE FIRST SCATTERING FACTOR
C
C       FOR MANY OF THE QUANTITIES WHICH MAY BE  BE REPLACED A FULL
C       DATA RE-REDUCTION IS PROBABLY IN ORDER AND WILL LEAD TO
C       FEWER POSSIBILITIES FOR ERROR
C
C       COMMON AND DIMENSION STATEMENTS
C
C       SYSTEM COMMON
C    MAIN PROGRAM
*       LABEL
CMIXUP   SUBROUTINE TO SORT EVEN OR ODD INDICES OF REFLECTIONS
        SUBROUTINE MIXUP(A,N,B,M)
C        VERSION OF 9 APR 63
C       THIS SUBROUTINE TAKES A AND B AND PUTS THEM IN ARRAY AND STUFF
C       RESPECTIVELY IN DESCENDING ORDER OF MAGNITUDE. THE NUMBER M
C       DETERMINES WHICH BLOCK OF THE ARRAY AND N DETERMINES WHERE IN THE
C       BLOCK.
C       THE BLOCKS ARE NOMINALLY 1500 LONG BUT MAY OF COURSE BE TWIDDLED
C       (TNX TO D.H.) IF THE NECESSARY CHANGES ARE MADE.
C       SYSTEM COMMON
*       LABEL
*MODPOS- CONVERT NUMBER INTO A POSITIVE MODULO VALUE.
*MODPOS  - REDUCE M MODULO N, POSITIVE      DARRELL HIGH
         ENTRY   MODPOS            CALL AS MODPOS(M,N)
*       LABEL
*NAME    - LEFT-JUSTIFY ALL NON-BLANK CHARACTERS IN ATOM NAME.
*                        18 SEPT 61
         ENTRY   NAME
         ENTRY   XNAME
* A FORTRAN CLOSED-SUBROUTINE FUNCTION TO LEFT-JUSTIFY ALL NON-BLANK
* CHARACTERS IN A 6-CHARACTER BCD NAME, FILLING OUT WITH BLANKS.
*        NOTE - THIS SUBROUTINE USES ERASEABLE STORAGE IN UPPER MEMORY.
* UNPACK CHARACTERS INTO 6 WORDS
*       LABEL
CNFIXER - A SUBROUTINE FOR FIXING A FLOATING POINT NUMBER
C
C      THE SECOND ARGUMENT,L, AMOUNTS TO A FLAG WHICH IN EFFECT GIVES THIS
C       FUNCTION TWO ENTRY POINTS.  IF L = 1 IN THE CALLING SEQUENCE, THE
C       OUTPUT VALUE OF THE FUNCTION WILL BE THE FIXED PT. NUMBER
C       OBTAINED BY ROUNDING THE ARGUMENT TO AN INTEGER.  IF L = 2 IN THE
C       CALLING SEQUENCE, THE OUTPUT VALUE WILL BE THE SIGN OF THE
C       ARGUMENT TIMES THE SMALLEST INTEGER EQUAL TO OR GREATER THAN THE
C       MAGNITUDE OF THE ARGUMENT.
C
    MAIN PROGRAM
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*       LABEL
*NOCALL - CUT-DOWN VERSION OF CALLER FOR NON-CHAIN OPERATION
        ENTRY   CALLER
        ENTRY   EXIT
        ENTRY   LINK
        ENTRY   IFFW
        ENTRY   IFFI
        ENTRY   IFFC
        ENTRY   (BSH)
        ENTRY   (CSH)
        ENTRY   LINES
        ENTRY   NPS
* THE SET OF SUBROUTINES IN THIS PACKAGE PERFORM MANY CONTROL FUNCTIONS.
* ALL INPUT-CARD RECORDS ARE READ BY CALLER, IFFI, OR EXIT.  A *DATA
* CARD IS RECOGNIZED AT ANY TIME AND CAUSES IMMEDIATE INITIALIZATION OF
* THE SYSTEM.  CERTAIN CARDS WILL BE RECOGNIZED AT ANY TIME BY CALLER
* AND IFFI, WHICH WILL PERFORM THE REQUIRED OPERATION AND CONTINUE
* READING.  (SEE TABLE BELOW.)  SEE INDIVIDUAL ENTRY LOCATIONS FOR
* FURTHER INFORMATION.
*
*       LABEL
CNWAX   CALCULATE NEW CELL DIMENSIONS AND ANGLES
        SUBROUTINE NWAX
C       SYSTEM COMMON ASSIGNMENTS
*       LABEL
CORBET          ORFLS PATCH FOR BETAS NO ATOMS TO BE RESET
        SUBROUTINE RESETB(BETA,ATOM,NA)
*       LABEL
*ORDNL - MAKES PROPER SUFFIX FOR ORDINAL NUMBERS.
*ORDNL - SUBROUTINE TO GET ORDINAL SUFFIXES      HIGH      AUG 61
        ENTRY   ORDNL
        ENTRY   XORDNL
* A FORTRAN CLOSED-SUBROUTINE FUNCTION TO GET THE BCD SUFFIX FOR AN
* ORDINAL NUMBER, GIVEN THE CARDINAL NUMBER AS A B17 INTEGER.
* CALL IN STATEMENTS LIKE A=ORDNLF(I) OR N=XORDNLF(I), WHERE I IS THE
* NAME OF THE INTEGER FOR WHICH A SUFFIX IS DESIRED, A OR N IS THE NAME
* OF THE FLOATING- OR FIXED-POINT VARIABLE WHERE THE SUFFIX IS TO BE
* STORED.  THE SUFFIX IS IN BCD, SUITABLE FOR OUTPUT WITH AN A3 FORMAT
* FOR THE PLURAL OR A2 FOR THE SINGULAR.
*       LABEL
CORFE           X-RAY VERSION OF ORFFE OF BUSING AND LEVY
C       BUSING-LEVY FUNCTION AND ERROR PROGRAM
C       SYSTEM DIMENSION
   MAIN PROGRAM
*       LABEL
CSUB8
        SUBROUTINE SUB8
C       COMPUTE ALL DISTANCES BETWEEN TWO ASYMMETRIC UNITS
C       SYSTEM DIMENSION
*       LABEL
CSB10
        SUBROUTINE SUB10
C       MULTIVALUED FUNCTIONS 7, 8, AND 9
C       SYSTEM DIMENSION
*       LABEL
CSB11
        SUBROUTINE SUB11
C       MULTIVALUED FUNCTIONS 10 AND 11
C       SYSTEM DIMENSION
*       LABEL
CSB19
        SUBROUTINE SUB19
C       FUNCTION AND ERROR CALCULATION
C       SYSTEM DIMENSION
*       LABEL
CSB21
        SUBROUTINE SUB21
C       COMPUTE MULTIVALUED FUNCTIONS
C       SYSTEM DIMENSION
*       LABEL
CHEDI
        SUBROUTINE HEDI(I)
C       SELECT THE HED SUBROUTINE TO BE ENTERED
*       LABEL
CPREI
        SUBROUTINE PREI(I)
C       SELECT THE PRE SUBROUTINE TO BE ENTERED
*       LABEL
CFUNI
        SUBROUTINE FUNI(I)
C       SELECT THE FUN SUBROUTINE TO BE ENTERED
C       SYSTEM DIMENSION
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*       LABEL
COUTI
        SUBROUTINE OUTI(I)
C       SELECT THE OUT SUBROUTINE TO BE ENTERED
*       LABEL
CSTKX
        SUBROUTINE SETKX(I)
C       SET KEY WORDS FOR ATOM COORDINATES
C       SYSTEM DIMENSION
*       LABEL
CSTKB
        SUBROUTINE SETKB(I)
C       SET KEY WORDS FOR ATOM BETAS
C       I=IN(K), THE INSTRUCTION INTEGER SPECIFYING THE ATOM NUMBER
C       SYSTEM DIMENSION
*       LABEL
CSTBB
        SUBROUTINE STOBB
C       STORE RECIPROCAL METRIC TENSOR
C       SYSTEM DIMENSION
*       LABEL
CATOM
        SUBROUTINE ATOM(I,Z)
C       ATOM COORDINATE SUBROUTINE
C       SYSTEM DIMENSION
*       LABEL
CBETA
        SUBROUTINE BETA(INS,Z)
C       STORE TRANSFORMED ANISOTROPIC TEMP FACTOR MATRIX
C       INS IS ATOM DESCRIPTION, Z IS TRANSFORMED MATRIX
C       SYSTEM DIMENSION
*       LABEL
CMM
        SUBROUTINE MM(X,Y,Z)
C       MULTIPLY TWO MATRICES
C       Z(3,3)=X(3,3)*Y(3,3)
*       LABEL
CVM
        SUBROUTINE VM(X,Y,Z)
C       TRANSPOSED VECTOR TIMES MATRIX
C       Z(3)=X(3)*Y(3,3)
*       LABEL
CVV
   MAIN PROGRAM
*       LABEL
CVMV
   MAIN PROGRAM
*       LABEL
CDIFV
        SUBROUTINE DIFV(X,Y,Z)
C       VECTOR - VECTOR
C       Z(3)=X(3)-Y(3)
*       LABEL
CSUMV
        SUBROUTINE SUMV(X,Y,Z)
C       COMPUTE THE SUM OF TWO VECTORS
C       Z(3)=X(3)+Y(3)
*       LABEL
CCSVV
   MAIN PROGRAM
*       LABEL
CARCS
   MAIN PROGRAM
*       LABEL
CNORM
        SUBROUTINE NORM(X,Y,Z)
C       STORE A VECTOR Z NORMAL TO VECTORS X AND Y
C       SYSTEM DIMENSION
*       LABEL
CAXES
        SUBROUTINE AXES(U,V,X)
C       STORE THREE MUTUALLY PERPENDICULAR
C          VECTORS X(I,1), X(I,2), AND X(I,3) GIVEN
C          VECTORS U AND V.
*       LABEL
CEGVL
        SUBROUTINE EIGVAL(W,Y)
C       FIND EIGENVALUES Y OF MATRIX W
C       SYSTEM DIMENSION
*       LABEL
CEGVC
        SUBROUTINE EIGVEC(W,Y,Z)
C       COMPUTE EIGENVECTOR Z OF MATRIX
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C        W GIVEN EIGENVALUE Y
C     SYSTEM DIMENSION
```

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*       LABEL
CTRCE
   MAIN PROGRAM
*       LABEL
CFUNA
   MAIN PROGRAM
*       LABEL
CFUND
   MAIN PROGRAM
*       LABEL
CHED1
        SUBROUTINE HED1
C       HEADING 1
C       SYSTEM DIMENSION
*       LABEL
CPRE1
        SUBROUTINE PRE1
C       SET KEY WORDS FOR INTERATOMIC DISTANCE
C       SYSTEM DIMENSION
*       LABEL
CFUN1
        SUBROUTINE FUN1
C       COMPUTE INTERATOMIC DISTANCE
C       SYSTEM DIMENSION
*       LABEL
COUT1
        SUBROUTINE OUT1
C       PUT OUT DESCRIPTION OF INTERATOMIC DISTANCE
C       SYSTEM DIMENSION
*       LABEL
CHED2
        SUBROUTINE HED2
C       HEADING 2
C       SYSTEM DIMENSION
*       LABEL
CSB13
        SUBROUTINE SUB13
C       ERROR CALCULATION AND OUTPUT
C       SYSTEM DIMENSION
*       LABEL
CPRE2
        SUBROUTINE PRE2
C       PRELIMINARY SUBROUTINE 2
C       SYSTEM DIMENSION
*       LABEL
CFUN2
        SUBROUTINE FUN2
C       BOND ANGLE SUBROUTINE
C       SYSTEM DIMENSION
*       LABEL
COUT2
        SUBROUTINE OUT2
C       OUTPUT DESCRIPTION 2
C       SYSTEM DIMENSION
*       LABEL
CHED3
        SUBROUTINE HED3
C       HEADING 3
C       SYSTEM DIMENSION
*       LABEL
CPRE3
        SUBROUTINE PRE3
C       PRELIMINARY SUBROUTINE 3
C       SYSTEM DIMENSION
*       LABEL
CFUN3
        SUBROUTINE FUN3
C       DIHEDRAL ANGLE SUBROUTINE
C       SYSTEM DIMENSION
*       LABEL
COUT3
        SUBROUTINE OUT3
C       OUTPUT DESCRIPTION 3
C       SYSTEM DIMENSION
*       LABEL
CHED4
        SUBROUTINE HED4
C       HEADING 4
C       SYSTEM DIMENSION
```

```
*       LABEL
CPRE4
        SUBROUTINE PRE4
C       PRELIMINARY SUBROUTINE 4
C       SYSTEM DIMENSION
*       LABEL
CFUN4
        SUBROUTINE FUN4
C       DIFFERENCE BETWEEN BOND DISTANCES
C       SYSTEM DIMENSION
*       LABEL
COUT4
        SUBROUTINE OUT4
C       OUTPUT DESCRIPTION 4
C       SYSTEM DIMENSION
*       LABEL
CHED5
        SUBROUTINE HED5
C       HEADING 5
C       SYSTEM DIMENSION
*       LABEL
CFUN5
        SUBROUTINE FUN5
C       DIFFERENCE BETWEEN BOND ANGLES
C       SYSTEM DIMENSION
*       LABEL
CHED6
        SUBROUTINE HED6
C       HEADING 6
C       SYSTEM DIMENSION
*       LABEL
CPRE6
        SUBROUTINE PRE6
C       PRELIMINARY SUBROUTINE 6
C       SYSTEM DIMENSION
*       LABEL
CFUN6
        SUBROUTINE FUN6
C       SUM OF BOND ANGLES
C       SYSTEM DIMENSION
*       LABEL
COUT6
        SUBROUTINE OUT6
C       OUTPUT DESCRIPTION 6
C       SYSTEM DIMENSION
*       LABEL
CFUN8
        SUBROUTINE FUN8(W,Z,Z1)
C       SET UP MATRIX AND GET EIGENVALUE
C       SYSTEM DIMENSION
*       LABEL
CFUNC
        SUBROUTINE FUNC(C,Z)
C       COS ANGLE OF PRINCIPAL AXIS AND VECTOR
C       SYSTEM DIMENSION
*       LABEL
CFUNX
        SUBROUTINE FUNX(C,Z)
C       COS ANGLE OF PRINCIPAL AND CARTESIAN AXES
C
C       SYSTEM DIMENSION
*       LABEL
CPRE7
        SUBROUTINE PRE7
C       PRELIMINARY SUBROUTINE 7
C       SYSTEM DIMENSION
*       LABEL
CFUN7
        SUBROUTINE FUN7
C       RMS PRINCIPAL DISPLACEMENT
C       SYSTEM DIMENSION
*       LABEL
COUT7
        SUBROUTINE OUT7
C       OUTPUT DESCRIPTION 7
C       SYSTEM DIMENSION
*       LABEL
CHED8
        SUBROUTINE HED8
C       HEADING 8
C       SYSTEM DIMENSION
*       LABEL
CPRE8
```

```
      SUBROUTINE PRE8                                                   ORFFP
C     PRELIMINARY SUBROUTINE 8                                          ORFFP
C     SYSTEM DIMENSION                                                  ORFFP
*     LABEL                                                             ORFFQ
CFUN8                                                                   ORFFQ
      SUBROUTINE FUN8                                                   ORFFQ
C     ANGLE BETWEEN PRINCIPAL AXIS AND VECTOR                           ORFFQ
C     SYSTEM DIMENSION                                                  ORFFQ
```

```
*       LABEL
COUT8
        SUBROUTINE OUT8
C       OUTPUT DESCRIPTION 8
C       SYSTEM DIMENSION
*       LABEL
CHED9
        SUBROUTINE HED9
C       HEADING 9
C       SYSTEM DIMENSION
*       LABEL
CFUN9
        SUBROUTINE FUN9
C       PRINCIPAL AXIS PROJECTED ON VECTOR
C       SYSTEM DIMENSION
*       LABEL
CPR10
        SUBROUTINE PRE10
C       PRELIMINARY SUBROUTINE 10
C       SYSTEM DIMENSION
*       LABEL
CFN10
        SUBROUTINE FUN10
C       ANGLE BETWEEN PRINCIPAL AND CARTESIAN AXES
C       SYSTEM DIMENSION
*       LABEL
COT10
        SUBROUTINE OUT10
C       OUTPUT DESCRIPTION 10
C       SYSTEM DIMENSION
*       LABEL
CHD11
        SUBROUTINE HED11
C       HEADING 11
C       SYSTEM DIMENSION
*       LABEL
CFN11
        SUBROUTINE FUN11
C       PRINCIPAL AXIS PROJECTED ON CARTESIAN AXIS
C       SYSTEM DIMENSION
*       LABEL
CFUNR
        SUBROUTINE FUNR(I,RSQ)
C       MEAN SQUARE RADIAL DISPLACEMENT
C       SYSTEM DIMENSION
*       LABEL
CFNCR
        SUBROUTINE FUNCR(C,R)
C       COMPUTE QUANTITIES FOR MEAN BOND DISTANCE
C       SYSTEM DIMENSION
*       LABEL
CFNXI
        SUBROUTINE FUNXI(I,J,XISQ)
C       MEAN SQUARE DISPLACEMENT IN GIVEN DIRECTION
C       SYSTEM DIMENSION
*       LABEL
CHD12
        SUBROUTINE HED12
C       HEADING 12
C       SYSTEM DIMENSION
*       LABEL
CPR12
        SUBROUTINE PRE12
C       PRELIMINARY SUBROUTINE 12
C       SYSTEM DIMENSION
*       LABEL
CFN12
        SUBROUTINE FUN12
C       RMS DISPLACEMENT IN GIVEN DIRECTION
C       SYSTEM DIMENSION
*       LABEL
COT12
        SUBROUTINE OUT12
C       OUTPUT DESCRIPTION 12
C       SYSTEM DIMENSION
*       LABEL
CHD13
        SUBROUTINE HED13
C       HEADING 13
C       SYSTEM DIMENSION
*       LABEL
CFN13
        SUBROUTINE FUN13
```

```
C     RMS RADIAL DISPLACEMENT                                           ORFG80
C     SYSTEM DIMENSION                                                  ORFG80
```

```
*       LABEL
COT13
        SUBROUTINE OUT13
C       OUTPUT DESCRIPTION 13
C       SYSTEM DIMENSION
*       LABEL
CHD14
        SUBROUTINE HED14
C       HEADING 14
C       SYSTEM DIMENSION
*       LABEL
CPR14
        SUBROUTINE PRE14
C       PRELIMINARY SUBROUTINE 14
C       SYSTEM DIMENSION
*       LABEL
CHD15
        SUBROUTINE HED15
C       HEADING 15
C       SYSTEM DIMENSION
*       LABEL
CFN15
        SUBROUTINE FUN15
C       MEAN INTERATOMIC DISTANCE ASSUMING INDEPENDENT MOTION
C       SYSTEM DIMENSION
*       LABEL
CSETA
        SUBROUTINE SETA(A)
C       DUMMY SUBROUTINE. MAY BE CHANGED BY USER.
*       LABEL
CSETP
        SUBROUTINE SETP(P)
C       DUMMY SUBROUTINE. MAY BE CHANGED BY USER.
*       LABEL
CSTAA
        SUBROUTINE STCAA
C       STORE METRIC TENSOR
C       SYSTEM DIMENSION
*       LABEL
CXMV          JRH SHOULD LABEL SUBROUTINES
        SUBROUTINE MV(X,Y,Z)
C       MATRIX * VECTOR
C       Z(3)=X(3,3)*Y(3)
*       LABEL
CORFLS    MODIFICATION AND SYSTEMIZATION OF OAK RIDGE FULL M. LEAST SQR.
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES
C       CALLING PROGRAM, AMODIFICATION OF A MODIFICATION OF A ..........
C       VERSION OF 18 MAY 1963
C
C
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY
C
   MAIN PROGRAM
*       LABEL
CORFUN          NEW VERSION OF ORFUN (FLSFUN)
        SUBROUTINE FLSFUN(ICONTR)
C       VERSION 1 JUNE 1963
C
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY
C
*       LABEL
CORIN           SUBROUTINE TO READ REFLECTION RECORDS FOR ORFLS.
        SUBROUTINE FLSIN
C       VERSION OF 18 MAY 1963
C
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY
C
*       LABEL
CORCAL     M   DRASTIC REVISION OF ORCAL  BY-PASS UNNECESSARY DIRIVATIVES
        SUBROUTINE CALC(Y,PAR,DER,ICONTR)
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES
C       CALCULATE STRUCTURE FACTOR AND DERIVATIVES FOR ONE REFLECTION
C       VERSION OF MARCH 1964
C
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY
C
*       LABEL
CORCUT          SUBROUTINE TO READ OUT REFLECTION RECORDS FOR ORFLS.
        SUBROUTINE FLSOUT
C       VERSION OF 18 MAY 1963
C
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY
C
```

```
*       LABEL                                                           ORPAC
CORPAC        DUMMY PATCH ROUTINE FOR ORFLS NO ATOMS IN SPECIAL POS.    ORPAC
        SUBROUTINE PATCH(IMSYM,I,TJ,HJ,HHJ,IREJKT,ATOM )                ORPAC
*       LABEL                                                           ORPRO
CORPRE      DRASTICALLY CHANGED  SUBROUTINE PRELIM OF ORFLS             ORPRO
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                  ORPRO
C       READ CRYSTAL STRUCTURE DATA AND STORE PARAMETERS                ORPRO
        SUBROUTINE PRELIM                                               ORPRO
C       VERSION OF 18 MAY 1963                                          ORPRO
C                                                                       ORPRO
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY ORPRO
C                                                                       ORPRO
*       LABEL                                                           ORPTO
CORPTO        SUBROUTINE PTOSB OF ORFLS (COPY PARAMETERS)               ORPTO
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                  ORPTO
C       COPY PARAMETERS FROM ARRAY P TO ARRAYS USED BY SUBROUTINES      ORPTO
        SUBROUTINE PTOSB(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NO,NP)           ORPTO
C       NOTE THAT THE FOLLOWIN DIMENSION STATEMENT IS ILLUSORY          ORPTO
*       LABEL                                                           ORRES
CORRES        DUMMY PATCH FOR ORFLS NO XYZ TO BE RESET                  ORRES
        SUBROUTINE RESETX(XYZ,ATOM,NA)                                  ORRES
*       LABEL                                                           ORSBT
CORSBT        SUBROUTINE SBTOP OF ORFLS (COPY PARAMETERS)               ORSBT
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                  ORSBT
C       COPY PARAMETERS FROM ARRAYS USED BY SUBROUTINES TO ARRAY P      ORSBT
        SUBROUTINE SBTOP(P,SC,TO,SF,AI,XYZ,BETA,ITF,NA,NO,NP)           ORSBT
C       NOTE THAT THE FOLLOWIN DIMENSION STATEMENT IS ILLUSORY          ORSBT
*       LABEL                                                           ORSMO
*ORSMI       SYMMETRIC MATRIX INVERTER OF BUSING AND LEVY (UNMODIFIED)  ORSMO
         ENTRY   SMI                                                    ORSMO
*       LABEL                                                           ORTOO
CORT     ORTHOR DEAL WITH ORTHORHOMBIC  SYSTEM                          ORTOO
        SUBROUTINE ORTHOR (TRNX)                                        ORTOO
C       SYSTEM COMMON ASSIGNMENTS                                       ORTOO
*       LABEL                                                           ORTSO
CORTES        SUBROUTINE TEST OF ORFLS                                  ORTSO
C       OR FLS, FORTRAN CRYSTALLOGRAPHIC LEAST SQUARES                  ORTSO
C       TEST FOR NON-POSITIVE-DEFINITE TEMPERATURE FACTORS              ORTSO
        SUBROUTINE TEST(SHIFT)                                          ORTSO
C                                                                       ORTSO
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY ORTSO
C                                                                       ORTSO
*       LABEL                                                           ORTRO
*ORTRIG   FLOATING POINT TABLE LOOK-UP COS OR SIN FUNCTIONS              ORTRO
         ENTRY   TRIG                                                   ORTRO
         ENTRY   HIFI                                                   ORTRO
         ENTRY   LOFI                                                   ORTRO
*                                                                       ORTRO
*  THE FOLLOWING IS A FLOATING POINT ADAPTATION OF THE FC SIN-COS TLU   ORTRO
*       CALL TRIG(ARG,COS,SIN)      IS CORRECT CALLING SEQUENCE         ORTRO
*       ''''''OVERFLOW INDICATORS WILL BE TURNED OFF '''                ORTRO
*                                                                       ORTRO
*       LABEL                                                           ORWTO
CORWT       REWRITE NEW PARAMETERS ON FRONT OF BINARY OUTPUT FROM ORFLS(UW)ORWTO
        SUBROUTINE ORWT                                                 ORWTO
C       VERSION OF 25 JUNE 1963                                         ORWTO
C                                                                       ORWTO
C                                                                       ORWTO
C       COMMON AND DIMENSION STATEMENTS FOR ORFLS AS MODIFIED FOR X-RAY ORWTO
C                                                                       ORWTO
*       LABEL                                                           OUTPO
COUTPUT- (DUMMY) FOR WRITING OUT ANY NON-STANDARD SPECIAL RESULTS.      OUTPO
        SUBROUTINE OUTPUT(KWRITE)                                       OUTPO
C       VERSION OF NOV 62                                               OUTPO
C       PRESERVE THE ORDER OF THE COMMON STORAGE OR ELSE REMEMBER TO    OUTPO
C       CHANGE COMMON IN SUBROUTINES.                                   OUTPO
C       SYSTEM COMMON ASSIGNMENTS                                       OUTPO
*       LABEL                                                           PATPO
CPATPAT- PATCH TO PERMIT CALCULATION OF ANY TYPE OF FOURIER FUNCTION.   PATPO
        SUBROUTINE PATPAT(KPAT)                                         PATPO
C       VERSION OF NOV 62                                               PATPO
C      THIS VERSION MAKES COEFFICIENTS FOR A STANDARD FU**2 PATTERSON   PATPO
C       COMMON AND DIMENSION STATEMENTS FOR FOURIER ROUTINES            PATPO
C                                                                       PATPO
C       SYSTEM COMMON ASSIGNMENTS                                       PATPO
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*       LABEL                                                           PLOTOOO
*PLOTER - A SUBPROGRAM TO ASSIST IN THE PLOT OF A GRAPH OF DELTA F VS FLPLOTOO2
        ENTRY   PLOTER                                                  PLOTOO4
*                                                                       PLOTOO5
*       CALLED BY--CALL PLOTER (NTAPE,N,KREJ)  WHERE NTAPE IS OUTPUT TAPE,PLOTOO6
*        N IS THE ORDINATE AS A FORTRAN INTEGER, AND KREJ IS A CODE FOR PLOTOO7
*        TESTING IF N IS GREATER THAN 1000.  KREJ IS -1 IF N IS GREATER PLOTOO8
*        THAN 1000 OR +1 IF N IS LESS-THAN OR EQUAL TO 1000.  IF N IS   PLOTOO9
*        GREATER THAN 100 IT WILL BE MADE MODULO 100.  THIS IS BECAUSE  PLOTO10
*        THE GRAPH PRINTED HAS AN ORDINATE RANGE OF ZERO THRU 100.      PLOTO11
*                                                                       PLOTO12
*        THE FUNCTION OF THIS ROUTINE IS TO PRINT THE LINES OF A GRAPH  PLOTO13
*        WHICH CONTAIN THE PLOTTED POINTS.  THIS IS ACCOMPLISHED BY     PLOTO14
*        RECEIVING THE ORDINATE IN BINARY FORM, CONVERTING IT TO BCD,   PLOTO15
*        AND THEN STUFFING IT INTO A FORMAT STATEMENT.                  PLOTO16
*                                                                       PLOTO17
*       LABEL                                                           PMVOOOO
CPMV    - MATRIX VECTOR PRODUCT.                                        PMVOOO1
        SUBROUTINE PMV(X,V1,V2)                                         PMVOOO2
C       V2 BECOMES V1 PRENULTIPLIED BY X.                               PMVOOO3
*       LABEL                                                           PSVOOOO
CPSV    - SCALAR VECTOR PRODUCT.                                        PSVOOO1
        SUBROUTINE PSV(S,V1,V2)                                         PSVOOO2
C       V2 BECOMES S TIMES V1.     V1 = V2 IS OK.                       PSVOOO3
*       LABEL                                                           PVMVOOO
CPVMV   - VECTOR MATRIX VECTOR PRODUCT.                                 PVMVOO1
   MAIN PROGRAM
*       LABEL                                                           RANDYOO
*RANDY  FORTRAN FUCTION SUB-PROGRAM TO GENERATE RANDOM ERRORS           RANDYO2
        ENTRY   RANDY              IN FORTRAN     X= RANDYF(X)          RANDYO5
*       CALLING SEQUENCE   TSX RANDY,4 OR  X=RANDYF(DUMMY)              RANDYO8
*       THE PROGRAM GENERATES TWO RANDOM NUMBERS THE FIRST SERVES AS AN RANDYO9
*       ARGUMENT X THE SECOND AS A POSSIBLE F OF X. THE FIRST RANDOM    RANDY10
*       NUMBER IS PLACED IN THE RANGE + OR - 3.2 BY X=6.4*R1-3.2 .      RANDY11
*       THE ROUTINE THEN FINDS EXPF(X**2/2.0) AND CALLS THIS FOFX.      RANDY12
*       A SECOND RANDOM NUMBER BETWEEN 0 AND 1 IS GENERATED. IF R2 IS   RANDY13
*       GREATER THAN FOFX OTHER PAIRS ARE GENERATED UNTIL AN X IS FOUND. RANDY14
*       THIS VALUE IS RETURNED IN THE ACCUMULATOR AS A FLOATING POINT   RANDY15
*       QUANTITY. OVER A NUMBER OF CALLS-MEAN ZERO, STD DEV 1, LIM 3.2 . RANDY16
*       LABEL                                                           RCALOOO
CRCAL     CALCULATION OF R FOR =RPLANE=                                 RCALOO1
        SUBROUTINE RCALC                                                RCALOO2
C       SYSTEM COMMON ASSIGNMENTS                                       RCALOO3
*       LABEL                                                           RCOROOO
CRCOR     MOVES MOLECULE FOR =RPLANE=                                   RCOROO1
        SUBROUTINE RCOOR                                                RCOROO2
C       SYSTEM COMMON ASSIGNMENTS                                       RCOROO3
*       LABEL                                                           REDUOOO
CREDUC            REDUCE TRICLINIC CELL                                 REDUOO1
        SUBROUTINE REDUC (S1,S2)                                        REDUOO2
C       SYSTEM COMMON ASSIGNMENTS                                       REDUOO3
*       LABEL                                                           REFLNOO
CREFLN    REFLECTION READING SUBROUTINE OF SHLPAT                       REFLNO1
        SUBROUTINE REFLTN                                               REFLNO2
C       SYSTEM COMMON ASSIGNMENTS                                       REFLNO3
*       LABEL                                                           REROOOO
*RERW   - MODIFIED FORTRAN TAPE READ ERROR (9RER) - SKIP NOISE RECORDS. REROOO1
*(RER)        READ TAPE ERROR          USED BY (TSH) AND (TSB).        REROOO2
*                                                                       REROOO3
        ENTRY   (RER)                                                   REROOO4
        ENTRY   -(ROC)                                                  REROOO5
*                                                                       RERO001
*       LABEL                                                           RHHOOOO
CRHH    RHOMBH DEAL WITH RHOMBOHEDRAL SYSTEM                            RHHOOO1
        SUBROUTINE RHOMBH (AL,ARH,COA,AHX,CHX)                          RHHOOO2
*       LABEL                                                           RHOTOOO
CRHOTP          PRINT C/A,A HEX,C HEX, IN ACCORDANCE WITH THE ACCURACY  RHOTOO1
        SUBROUTINE RHOTP (SYS1,COA,AHX,CHX,IDEC)                        RHOTOO2
C       SYSTEM COMMON ASSIGNMENTS                                       RHOTOO3
*       LABEL                                                           RPLAOOO
CRPLAN    CALCULATE R OVER A PROJECTION (LINK 12000)                    RPLAOO1
C       SYSTEM COMMON ASSIGNMENTS                                       RPLAOO2
   MAIN PROGRAM
*       LABEL                                                           RRREOOO
CRRRE     CALCULATE PRINT OUT AND R FOR R-LIST                          RRREOO1
        SUBROUTINE RARE(I)                                              RRREOO2
C                                                                       RRREOO3
C                                                                       RRREOO4
C       COMMON AND DIMENSION STATEMENTS                                 RRREOO5
C       SYSTEM COMMON                                                   RRREOO6
```

```
*       LABEL
CRRLS          CLASSIFIES REFLECTIONS FOR R LISTING PROGRAM
        SUBROUTINE RCLS(NC)
C       VERSION  OF FEB. 11,1964
C
C
C       COMMON AND DIMENSION STATEMENTS
C       SYSTEM COMMON
*       LABEL
CRRIS          MAIN PROGRAM FOR PREPARING LIST OF R 'S
C       VERSION OF FEB. 11,1964
C
C
C       MAXLEV(I) = MAX. ABSOLUTE VALUE OF N FOR LEVELS
C       IHLEMI(I) = MAX. NEGATIVE N  FOR LEVELS
C       IHLEMA(I) = MAX. POSITIVE N FOR LEVELS
C        IAMMED = LAST NO. OF GROUPS  +7
C        IAM DESIGNATES ROW ON WHICH VALUE IS TO BE PLACED
C       COMMON AND DIMENSION STATEMENTS
C       SYSTEM COMMON
   MAIN PROGRAM
*       LABEL
CRREA          READS REFLECTIONS FOR R LIST PROGRAM
        SUBROUTINE RREA(IGC)
C       VERSION OF FEB. 11,1964
C
C
C       COMMON AND DIMENSION STATEMENTS
C       SYSTEM COMMON
*       LABEL
CRRUM     MAKES SUMS FOR R LIST
        SUBROUTINE RSUM(I)
C       VERSION OF FEB.11,1964
C
C
C       COMMON AND DIMENSION STATEMENTS
C       SYSTEM COMMON
*       LABEL
CRTABL    GENERATES TABLE OF TRIG FUNCTIONS FOR =RPLANE=
        SUBROUTINE RTABLE
C       SYSTEM COMMON ASSIGNMENTS
*       LABEL
*RWTUW - FORTRAN REWIND TAPE (9RWT).
*              REWIND N                    LINKAGE COMPILED BY I/O TRANSLATOR.
*
*A       CAL  N                            UNIT DESIGNATION.
*        TSX  (RWT),4                      REWIND TAPE.
*
         ENTRY   (RWT)
*       LABEL
CSCAL   CALCULATE SCALAR PRODUCTS A.A,A.B,A.C,B.B,B.C,C.C
        SUBROUTINE SCAL
C       SYSTEM COMMON ASSIGNMENTS
*       LABEL
*SCNUW - FORTRAN FLOATING POINT SIN AND COSINE ROUTINE (9SCN).
         ENTRY   COS
         ENTRY   SIN
*       LABEL
CSHLP      PATTERSON SHELL PROGRAM   (LINK 5500.
C       VERSION OF 9 MAY 1963
C       SYSTEM COMMON ASSIGNMENTS
   MAIN PROGRAM
*       LABEL
CSHORT         FIND THE SHORTEST TRANSLATION IN A PLANE
        SUBROUTINE SORT (C1,CA1,A1,C2,CA2,A2,W)
*       LABEL
*SLASH  CHANGES BLANK TO SLASH IN FRONT OF M,A,B,C,N, OR *
         ENTRY   SLASH
* A SUBROUTINE TO CHANGE BLANK TO SLASH IN FRONT OF M,A,B,C,N OR *
* ARG. BY A2 FORMAT (1ST A1 BE BLANK SPACE)  OF MONOCLINIC SM2=SM(2)
* CALLING SEQUENCE ... CALL SLASH (SM2)
* THE ROUTINE MAKES P21 C  TO P21/C  ,FOR EXAMPLE.
*       LABEL
*SLIUW - FORTRAN SHORT LIST INPUT (9SLI).
*              SHORT LIST INPUT            LINKAGE COMPILED BY I/O TRANSLATOR.
*
*        TSX  (SLI),4                      FOR INPUT OF NON-SUBSCRIPTED LIST.
*        PZE  SYMBOL+1                     LOCATION OF THE ARRAY +1.
*        PZE  N                            NUMBER OF ELEMENTS.
*
         ENTRY   (SLI)
```

```
*       LABEL
*SLOUW - FORTRAN SHORT LIST OUTPUT (9SLO).
*            SHORT LIST OUTPUT          LINKAGE COMPILED BY I/O TRANSLATOR.
*
*       TSX   (SLO),4                   FOR OUTPUT OF NON-SUBSCRIPTED LIST.
*       PZE   SYMBOL+1                  LOCATION OF THE ARRAY +1.
*       PZE   N                         NUMBER OF ELEMENTS.
*
        ENTRY    (SLO)
*       LABEL
CSMINP       CONVERT INPUT FORM OF SPACE-GROUP SYMBOL TO INTERNAL FORM
        SUBROUTINE SMINP (QSM,SM,KZZ)
*       LABEL
CSMTR   INTERCHANGE  SYMMETRY SYMBOL
        SUBROUTINE SMTR (BL1,BL2,GP1,GP2)
C       SYSTEM COMMON ASSIGNMENTS
*       LABEL
*SOR     SUBROUTINE TO SORT REFLECTIONS ON INDECES
        ENTRY    PRIME
        ENTRY    SORT
*    THIS IS A SUBROUTINE TO SORT REFLECTIONS AND THEIR E VALUES
*    IN ANY ORDER AS SPECIFIED ON A CARD WHICH IS READ BY THE
*    MAIN PROGRAM AND IS TRANSMITTED TO THE SUBROUTINE IN A CALLING
*    SEQUENCE ALONG WITH THE DIMENSION OF THE REFLECTIONS ON WHICH
*    THE SORT IS TO TAKE PLACE(I.E.,CALL PRIME(MH,MK,ML,IDSORT),
*    WHERE MH=1,MK=2,ML=3,IDSORT=2)
*    TO OBTAIN THE SORTING CALL SORT(E1,NUMBER OF REFLECTIONS OF THIS
*    CLASS,CRAMMED INDICES,CLASS OF REFLECTION AS DIMEN SEES IT)
*       LABEL
*SPHW   -   MODIFIED FORTRAN STORAGE-TO-PRINTER HOLLERITH (9SPH).
*            PRINT K                    LINKAGE COMPILED BY I/O TRANSLATOR.
*
*A      TSX   (SPH),4                   STORAGE TO PRINTER HOLLERITH.
*       PZE   8)K                       FORMAT DESIGNATION.
*A1    ...   ..                        INDEXING.
*B      LDQ   SYMBOL,TAG                OUTPUT LIST.
*       STK                             ..
*B1    ...   ..                        INDEXING.
*C      TSX   (FIL),4                   FILL OUT LINE.
*
        ENTRY    (SPH)
        ENTRY    .SPH.
*
*       LABEL
CSPREO       REORIENT SPACE-GROUP SYMBOL OF MONOCLINIC SYSTEM
        SUBROUTINE SPREO (W)
C       SYSTEM COMMON ASSIGNMENTS
*       LABEL
*SQRUW - FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR).
        ENTRY    SQRT
*       LABEL
*SQUASH- PACKS ATOM PARAMETER STORAGE DEPENDING ON TEMP. FACTOR.
*SQUASH - COMPRESS ATOM-STORAGE BAND FOR PARAM LOADER    HIGH
*                        15 SEPT 61
        ENTRY    SQUASH
* FORTRAN SUBROUTINE SUBPROGRAM TO COMPRESS ATOM PARAMETER STORAGE FOR
* THE PARAMETER LOADER.  FOR INDIVIDUAL TEMPERATURE FACTORS, STORAGE IS
* INITIALLY 14 CELLS/ATOM.  IF ALL TEMP. FACTORS TURN OUT TO BE ISO-
* TROPIC, THIS SUBROUTINE IS USED TO REDUCE THE STORAGE TO 8 CELLS/ATOM.
* CALL SQUASH(ILD,INDXC,B) WHERE INDXC IS NUMBER OF CELLS/ATOM, ILD IS
* (NUMBER OF ATOMS LOADED - 1)*INDXC + 1, B IS THE FIRST (LARGEST-
* -ADDRESSED) LOCATION OF THE ATOM PARAMETER ARRAY.
*       LABEL
*STBUW - FORTRAN STORAGE TO TAPE BINARY (9STB).   (JAN. 1960)
*
*            WRITE TAPE N      LINKAGE COMPILED BY I/O TRANSLATOR.
*
*A      CAL      N              UNIT DESIGNATION.
*       TSX      (STB),4        STORAGE TO TAPE BINARY.
*A1    ...      ..             INDEXING.
*B      LDQ      SYMBOL, TAG    OUTPUT
*       STR                     LIST.
*B1    ...      ..             INDEXING.
*C      TSX      (WLR),4        WRITE LAST RECORD.
*
        ENTRY    (STB)
        ENTRY    (WLR)
*
*
```

```
*       LABEL
*STHW   -   MODIFIED FORTRAN STORAGE-TO-TAPE HOLLERITH (9STH).                STH000
*           WRITE OUTPUT TAPE N,K     LINKAGE COMPILED BY I/O TRANSLATOR.STH000
*                                                                            STH000
*A      CAL  N                        UNIT DESIGNATION.                      STH000
*       TSX  (STH),4                  STORAGE TO TAPE HOLLERITH.             STH000
*       PZE  8)K                      FORMAT DESIGNATION.                    STH000
*A1     ...  ..                       INDEXING.                              STH001
*B      LOQ  SYMBOL,TAG               OUTPUT                                 STH001
*       STR                           LIST.                                  STH001
*B1     ...  ..                       INDEXING.                              STH001
*C      TSX  (FIL),4                  FILL OUT RECORD.                       STH001
*                                                                            STH001
        ENTRY   (STH)                                                        STH001
        ENTRY   (STHM)                                                       STH001
        ENTRY   .STH.             ENTRY FOR TRANSMISSION ONLY                STH001
*                                                                            STH002
*       LABEL                                                                STUJ00
CSTUJ        STUDENT PROBLEM GENERATOR                                       STUJ00
C       VERSION OF 13 FEB 1964                                               STUJ00
C       A PROGRAM TO PRODUCE A LIST OF WEISSENBERG COORDINATES               STUJ00
C       AND RELATIVE INTENSITIES FOR PROBLEMS IN X-RAY                       STUJ00
C       CRYSTALLOGRAPHY (2-DIMENSIONAL)                                      STUJ00
C                                                                            STUJ00
C       SYSTEM COMMON                                                        STUJ00
   MAIN PROGRAM
*       LABEL                                                                STUN00
CSTUN ATOMIC WEIGHT RETRIVAL FROM SYMBOL                                     STUN00
C       VERSION OF 13 FEB 1964                                               STUN00
C       GIVEN AN A2 SYMBOL FOR THE ELEMENT                                   STUN00
C       THIS PROGRAM RETURNS THE ATOMIC WEIGHT AND NUMBER ON THE             STUN00
C       CHEMISTS CARBON SCALE                                                STUN00
        SUBROUTINE STUN (ARG,WEIGHT,ATNUM,IGO)                               STUN00
*       LABEL                                                                STUPI0
*STUPID     PUT PARENTHESIS AROUND A A FORMAT WORD  BEST BE (A4  )           STUPI0
        ENTRY   STUPID                                                       STUPI0
*                                                                            STUPI0
*   A FUNCTION SUBROUTINE    USUALLY USED..  A = STUPIOF(NAMEF(A))           STUPI0
*   NAMEF REMOVES BLANKS AND LEFT JUSTIFIES THE BCD CHARACTERS               STUPI0
*   THIS SUBROUTINE THEN SHIFTS AND PUTS PARENS AROUND THE FIRST FOUR BCDSTUPI0
*   CHARACTERS OF THE ORIG WORD  (GOOD LUCK TO THE LAST TWO BCD CHAR)        STUPI1
*    IF STUPID IS HANDED BLANKS IN THE FIRST PLACE IT RETURNS BLANKS         STUPI1
*                                                                            STUPI1
*       LABEL                                                                SYM200
*SYMTR2 - INTERPRET SYMMETRY CARD (FLOATING POINT)     HIGH  MAY 61          SYM200
        ENTRY   SYMTR2                                                       SYM200
* A FORTRAN FUNCTION SUBPROGRAM TO SCAN A SYMMETRY CARD AND BUILD            SYM200
* THE CORRESPONDING SYMMETRY-OPERATION MATRIX.  THE CONTENTS OF THE          SYM200
* CARD ARE WRITTEN OFF-LINE.  IN CASE OF ERROR, AN ERROR MESSAGE IS          SYM200
* WRITTEN ON- AND OFF-LINE.  THE FUNCTIONAL VALUE IS NORMALLY NON-ZERO,      SYM200
* WHEN AN ERROR HAS BEEN DETECTED IT IS ZERO.                                SYM201
*                                                                            SYM201
* THE CALLING PROGRAM MUST READ THE CARD RECORD WITH A 12A6 FORMAT INTO      SYM201
* A 12-WORD ARRAY BEGINNING AT THE ORIGIN OF COMMON, AND ASCERTAIN THAT      SYM201
* THE ID IS CORRECT.  THE ROUTINE IS CALLED AS A FORTRAN FUNCTION            SYM201
* SYMTR2(SYMOP) WHERE SYMOP IS THE FIRST ELEMENT OF THE 3X4 ARRAY WHERE      SYM201
* THE SYM. OP. IS TO BE STORED (IN STANDARD FORTRAN ORDER).                  SYM201
* SYM. OP. ELEMENTS ARE NORMALIZED FLOATING-POINT.                           SYM201
*       LABEL                                                                SYM300
*SYMTR3 - INTERPRET SYMMETRY CARD (GENERAL EXPRESSION)   HIGH  JUNE 61       SYM300
        ENTRY   SYMTR3                                                       SYM300
* A FORTRAN FUNCTION SUBPROGRAM TO SCAN A SYMMETRY CARD AND BUILD            SYM300
* THE CORRESPONDING SYMMETRY-OPERATION MATRIX.  THE CONTENTS OF THE          SYM300
* CARD ARE WRITTEN OFF-LINE.  IN CASE OF ERROR, AN ERROR MESSAGE IS          SYM300
* WRITTEN ON- AND OFF-LINE.  THE FUNCTIONAL VALUE IS NORMALLY NON-ZERO,      SYM300
* WHEN AN ERROR HAS BEEN DETECTED IT IS ZERO.                                SYM301
*                                                                            SYM301
* THE CALLING PROGRAM MUST READ THE CARD RECORD WITH A 12A6 FORMAT INTO      SYM301
* A 12-WORD ARRAY BEGINNING AT THE ORIGIN OF COMMON, AND ASCERTAIN THAT      SYM301
* THE ID IS CORRECT.  THE ROUTINE IS CALLED AS A FORTRAN FUNCTION            SYM301
* SYMTR3(SYMOP,M) WHERE SYMOP IS THE 1ST ELEMENT OF THE 3X4 ARRAY WHERE      SYM301
* THE SYM. OP. IS TO BE STORED (IN STANDARD FORTRAN ORDER).                  SYM301
* INTEGER M WILL BE PREFIXED TO THE LISTING OF THE SYMTRY CARD.              SYM301
* SYM. OP. ELEMENTS ARE NORMALIZED FLOATING-POINT.                           SYM301
*                                                                            SYM301
* THIS ROUTINE DIFFERS FROM SYMTR2 CHIEFLY IN ACCEPTING ARBITRARY            SYM302
* RELATIONSHIPS SUCH AS ARE NEEDED IN BOND-LENGTH OR PROJECTION PRO-         SYM302
* GRAMS, WHERE THE SYMOP CANNOT BE ARBITRARILY REDUCED MODULO 1.             SYM302
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*     LABEL                                                          SYMYO
*SYMTRY- STORES SYMMETRY OPERATIONS IN FORTRAN MATRIX ARRAY.          SYMYO
      ENTRY   SYMTRY                                                 SYMYO
* A FORTRAN FUNCTION SUBPROGRAM TO SCAN A SYMMETRY CARD AND BUILD     SYMYO
* THE CORRESPONDING SYMMETRY-OPERATION MATRIX.  THE CONTENTS OF THE   SYMYO
* CARD ARE WRITTEN OFF-LINE.  IN CASE OF ERROR, AN ERROR MESSAGE IS   SYMYO
* WRITTEN ON- AND OFF-LINE.  THE FUNCTIONAL VALUE IS NORMALLY NON-ZERO, SYMYO
* WHEN AN ERROR HAS BEEN DETECTED IT IS ZERO.                         SYMYO
*                                                                     SYMYO
* THE CALLING PROGRAM MUST READ THE CARD RECORD WITH A 12A6 FORMAT INTO SYMYO
* A 12-WORD ARRAY BEGINNING AT THE ORIGIN OF COMMON, AND ASCERTAIN THAT SYMYO
* THE ID IS CORRECT.  THE ROUTINE IS CALLED AS A FORTRAN FUNCTION     SYMYO
* SYMTRY(MSYM) WHERE MSYM IS THE FIRST ELEMENT OF THE 3X4 ARRAY WHERE SYMYO
* THE SYM. OP. IS TO BE STORED (IN STANDARD FORTRAN ORDER).           SYMYO
* SYM. OP. ELEMENTS ARE 817 FIXED-POINT NUMBERS.                      SYMYO
*     LABEL                                                          SYSBO
*SYSBEL - SUBROUTINE TO INITIALIZE SYSTEM COMMON. BELL IOU TABLE.     SYSBO
      ENTRY   SYSCOM                                                 SYSBO
*                                                                     SYSBO
* FOR ANY UNDEFINED SYSTEM TAPE, ETC., USE THE USUAL VALUE            SYSBO
*     LABEL                                                          SYSCO
*SYSCOM - SUBROUTINE TO INITIALIZE SYSTEM COMMON                      SYSCO
      ENTRY   SYSCOM                                                 SYSCO
*                                                                     SYSCO
* FOR ANY UNDEFINED SYSTEM TAPE, ETC., USE THE USUAL VALUE            SYSCO
*     LABEL                                                          TABLE
CTABLE                                                               TABLE
      SUBROUTINE TABLE                                               TABLE
C     SYSTEM COMMON ASSIGNMENTS                                      TABLE
*     LABEL                                                          TCLOO
CTCL   TRICLI DEAL WITH TRICLINIC SYSTEM                             TCLOO
      SUBROUTINE TRICLI (VOO,Z)                                      TCLOO
C     SYSTEM COMMON ASSIGNMENTS                                      TCLOO
*     LABEL                                                          TESOO
*TESUW - FORTRAN TEST LAST WRITE (9TES).                              TESOO
      ENTRY   (TES)                                                  TESOO
*     LABEL                                                          TIMEO
*TIME  - SUBROUTINE TO READ CLOCK.                                    TIMEO
      ENTRY   TIME                                                   TIMEO
*  CALLING SEQUENCE-TSX TIME,4.  RETURN WITH FLOATING PT. IN AC      TIMEO
*     LABEL                                                          TIMEM
*TIMEM   TIME FUNCTION FOR READING CLOCK THAT UPS MEMORY LOC 5        TIMEM
      ENTRY   TIME                                                   TIMEM
*                                                                     TIMEM
*                                                                     TIMEM
*     LABEL                                                          TINOL
*TINOL  TIME FUNCTION SUBROUTINE FOR READING CLOCK AT NAVAL ORD. LAB  TINOL
      ENTRY   TIME                                                   TINOL
*     CALLING SEQUENCE TSX  TIME,4                                   TINOL
*     ACTUALLY NO ARGUMENT NEEDS TO BE IN THE ACC AS PRINTER SUPPLIES TINOL
*        THE CLOCK READINGS AND TIME SPITS BACK THE MIN IN FLOATING PTTINOL
*                                                                     TINOL
*     LABEL                                                          TRACO
*TRACE - FLOW TRACE FOR FORTRAN MONITOR SYSTEM.                       TRACO
      ENTRY   TRACE          INITIALIZE TRACE ON TAPE 6              TRACO
      ENTRY   TRACEN         INITIALIZE TRACE ON TAPE SPECIFIED      TRACO
      ENTRY   UNTRAP         DISCONTINUE TRACING                     TRACO
* WRITES ON TAPE THE LOCATIONS OF ALL EXECUTED TRANSFERS EXCEPT TIR,  TRACO
* 20 LOCATIONS PER LINE.  DETECTS AND GROUPS REPEATED SEQUENCES OF    TRACO
* ONE OR TWO LOCATIONS.                                               TRACO
* FORTRAN I/O LIBRARY IS USED FOR OUTPUT, THERE IS NO CONFLICT WITH   TRACO
* PROGRAM OUTPUT.  HOWEVER, IOH AND IOB CANNOT BE TRACED BECAUSE OF   TRACO
* CONFLICT WITH STR.                                                  TRACO
* CALLING SEQUENCES -                                                 TRACO
*     CALL    TRACE,I        TO START TRACING, OUTPUT ON TAPE 6       TRACO
*     CALL    TRACEN,N,I     TO START TRACING, OUTPUT ON TAPE N       TRACO
*     CALL    UNTRAP         TO STOP TRACING AND/OR WRITE OUT         TRACO
*                              ANY PARTIALLY-FILLED LINE              TRACO
*                              (IN MACHINE-LANGUAGE PROGRAMS,         TRACO
*                              TRACING CAN  BE SUSPENDED AND RESUMED  TRACO
*                              BY GIVING LTM AND ETM INSTRUCTIONS,    TRACO
*                              RESPECTIVELY.)                         TRACO
* I IS A RELOCATION INCREMENT TO BE SUBTRACTED FROM THE LISTED ADDRESSESTRACO
*     LABEL                                                          TRANO
CTRANS CALCULATE  PRODUCTS OF TRANSFORMATION MATRIX                  TRANO
      SUBROUTINE TRANS (U11,U12,U13,U21,U22,U23,U31,U32,U33,INFO)    TRANO
C     SYSTEM COMMON ASSIGNMENTS                                      TRANO
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*       LABEL                                                           TSB00
*TSBUW - FORTRAN TAPE TO STORAGE BINARY (9TSB). (JAN. 1960)             TSB00
*                                                                       TSB00
*               READ TAPE N        LINKAGE COMPILED BY I/O TRANSLATOR.  TSB00
*                                                                       TSB00
*A      CAL     N                  UNIT DESIGNATION.                    TSB00
*       TSX     (TSB),4            TAPE TO STORAGE BINARY.              TSB00
*A1     ...     ..                 INDEXING.                            TSB00
*B      STR                        INPUT                                TSB00
*       STQ     SYMBOL,TAG         LIST.                                TSB00
*B1     ...     ..                 INDEXING.                            TSB00
*C      TSX     (RLR),4            READ LAST RECORD.                    TSB00
*                                                                       TSB00
        ENTRY   (TSB)                                                   TSB00
        ENTRY   (RLR)                                                   TSB00
*                                                                       TSB00
*       LABEL                                                           TSH00
*TSHUW - FORTRAN TAPE TO STORAGE HOLLERITH (9TSH).                      TSH00
*               READ INPUT TAPE N,K       LINKAGE COMPILED BY I/O TRANSLATOR.TSH00
*                                                                       TSH00
*A      CAL  N                           UNIT DESIGNATION.              TSH00
*       TSX  (TSH),4                     TAPE TO STORAGE HOLLERITH.     TSH00
*       PZE  8)K                         FORMAT DESIGNATION.            TSH00
*A1     ...  ..                          INDEXING.                      TSH00
*B      STR                              INPUT                          TSH00
*       STQ  SYMBOL,TAG                  LIST.                          TSH00
*B1     ...  ..                          INDEXING.                      TSH00
*C      TSX  (RTN),4                     RETURN.                        TSH00
*                                                                       TSH00
        ENTRY (TSH) SET BY FORTRAN COMPILER.                            TSH00
        ENTRY (TSHM) SET BY MONITOR AT OBJECT TIME.                     TSH00
*                                                                       TSH00
*       LABEL                                                           UCROS
CUCROSS- NORMALIZED CROSS PRODUCT BETWEEN TWO VECTORS.                  UCROS
   MAIN PROGRAM
*       LABEL                                                           UKEEP
CUKEEP        KEEP U(I,J)                                               UKEEP
        SUBROUTINE UKEEP ( U,INFO)                                      UKEEP
*       LABEL                                                           UNITV
CUNITV - NORMALIZE VECTOR.                                              UNITV
   MAIN PROGRAM
*       LABEL                                                           VOL00
CVOL    CALCULATE CELL VOLUME                                           VOL00
   MAIN PROGRAM
*       LABEL                                                           WERW0
*WERW   -   WRITE ERROR SUBROUTINE (MODIFIED FORTRAN 9WER)              WERW0
*(WER)        WRITE TAPE ERROR          USED BY (STH) AND (STB).        WERW0
*                                                                       WERW0
        ENTRY   (WER)                                                   WERW0
        ENTRY   -(WTC)                                                  WERW0
        ENTRY   RERITE                                                  WERW0
        ENTRY   IFEOT                                                   WERW0
*                                                                       WERW0
*       LABEL                                                           WTFN0
CWTFN   - CALCULATION OF SPECIAL LEAST SQUARES WEIGHTING FACTORS.       WTFN0
   MAIN PROGRAM
*       LABEL                                                           XLS00
*XLSOUT - WRITE ORXLS-TYPE BINARY REFLECTION RECORD                     XLS00
        ENTRY   XLSOUT            CALL XLSOUT(NTAPE,ORIGIN,LENGTH)      XLS00
*       LABEL                                                           XMIX0
*XMIX   - CONVERT FLOATING POINT NUMBER TO FIXED POINT NUMBER.           XMIX0
*XMIX - FLOATING/POINT TO 817 FIXED-POINT MIXED FRACTION    HIGH  FEB 61XMIX0
        ENTRY   XMIX                                                    XMIX0
* A FORT-AN CLOSED-FUNCT+ON SUBROUTINE TO CONVERT A FLOATING-PO+NT      XMIX0
* NUMBER TO FIXED-POINT WITH 817 SCALING.                               XMIX0
* NUMBERS ABSOLUTELY EXCEEDING 2**17 WILL CAUSE AC OVERFLOW.  FLOAT.-   XMIX0
* PT. ARGUMENT IN AC, FIX.-PT. RESULT IN AC ROUNDED TO 18 BINARY PLACES.XMIX0
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*       LABEL                                                           XMODT00
*XMODTW- CONVERT FIXED POINT BIN FRACTION TO INTEGERS IN 0-11 TWELFTHS. XMODT02
*XMODTW A SUBROUTINE OF GENCHK OF DATA REDUCTION                        XMODT04
*        TO MAKE FIXED POINT BINARY (B17) FRACTIONS INTO B17 INTEGERS IN XMODT05
*        THE RANGE 0-11 (TWELFTHS).                                     XMODT06
*        CALLING SEQUENCE AT 1603 IN GENCHK AS CALL XMODTW(MSYM(I,4,J)) XMODT07
*        WHICH ARE THE TRANSLATION VECTORS OF THE J SYMMETRY OPERATIONS. XMODT08
         ENTRY   XMODTW                                                 XMODT09
*       LABEL                                                           XNOOOOO
*XNOO  - MAKES INTEGERS FROM B17 TRANSLATION FRACTION, 1-12=0/12-11/12. XNOOOO2
*XNOO   FUNCTION SUBROUTINE TO ADJUST (H*T+1) TO NUMBER BETWEEN 1 AND 12XNOOOO4
         ENTRY   XNOO                                                   XNOOOO5
*  THIS PROGRAM IS REQUIRED BY GEN OF DATA REDUCTION.                   XNOOOO6
*  CALLED AT STEP 1601 IN GEN.                                          XNOOOO7
*       LABEL                                                           XP2UW00
*XP2UW - FORTRAN EXPONENTIAL ROUTINE - FLOAT.PT. BASE, FIXED PT. EXPON. XP2UW02
         ENTRY   EXP(2                                                  XP2UW05
*       LABEL                                                           XP3U000
*XP3UW - FORTRAN EXPONENTIAL ROUTINE FLOAT.PT. BASE AND EXPONENT (9XP3) XP3U002
         ENTRY   EXP(3                                                  XP3U005
*       LABEL                                                           XRNOOOO
*XRND  - PROPERLY FIXES AND ROUNDS OFF FLOATING-POINT NUMBER.            XRNOOO2
*XRNOF - ROUND AND FIX                HIGH      JUNE 61                 XRNOOO4
         ENTRY   XRNO                                                   XRNOOO5
* A FORTRAN CLOSED-SUBROUTINE FUNCTION TO CONVERT A FLOATING-POINT       XRNOOO6
* NUMBER TO THE NEAREST B17 INTEGER.                                     XRNOOO7
* THE OVERFLO LITE IS TURNED ON                                          XRNOOO8
*       LABEL                                                           ZZZZ000
$IBSYS                                                                  ZZZZ001
*       LABEL                                                           RTRV000
                 JOB          XRAY PROGRAM RETRIEVAL                    RTRV001
*       LABEL                                                           UPDT000
                 JOB  GENERATE AND UPDATE XRAY SYMBOLIC TAPE             UPDT001
*       LABEL                                                           UPDC000
*       LABEL                                                           ZZZZ200
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APPENDIX I

SUBROUTINES REQUIRED BY THE PROGRAMS

A. SYSTEM PROGRAMS AND SUBROUTINES.

ABSORB - BOND ABSORPTION CORRECTION FOR EACH REFLECTION. (STEWART AND MCROSIN)

AINPT - CONVERT A,B,C BY 24A1 TO FLOATING POINT NUMBER (A(I),I=1,3) (HOLDEN)

ADUTP - PRINT OUT A/B,C/B,A,B,C IN ACCORDANCE WITH ACCURACY (TAKEDA)

ARCTN - FIXED POINT ARCTANGENT ROUTINE (IBM-SHARE)

ARR - ARRANGE SCALAR PRODUCTS IN DECREASING ORDER (TAKEDA)

ATN - LOOK-UP ATOM NAME IN ATOM-TYPE DICTIONARY (HIGH)

ATNAME - PREPARE ATOM-TYPE NAME FOR DICTIONARY (HIGH)

ATNUM - GET ATOM TYPE NUMBER FROM ATOM AND DICTIONARY NAME (STEWART)

ATNUW - FORTRAN FLOATING POINT ARCTANGENT ROUTINE (9ATN)

ATOFL - BCD INTEGERS TO FLOATING POINT NUMBERS (STEWART)

B5BELL - PROGRAM TO USE X-RAY SYSTEM UNDER THE BELL MONITOR (STEWART)

B5FOR - PROGRAM TO CALL X-RAY SYSTEM FROM B5 (HIGH)

B5IBSY - PROGRAM TO USE X-RAY SYSTEM UNDER THE IBSYS MONITOR (STEWART)

BANGL - COMPUTE BOND ANGLE FOR =BONDLA=. (CHASTAIN AND STEWART)

BDIST - COMPUTE BOND DISTANCE FOR =BONDLA=. (CHASTAIN AND STEWART)

BDDIS - COMPUTE DEVIATIONS OF BOND DISTANCES (CHASTAIN AND STEWART)

BDZ - BINARY TO ZONED DECIMAL (HIGH)

BEGIN - SYSTEM BEGIN ROUTINE AND BSS LOADER (HIGH)

BLANK - INSERT A BLANK CHARACTER IN AN =A= FORMAT WORD (STEWART)

BONSEK - BOND SEEKING PROGRAM FOR =BONDLA= (CHASTAIN AND STEWART)

BONDLA - PROGRAM FOR CALCULATING BOND LENGTHS AND ANGLES (LINK 6000) (CHASTAIN AND STEWART)

BSTUW - FORTRAN BACKSPACE TAPE (9BST)

BTSNU - CONVERT SIGN-OVER-UNITS BCD INTEGERS TO BINARY (MODIFIED FROM FORTRAN BY F.NUSSBAUM (D.C.T.) AND BY HIGH)

BYEBYE - PREPARE 650 CARDS OR BUSING TAPE FROM SYSTEM REFLECTION TAPE (LINK 31000) (CHASTAIN AND STEWART)

CALLER - -CONTROL SUBROUTINE FOR X-RAY SYSTEM (HIGH)

CELFAC - CALCULATES CELL CONSTANTS AND WRITES BINARY TAPE (STEWART)

CHAC - INTERCHANGE A AND C AXES (TAKEDA)

CHEK - CHECK TRANSFORMED CELL DIMENSIONS AND ANGLES (TAKEDA)

COMNT - PRINT MANY COMMENTS IN ACCORDANCE WITH NUMBER OF GROUP AND ENTRY (TAKEDA)

CONVO - REWRITE THE SPACE-GROUP SYMBOL TO OBEY PRIORITY RULES (TAKEDA)

CONVM - REWRITE THE SPACE-GROUP SYMBOL TO OBEY CONVENTION (TAKEDA)

COOR - SYMMETRY GENERATOR FOR FOURIER REFINEMENT (HOLDEN)

CRAM - SUBROUTINE TO STORE INTEGERS IN LEAST SIGNIFICANT DIGITS OF A FLOATING POINT NUMBER (STEWART)

DATFX - PROGRAM TO CALCULATE UNITARY STRUCTURE FACTORS (LINK 10500) (HOLDEN)

DATRD - PROGRAM FOR DATA REDUCTION (LINK 10000) (JARSKI, STEWART, MOROSIN, CHASTAIN)

DEGR - CONVERT RADIANS TO DEGREES (TAKEDA)

DELGRF - A PROGRAM TO PLOT A GRAPH (CHASTAIN)

DELPLT - PROGRAM TO ASSIST IN PLOTTING OF A GRAPH (CHASTAIN)

DELSIG - PROGRAM TO GIVE DELTA-F VS FO PLOT (LINK 8000) (CHASTAIN)

DIFSYN - PROGRAM FOR DIFFERENTIAL SYNTHESIS (LINK 2000) (MOROSIN)

DIM - SUBROUTINE TO DETERMINE DIMENSION OF A REFLECTION (DICKINSON)

DMPUW - FORTRAN DUMP ROUTINE (9DMP)

DOT - DOT PRODUCT BETWEEN TWO VECTORS (HIGH)

DPSUW - FORTRAN DOUBLE PRECISION ARITHMATIC SUBROUTINE (9DPS)

DSQUW - FORTRAN DOUBLE PRECISION SQUARE ROOT FUNCTION (9DSQ)

EDCAL - FOURIER BLOCK CALCULATOR OF FOURIER REFINEMENT (HOLDEN)

EDIT - EDITS SELECTED REFLECTIONS AT FC TIME (STEWART)

EFTUW - FORTRAN ENDFILE TAPE (9EFT)

ERASE - WRITES BLANK TAPE FOR RECORDS TO BE RE-WRITTEN (HIGH)

ERLINK - ERROR LINK PROGRAM (LINK 32700) (HIGH)

ERREC - ERROR RECORD SUBROUTINE (HIGH)

ESORT - PROGRAM TO SORT UNITARY STRUCTURE VALUES FROM TAPE (LINK 10800) (DICKINSON)

EX221 - EXAMINE THE SPACE GROUP SYMBOL WITH ONE 2-FOLD AXIS EXCEPT F,I (TAKEDA)

EXEMW - EXECUTION ERROR MONITOR FOR X-RAY SYSTEM (HIGH)

EXPAND - SUBROUTINE TO EXPAND ATOM PARAMETERS FOR INDIVIDUAL ANISOTROPIC TEMPERATURE FACTOR DATA (MOROSIN)

FCALC - CALCULATION OF STRUCTURE FACTORS (STEWART AND HIGH)

FCINPU - READS REFLECTION DATA FOR FC SUBROUTINE (STEWART)

FCONE - FC PROGRAM (LINK 1000) PARAMETER LOADER (STEWART AND HIGH)

FCOUTP - WRITE REFLECTION DATA FOR FC SUBROUTINE (STEWART)

FCPACH - (DUMMY) ALLOWS PATCHING OF FC (STEWART)

FCSUMS - ACCUMULATES SUMS FOR R AND RESCALE IN FC PROGRAM (STEWART)

FCTWO - FC PROGRAM (LINK 1001) FC STATISTICS (STEWART AND HIGH)

FOFUN - FOURIER REFLECTION READING, GENERATOR, AND FOSUM FEEDER (HIGH, STEWART AND HOLDEN)

FOOB - TO TAKE CARE OF BELL MONITOR ON-LINE CARDS (DICKINSON)

FOSUM - FOURIER SUMMATION SUBROUTINE (HIGH, STEWART, AND HOLDEN)

FOURR - CONTROL PROGRAM FOR FOURIER SYNTHESIS (LINK 4000) (HIGH, STEWART, AND HOLDEN)

FPTUW - FORTRAN FLOATING POINT TRAP ROUTINE (9FPT)

FOREF - FOURIER REFINEMENT PROGRAM (LINK 5000) (HOLDEN)

GEN - DEVELOPS FOURIER DIRECTING CODES FOR EACH REFLECTION (STEWART)

GENCHK - ARRANGES AND CHECKS SYMMETRY OPERATIONS FOR GEN (STEWART)

GENRAT - GENERATION OF SYMMETRIC ATOMS FROM SPACE-GROUP (HIGH)

GU - IDENTIFIES EVEN-ODD CONDITIONS OF INDICES (DICKINSON)

HOLLER - TO MAKE BCD CHARACTER FOR CRYSET (STEWART)

INABS - INITIALIZES ABSORPTION CORRECTION SUBROUTINE ABSORB (MOROSIN)

INPUT - READS REFLECTION DATA FOR DATA REDUCTION (STEWART)

INV33 - INVERT 3X3 MATRIX (JORDAN/DEKKER MODIFIED BY HIGH)

IOBUW - FORTRAN INPUT-OUTPUT BINARY (9IOB)

IOHUW - FORTRAN INPUT-OUTPUT HOLLERITH (9IOH)

IOSW - INPUTOUTPUT SUPERVISOR (9IOS) MODIFIED FOR IOU IN COMMON. (IBM MODIFIED BY HIGH)

IOUBEL - INPUT-OUTPUT ROUTINE FOR BELL MONITOR. REPLACES FORTRAN (9IOU) (STEWART)

IOUW - INPUT-OUTPUT ROUTINE, UNIV. OF WASH. SPECIFIC. REPLACES FORTRAN (9IOU). (IBM MODIFIED BY HIGH)

LISTFC - PROGRAM FOR FINAL STRUCTURE FACTOR LISTING (LINK 11000) (HIGH AND STEWART)

LISTK - READ AND CHECK FIRST SEVEN RECORDS FOR =LISTFC= (STEWART)

LISTIN - READ THE BINARY REFLECTION RECORDS FOR =LISTFC= (STEWART)

LISTUP - LISTING TAPE UPDATE PROGRAM. (HIGH)

LOGUW - FORTRAN FLOATING POINT LOG ROUTINE (9LOG)

LSACS - ARCCOSINE ROUTINE (IBM-SHARE MODIFIED BY CHASTAIN)

LSCRT - ROOTS OF A CUBIC EQUATION (CHASTAIN)

LSHEQ - SOLUTIONS OF THREE HOMOGENEOUS EQUATIONS (CHASTAIN)

LSMIV - INVERSION OF A 3X3 MATRIX (CHASTAIN)

LSMMPY - MATRIX-MATRIX OR MATRIX-VECTOR MULTIPLY (CHASTAIN)

LSQPL - LEAST-SQUARES LINES AND PLANES PROGRAM (LINK 6500) (CHASTAIN)

MAP - SPECIAL FOURIER PRINT FEATURES. (HOLDEN, STEWART, DICKINSON)

MCL - DEAL WITH MONOCLINIC SYSTEM (TAKEDA)

MDIF - PROGRAM FOR UPDATING OR ALTERING A REFLECTION TAPE (LINK 10600) (STEWART)

MIXUP - SORTS EVEN OR ODD INDICES OF REFLECTIONS (DICKINSON)

MODPOS - CONVERT NUMBER INTO A POSITIVE MODULO VALUE (HIGH)

NAME - LEFT-JUSTIFY ALL NON-BLANK CHARACTERS IN ATOM NAME (HIGH)

NFIXER - SUBROUTINE FOR FIXING FLOATING POINT NUMBERS (CHASTAIN)

NOCALL - CUT-DOWN VERSION OF =CALLER= FOR NON-CHAIN OPERATION (HIGH)

NWAX - CALCULATE NEW CELL DIMENSIONS AND ANGLES (TAKEDA)

ORBET - RESET RELATIONSHIP FOR BETAS WHEN SPECIAL POSITION PATCHING IS REQUIRED (USER SUPPLIED PATCH FOR =ORFLS=)

ORCAL - CALCULATES STRUCTURE FACTORS AND DERIVATIVES FOR =ORFLS= (BUSING-MARTIN-LEVY MODIFIED BY STEWART)

ORDNL - MAKES PROPER SUFFIX FOR ORDINAL NUMBERS (HIGH)

ORFLS - FULL-MATRIX LEAST-SQUARES REFINEMENT PROGRAM (BUSING-MARTIN-LEVY MODIFIED FOR SYSTEM BY STEWART)

ORFUN - USES SYSTEM CODES TO GENERATE REFLECTIONS (STEWART)

ORIN - READS BINARY REFLECTION TAPE (STEWART)

OROUT - WRITES BINARY REFLECTION TAPE (STEWART)

ORPAC - CORRECTION FOR SPECIAL POSITIONS FOR =ORFLS= (BUSING-MARTIN-LEVY MODIFIED BY STEWART)

ORPRE - SETTING-UP OF PRELIMINARY DATA FROM REFLECTION TAPE (STEWART)

ORPT - COPY PARAMETERS FROM ONE STORAGE ARRAY TO ANOTHER (BUSING-MARTIN-LEVY)

ORRES - RESET RELATIONSHIP FOR POSITONAL PARAMETERS WHEN SPECIAL POSITONAL PATCHING IS REQUIRED (USER SUPPLIED PATCH =ORFLS=)

ORSBT - COPY PARAMETERS FROM ONE STORAGE ARRAY TO ANOTHER (BUSING-MARTIN-LEVY)

ORSMI - SYMMETRIC MATRIX INVERSION (BUSING-MARTIN-LEVY)

ORT - DEAL WITH ORTHORHOMBIC SYSTEM (TAKEDA)

ORTES - TEMPERATURE FACTOR EVALUATION (BUSING-MARTIN-LEVY MODIFIED BY STEWART)

ORTRIG - TRIG FUNCTION ADOPTED FROM SYSTEM =FCALC= SUBROUTINE FOR =ORFLS= (STEWART)

ORWT - WRITE NEW PARAMETERS ON FRONT OF BINARY INPUT TAPE (STEWART)

OUTPUT - (DUMMY) FOR WRITING OUT ANY NON-STANDARD SPECIAL RESULTS (STEWART)

PATPAT - PATCH TO PERMIT CALCULATION OF ANY TYPE OF FOURIER FUNCTION (STEWART AND HOLDEN)

PKCAL - PEAK CALCULATOR FOR FOURIER REFINEMENT PROGRAM (HOLDEN)

PMV - MATRIX VECTOR PRODUCT (HIGH)

PSV - SCALAR VECTOR PRODUCT (HIGH)

PVMV - VECTOR MATRIX VECTOR PRODUCT (HIGH)

RANDY - FUNCTION SUBROUTINE TO GENERATE RANDOM ERRORS (STEWART)

RANGL - IF 90-ANGLE WERE ACUTE, IT GIVES GAMMA AND TRANSFORMATION MATRIX FOLLOWS (TAKEDA)

RCAL - CALCULATION OF R FOR R-PLANE PROGRAM (HOLDEN)

RCOR - MOVES MOLECULE FOR R-PLANE PROGRAM (HOLDEN)

REDUC - REDUCE TRICLINIC CELL (TAKEDA)

REFLN - REFLECTION READING SUBROUTINE FOR =SHLPAT= (HOLDEN)

RERW - MODIFIED FORTRAN TAPE READ ERROR (9RER) - SKIP NOISE RECORDS (IBM MODIFIED BY STEWART AND HIGH)

RHH - =RHOMBH= DEALS WITH RHOMBOHEDRAL SYSTEM (TAKEDA)

RHOTP - PRINT C/A, A HEX, C HEX, IN ACCORDANCE WITH ACCURACY (TAKEDA)

RPLAN - CALCULATE R OVER A PROJECTION FOR MOVED MOLECULES (LINK 12000) (HOLDEN)

RTABL - GENERATES TABLE OF TRIG FUNCTIONS FOR R-PLANE PROGRAM (HOLDEN)

RWTUW - FORTRAN REWIND TAPE (9RWT)

BONSEK	BONSEK
BTCBZ1	BTSNU
BTSNU	BTSNU
CALC	CRCAL
CALLER	CALLER
CALLER	NOCALL (NON-CHAIN OPERATION)
CELFAC	CELFAC
CERUTS	LSCRT

SAME - PRINT OUT ANOTHER TRANSFORMATION MATRIX IF CELL HAS SOME EDGES (TAKEDA)

SCAL - CALCULATES SCALAR PRODUCTS A.A, A.B, A.C, B.B, B.C, C.C (TAKEDA)

SCNUW - FORTRAN FLOATING POINT SINE AND COSINE ROUTINE (9SCN)

SFCAL - STRUCT. FACTOR CALC. OF FOURIER REFINEMENT PROGRAM (HOLDEN)

SHLP - SHELL PATTERSON PROGRAM (LINK 5500) (HOLDEN)

SHORT - FIND THE SHORTEST TRANSLATION IN A PLANE (TAKEDA)

SLASH - CHANGES BLANK TO SLASH IN FRONT OF M,A,B,C,N, OR * (STEWART)

SLIUW - FORTRAN SHORT LIST INPUT (9SLI)

SLOUW - FORTRAN SHORT LIST OUTPUT (9SLO)

SMINP - CONVERT INPUT FORM OF SPACE-GROUP SYMBOL TO INTERNAL FORM (TAKEDA)

SMTR - INTERCHANGE SYMMETRY SYMBOL (TAKEDA)

SOLVPM - SUBROUTINE TO SOLVE PARAMETER SHIFTS FOR =DIFSYN= (MOROSIN)

SOLVTM - SUBROUTINE TO SOLVE TEMP. FACT. SHIFTS FOR =DIFSYN= (MOROSIN)

SOR - SUBROUTINE TO SORT REFLECTIONS ON INDICES (DICKINSON)

SPHW - MODIFED FORTRAN STORAGE-TO-PRINTER HOLLERITH (9SHP) (IBM MODIFIED BY HIGH)

SPREO - REORIENT SPACE-GROUP SYMBOL OF MONOCLINIC SYSTEM (TAKEDA)

SQRUW - FORTRAN FLOATING POINT SQUARE ROOT ROUTINE (9SQR)

SQUASH - PACKS ATOM PARAMETERS STORAGE DEPENDING ON TEMPERATURE FACTOR (HIGH)

STBUW - FORTRAN STORAGE-TO-TAPE BINARY (9STB)

STHW - MODIFIED FORTRAN STORAGE-TO-TAPE HOLLERITH (9STH) (IBM MODIFIED BY HIGH)

SYMTR2 - INTERPRET SYMMETRY CARD (FLOATING POINT) (HIGH)

SYMTR3 - INTERPRET SYMMETRY CARD (GENERAL EXPRESSION) (HIGH)

SYMTRY - STORES SYMMETRY OPERATIONS IN A FORTRAN MATRIX ARRAY (HIGH)

SYSBEL - INITIALIZES SYSTEM COMMON - BELL IOU TABLE (STEWART)

SYSCOM - INITIALIZES SYSTEM COMMON - FORTRAN IOU TABLE (HIGH)

TABLE - GENERATES TABLE OF TRIG FUNCTIONS FOR =FOUREF= (HOLDEN)

TCL - TRICLI - DEALS WITH TRICLINIC SYSTEM (TAKEDA)

TESUW - FORTRAN TEST LAST WRITE (9TES)

TIME - READS CLOCK AT UNIV. OF WASH. (BISSET (RCL) AND HIGH)

TIMEM - TIME FUNCTION FOR READING THE CLOCK THAT UPS MEMORY LOC. 5 (STEWART)

TINOL - TIME FUNCTION FOR READING THE CLOCK AT NAVAL ORDNANCE LABORATORY (STEWART)

TRACE - FLOW TRACE FOR FORTRAN MONITOR SYSTEM (HIGH)

TRANS - CALCULATE PRODUCTS OF TRANSFORMATION MATRIX (TAKEDA)

TRIGF - FLOATING POINT TABLE LOOK-UP OF COS OR SIN FUNCTIONS (DICKINSON AND STEWART)

TRXLS - TRANSFORMATION OF CRYSTAL SETTING AND SPACE GROUP SYMBOL (LINK 11100) (DONNAY AND TAKEDA)

TSBUW - FORTRAN TAPE-TO-STORAGE BINARY (9TSB)

TSHUW - FORTRAN TAPE TO STORAGE HOLLERITH (9TSH)

UCROSS - NORMALIZED CROSS PRODUCT BETWEEN TWO VECTORS (HIGH)

UKEEP - KEEP U(I,J) (TAKEDA)

UNITV - NORMALIZED VECTOR (HIGH)

VOL - CALCULATES CELL VOLUME (TAKEDA)

WERE - MODIFIED FORTRAN WRITE ERROR ROUTINE (9WER) (IBM MODIFIED BY HIGH)

WTFN - CALC. OF SPECIAL LEAST SQUARES WEIGHTING FACTORS (STEWART)

XLSOUT - WRITE ORXLS-TYPE BUSING-LEVY REFLECTION RECORD (HIGH)

XMIX - CONVERT FLOATING POINT NUMBERS TO FIXED POINT NUMBER (HIGH)

XMODTW - CONVERT FIXED POINT BINARY FRACTION TO INTEGERS IN 0-11 TWELFTHS (STEWART)

XNOO - MAKES INTEGERS FROM B17 TRANSLATION FRACTION, 1-12 = 0/12 TO 11/12 (STEWART)

XPFUW - FORTRAN FLOATING POINT EXPONENTIAL FUNCTION (9XPF)

XP2UW - FORTRAN EXPONENTIAL ROUTINE - FLOATING POINT BASE AND FIXED POINT EXPONENT (9XP2)

XP3UW - FORTRAN EXPONENTIAL ROUTINE FLOAT.PT. BASE AND EXPONENT (9XP3)

XRND - PROPERLY FIXES AND ROUNDS OFF FLOATING POINT NUMBERS (HIGH)

B. INTERNAL 709-7090 SYSTEM AND FORTRAN SUBROUTINE ENTRY POINTS.

ENTRY	PROGRAM	
ABSORB	ABSORB	
AINPT	AINPT	
ANGLE	BANGL	
AOUTP	AOUTP	
ARCOS	LSACS	
ARCTAN	ARCTN	
ARCSIN	LSACS	
ARR	ARR	
ATAN	ATNUW	
ATN	ATNF	
ATNAME	ATNAME	
ATNUM	ATNUM	
ATOFL	ATOFL	
BDZIN	BDZ	
BDZFL	BDZ	
BDZFX	BDZ	
BLANK	BLANK	
CHAC	CHAC	
CHEK	CHEK	
COMNT	COMNT	
CONVO	CONVO	
CONVM	CONVM	
COOR	COOR	
COS	SCNUW	(FORTRAN FLOATING POINT SERIES EXPANSION)
COS	TRIGF	(FLOATING POINT TABLE LOOK-UP)
CRAM	CRAM	
CYCLES	TRIGF	
DDIST	BDDIS	
DEGR	DEGR	
DEGREE	TRIGF	
DIMEN	DIM	
DIST	BDIST	
DOT	DOT	
DSQRT	DSQUW	
DUMP	DMPUW	
EDCAL	EDCAL	
EDIT	EDIT	
ERASE	ERASE	
ERREC	ERREC	
EXIT	CALLER	
EXIT	NOCALL	(NON-CHAIN OPERATION)
EXP	XPFUW	
EXPAND	EXPAND	
EXP(2	XP2UW	
EXP(3	XP3UW	

ENTRY	PROGRAM	
EX221	EX221	
FCALC	FCALC	
FCINPU	FCINPU	
FCOUTP	FCOUTP	
FCPACH	FCPACH	
FCSUMS	FCSUMS	
FLSFUN	ORFUN	
FLSIN	ORIN	
FLSOUT	OROUT	
FOFUN	FOFUN	
FOOLBE	FOOB	
FOSUM	FOSUM	
GEEYOU	GU	
GEN	GEN	
GENCHK	GENCHK	
GENRAT	GENRAT	
GRAPH	DELGRF	
HIFI	ORTRIG	
HIFI	TRIGF	
HOLLER	HOLLER	
IFEOT	WERW	
IFFC	CALLER	
IFFC	NOCALL	(NON-CHAIN OPERATION)
IFFI	CALLER	
IFFI	NOCALL	(NON-CHAIN OPERATION)
IFFW	CALLER	
IFFW	NOCALL	(NON-CHAIN OPERATION)
IFFY	CALLER	
INABS	INABS	
INPUT	INPUT	
INV33	INV33	
LINES	CALLER	
LINES	NOCALL	(NON-CHAIN OPERATION)
LINK	CALLER	
LINK	NOCALL	(NON-CHAIN OPERATION)
LISTIN	LISTIN	
LISTK	LISTK	
LOFI	ORTRIG	
LOFI	TRIGF	
LOG	LOGUW	
LOGE	LOGUW	
LOGN	LOGUW	
LOG10	LOGUW	
LSHEQ	LSHEQ	
LSOPL	LSOPL	
MAP	MAP	
MATINV	LSMIV	
MATMPY	LSMMPY	
MIXUP	MIXUP	
MODPOS	MODPOS	
MONOCL	MCL	
NAME	NAME	
NFIXER	NFIXER	
NPS	CALLER	
NPS	NOCALL	(NON-CHAIN OPERATION)
NWAX	NWAX	
ORDNL	ORDNL	
ORTHOR	ORT	
ORWT	ORWT	
OUTPUT	OUTPUT	

ENTRY	PROGRAM	
PATCH	ORPAC	
PATPAT	PATPAT	
PDUMP	DMPUW	
PKCAL	PKCAL	
PLOTER	DELPLT	
PMV	PMV	
PRELIM	ORPRE	
PRIME	SOR	
PSV	PSV	
PTOSB	ORPT	
PVMV	PVMV	
RADIAN	TRIGF	
RANDY	RANDY	
RANGL	RANGL	
RCALC	RCAL	
RCCOR	RCOR	
REDUC	REDUC	
REFLTN	REFLN	
RERITE	WERW	
RESETB	ORBET	
RESETX	ORRES	
RHOMBH	RHH	
RHOTP	RHOTP	
RTABLE	RTABL	
SAME	SAME	
SBTOP	ORSBT	
SCAL	SCAL	
SEMIDN	FCALC	
SETFCP	FCPACH	
SFCAL	SFCAL	
SIN	SCNUW	(FORTRAN FLOATING POINT SERIES EXPANSION)
SIN	TRIGF	(FLOATING POINT TABLE LOOK-UP)
SLASH	SLASH	
SMI	ORSMI	
SMINP	SMINP	
SMTR	SMTR	
SOLVPM	SOLVPM	
SOLVTM	SOLVTM	
SORT	SHORT	
SORT	SOR	
SPREO	SPREO	
SQRT	SQRUW	
SQUASH	SQUASH	
SYMTRY	SYMTRY	
SYMTR2	SYMTR2	
SYMTR3	SYMTR3	
SYSCOM	SYSBEL	(BELL IOU TABLE)
SYSCOM	SYSCOM	(FORTRAN IOU TABLE)
TABLE	TABLE	
TEST	ORTES	
TIME	TIME	(CLOCK AT U OF W)
TIME	TIMEM	(INCREASES MEMORY LOCATION 5)
TIME	TINOL	(CLOCK AT NAVAL ORD. LABS)
TRACE	TRACE	
TRACEN	TRACE	
TRANS	TRANS	
TRICLI	TCL	
TRIG	ORTRIG	
UCROSS	UCROSS	
UKEEP	UKEEP	

ENTRY	PROGRAM	
UNCRAM	CRAM	
UNITV	UNITV	
UNTRAP	TRACE	
VOL	VOL	
WTFN	WTFN	
XBTSNU	BTSNU	
XLSOUT	XLSOUT	
XMIX	XMIX	
XMODTW	XMODTW	
XNAME	NAME	
XNOD	XNOD	
XORDNL	ORDNL	
XRND	XRND	
(BSH)	CALLER	
(BSH)	NOCALL	(NON-CHAIN OPERATION)
(BST)	BSTUW	
(DFAD)	DPSUW	
(DFDP)	DPSUW	
(DFMP)	DPSUW	
(DFSB)	DPSUW	
(CSH)	CALLER	
(CSH)	NOCALL	(NON-CHAIN OPERATION)
(EFT)	EFTUW	
(EXE)	ERREC	(ENTERED ONLY THROUGH EXEMW)
(EXE)	EXEMW	
(EXEM)	ERREC	(ENTERED ONLY THROUGH EXEMW)
(EXEM)	EXEMW	
(FIL)	IOHUW	
(FPT)	FPTUW	
(ICB)	IOBUW	
(ICH)	IOHUW	
(ICS)	IOSW	
(ICSW)	IOSW	
(ICU)	IOUBEL	(BELL MONITOR)
(ICU)	IOUW	(U OF W SPECIFIC)
(RER)	RERW	
(RLR)	TSBUW	
(RTN)	IOHUW	
(RWT)	RWTUW	
(SLI)	SLIUW	
(SLO)	SLOUW	
(SPH)	SPHW	
(STB)	STBUW	
(STH)	STHUW	
(STHM)	STHUW	
(TES)	TESUW	
(TSB)	TSBUW	
(TSH)	TSHUW	
(TSHM)	TSHUW	
(WER)	WERW	
(WLR)	STBUW	
.SPH.	SPHW	
.STH.	STHW	
.UNIT.	IOSW	

ENTRY	PROGRAM
-(BSR)	IOSW
-(ETT)	IOSW
-(EXB)	IOBUW
-(LCH)	IOSW
-(RCH)	IOSW
-(RDC)	RERW
-(RDS)	IOSW
-(REW)	IOSW
-(SCH.)	IOSW
-(TCO)	IOSW
-(TEF)	IOSW
-(TRC)	IOSW
-(WEF)	IOSW
-(WRS)	IOSW
-(WTC)	WERW

APPENDIX II

CARD FORMATS FOR X-RAY CRYSTALLOGRAPHY SYSTEM PROGRAMS.

REFER TO SECTION 2.0-D FOR STATEMENT REGARDING STANDARDIZATION OF CARD FORMATS WITHIN THE FORTRAN CONVENTIONS.

```
*DATA CARD - USED BY MONITOR AND CALLER TO DENOTE BEGINNING OF DATA
        DECK.  REQUIRED IN ALL PROGRAMS.
        FORMAT (A1,5X,A6)
            1      *                (ASTERISK)
          2- 6                      (BLANK)
          7-10      DATA
         11-72                      (BLANK)

650     - CARD TO SIGNAL INPUT 650-FORMAT CARDS FOR =LISTFC=.
        FORMAT (A6)
          1- 6        650$$$
          7-72                      BLANKS.

ABSORB - ABSORPTION CORRECTION CARD - TYPE I. (REQUIRES ONE CARD FOR
        EACH ENTRY IN TABLE.  TOTAL = 19 CARDS.)
        FORMAT (A6,1X,I1,I4,F4.0,2X,F10.3)
          1- 6      ABSORB
            7       $                BLANK
            8         X              ABSORPTION TYPE.    (1)/(2)  FOR (NO
                                       CORRECTION)/(SPHERE OR CYLINDER)  (I1)
                                     TYPE (1) IS USED TO CANCEL PREVIOUS
                                     TYPE CODES IF NO CORRECTIONS ARE DESIRED
                                     FOR FOLLOWING SET OF DATA.
          9-12      $$$I             GROUP NUMBER OF DATA ALONG THE AXIS OF
                                     ROTATION.    (I4)
         13-16        $XX.           TYRTA.    THETA, OR UPSILON/2 (BUERGERS
                                       NOTATION).    (F4.0)
                                     SEE W.L.BOND IN INTERNATIONAL TABLES,
                                     VOL 2, PP 291-306. USE TABLE 5.3.5B FOR
                                     CYLINDER (P 295-298) AND TABLE 5.3.6B
                                     FOR SPHERE (P 302-305).
         17-18        $$             BLANK.
         19-28      $XXXXX.XXX       ABSORPTION CORRECTION AS LISTED IN TABLE
         29-72      ANY DESIRED LEGAL PUNCHING OR BLANKS.

ABSORB - ABSORPTION CORRECTION CARD - TYPE II.
        FORMAT (A6,1X,I1, **********)  (FINAL FORMAT NOT SET)
          1- 6      ABSORB
            7       $                BLANK
            8         X              ABSORPTION TYPE.   (1)/(3)/(4)  FOR (NO
                                     CORRECTION)/(ELLIPSOIDAL)/(BUSING
                                     GENERAL CASE)    (I2)
                                     TYPE (1) USED TO CANCEL ANY PREVIOUS
                                     TYPE CODES IF NO CORRECTIONS ARE DESIRED
                                     FOR FOLLOWING SET OF DATA.
                                       NOTE= PRESENTLY (3) AND (4) CALCULATE
                                       LIKE (1) PENDING PROGRAMMING OF TYPE.
          9-72                       NO DETAILS OF CARD FORMAT SET
```

```
ANGLE   - CALCULATE A SPECIFIED =BOND= ANGLE.
          FORMAT (A6,4(1X,A6))
            1- 6        ANGLE$
              7         $           BLANK
            8-13                    ATOM ID FOR FIRST BONDED ATOM
             14         $           BLANK
           15-20                    ATOM ID FOR SECOND BONDED ATOM
             21         $           BLANK
           22-27                    ATOM ID OF THIRD BONDED ATOM
             28         $           BLANK
           29-34                    ATOM ID OF FOURTH BONDED ATOM
           35-72                    BLANKS
                      THE ANGLE CALCULATED IS THAT BETWEEN THE LINES
                      DEFINED BY A1-A2 AND A3-A4.  A1 AND A3 MAY BE
                      IDENTICAL TO GIVE =USUAL= BOND ANGLES.

ATOM    - ATOM PARAMETER CARD.
          FORMAT (A6,1X,3F8.4,F6.3,F5.2,3F8.5)
            1- 6      ATOM$$
              7       $           BLANK
            8-13                  ATOM NAME - CONSISTS OF TWO PARTS. THE
                                    FIRST, WHICH MUST NOT END IN A DIGIT, IS
                                    THE ATOM-TYPE NAME (SEE FORMFX). THE
                                    REST OF THE WORD, UP TO A TOTAL OF SIX
                                    COLUMNS, MAY BE NUMERIC IDENTIFICATION
                                    OF THE PARTICULAR ATOM. THIS SECOND PART
                                    MUST BE NUMERIC. BLANKS ARE IGNORED.
           14-21      $XX.XXXX   X   FRACTIONAL COORDINATE   (F8.4)
                                    DECIMAL POINT MUST BE PUNCHED IN ORDER
                                    TO SUPERCEDE FORMAT.
           22-29      $XX.XXXX   Y
           30-37      $XX.XXXX   Z
           38-43      $X.XXX     INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR.
                                    MAY BE ZEROS OR BLANK IF APPLYING OVER-
                                    ALL TEMPERATURE FACTOR OR IF A SEPARATE
                                    TEMPERATURE FACTOR CARD IS USED, SINCE
                                    THIS WORD IS THEN IGNORED.
           44-48      $X.XX      INDIVIDUAL ATOM SCALE FACTOR (F5.2).  MUST
                                    BE ZEROS OR BLANK TO BE IGNORED.
           49-56      $X.XXXXX   STANDARD DEVIATION IN X (REQUIRED ONLY IF
                                    REQUIRED BY PROGRAM BEING USED.)
           57-64      $X.XXXXX   STANDARD DEVIATION IN Y.
           65-72      $X.XXXXX   STANDARD DEVIATION IN Z.

ATOMG   - ATOMIC PARAMETER CARD BASED ON GRID POINTS.
          FORMAT (A6,1X,3F8.4,F6.3,F5.2,3F8.5)
            1- 6      ATOMG$
            7-72                  SAME AS ATOM CARD, WITH ATOMIC COORDINATES
                                    EXPRESSED AS GRID VALUES FROM FOURIER
                                    MAPS AS $XXX.XXX.  THE SET OF ATOMG
                                    CARDS MUST BE PRECEDED BY A LEADING
                                    GRID CARD.

B       - ISOTROPIC TEMPERATURE FACTOR CARD.
          FORMAT (A6,1X,A6,F8.4)
            1- 6      B$$$$$
              7       $           BLANK
            8-13                  COMPID IF OVERALL TEMPERATURE FACTOR.
            8-13                  NAMEAT IF INDIVIDUAL TEMPERATURE FACTOR.
           14-21      $XX.XXXX   B
           22-61                  MUST BE BLANK.
           62-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
BEGIN  - MARKS THE BEGINNING OF BINARY DECKS OF UNIVERSALLY USED
         SUBROUTINES THAT WILL BE STORED IN LOW CORE.
         FORMAT (A6)
           1- 6       BEGIN$
           7-72                    (IGNORED)

BETA   - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                    2*(PI**2)*ASTAR(I)*ASTAR(J)*U(I,J)=BETA(I,J)
         FORMAT (A6,1X,A6,6F8.4)
           1- 6     BETA$$
           7-61     FORMAT IDENTICAL WITH BIJ CARD
          62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BIJ    - ANISOTROPIC TEMPERATURE FACTOR CARD. IN FORTRAN NOTATION
                    8*(PI**2)*U(I,J)=B(I,J)
         FORMAT (A6,1X,A6,6F8.4)
           1- 6     BIJ$$$
               7    $              BLANK
           8-13                      NAMEAT.
          14-21     $XX.XXXX       B11   (F8.4)
          22-29     $XX.XXXX       B22
          30-37     $XX.XXXX       B33
          38-45     $XX.XXXX       B12
          46-53     $XX.XXXX       B13
          54-61     $XX.XXXX       B23
          62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BLINIT - CARD TO CONTROL ESTIMATION OF OVERALL ISOTROPIC TEMPERATURE
         FACTOR AND LEVEL SCALE FACTORS.
         FORMAT (A6,1X3F6.3)
           1- 6       BLINIT
               7      $          BLANK
           8-13       XX.XXX     MAXIMUM PERMISSIBLE ERROR IN ESTIMATED B
                                   (BLANK = 0.1)
          14-19       XX.XXX     MINIMUM PERMISSIBLE RATIO FOR AN ESTIMATED
                                   LEVEL SCALE FACTOR TO THE OVERALL ESTI-
                                   MATED SCALE FACTOR (BLANK = 1.0, I.E.
                                   NO VARIATION)
          20-25       XX.XXX     MAXIMUM PERMISSIBLE RATIO FOR A LEVEL
                                   SCALE FACTOR TO THE OVERALL SCALE FACTOR
                                   (BLANK = 1.0)
          26-72                  (IGNORED)

BNORM  - ANISOTROPIC TEMPERATURE FACTOR CARD, WHERE TEMPERATURE FACTOR
         IS EXPRESSED IN TERMS OF B(I) USING THREE PRINCIPAL AXES OF THE
         ELLIPSOID OF VIBRATION, AND THE E(I,J) ARE VECTORS WHICH
         EXPRESS THE DIRECTIONS OF TWO OF THE THREE PRINCIPAL AXES OF
         THE VIBRATION ELLIPSOID. THE THIRD IS ASSUMED TO BE NORMAL TO
         THESE TWO.
         FORMAT (A6,1X,A6,9F6.4)
           1- 6     BNORM$
               7    $              BLANK
           8-13                      NAMEAT.
          14-18     X.XXXX         B1    (F6.4)
          19-25     X.XXXX         B2
          26-31     X.XXXX         B3
          32-37     X.XXXX         E11
          38-43     X.XXXX         E12
          44-48     X.XXXX         E13
          49-54     X.XXXX         E21
          55-60     X.XXXX         E22
          61-66     X.XXXX         E23
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
BNORMG - ANISOTROPIC TEMPERATURE FACTOR CARD.  LIKE THE BNORM CARD
         EXCEPT THE COEFFICIENTS ARE BASED ON GRID POINTS.
         FORMAT (A6,1X,A6,9F6.4)
                  EXCEPT COEFFICIENTS ARE BASED ON GRID POINTS.
           1- 6   BNORMG
           7-66   FORMAT IDENTICAL WITH BNORM CARD.
          67-72   ANY LEGAL PUNCHING DESIRED, OR BLANKS.

BOND   - CALCULATE A SPECIFIED =BOND= DISTANCE.
         FORMAT (A6,2(1XA6))
           1- 6      BOND$$
             7       $          BLANK
           8-13                 ATOM ID FOR FIRST ATOM.
            14       $          BLANK
          15-20                 ATOM ID FOR BONDED ATOM
          21-72                 BLANKS

BONDLA - CALLING CARD FOR =BONDLA= PROGRAM (LINK 6000).
         FORMAT (A6,1X,A6,3(1XI4),3F6.2)
           1- 6      BONDLA
             7       $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-15      $X         (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                  =INTRAMOLECULAR= DISTANCES.
          16-17      $X         (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                  =INTRAMOLECULAR= ANGLES. (IGNORED IF
                                  COL 15 IS BLANK.)
          18-19      $X         (BLANK)/(1) FOR (DO NOT)/(DO) CALCULATE
                                  =INTERMOLECULAR= DISTANCES
          20-25      XXX.XX     MINIMUM =SIGNIFICANT= DISTANCE TO BE
                                  PRINTED.
          26-31      XXX.XX     MAXIMUM =SIGNIFICANT= DISTANCE TO BE
                                  PRINTED.
          32-37      XXX.XX     TEMPERATURE FACTOR TO BE PLACED ON GENERA-
                                  TED ATOMS (IF ANY). BLANK OR ZERO WILL
                                  CAUSE TEMPERATURE FACTOR OF BONDED
                                  =HEAVY= ATOM TO BE USED.
          38-72                 BLANKS

BYEBYE - CALLING CARD FOR NON-SYSTEM INPUT FORMATS.
         FORMAT (A6,1X,A6,I5,I3,2I2)
           1- 6      BYEBYE
             7                  BLANK
           8-13                 SIX COLUMNS OF HOLLERITH PUNCHING OR
                                  BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                  (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                  NOT ALLOWED. THIS IDENTIFICATION IS
                                  CHECKED BY VARIOUS PROGRAMS FOR
                                  CONSTANCY, SO CHOOSE CAREFULLY AND
                                  REMEMBER YOUR CHOICE.     (A6)
          14-18      $XXXX      650 REFLECTION DECK ID NUMBER.
          19-21      $XX        650 FC DECK TRIAL NUMBER.
          22-23      $X         OUTPUT TYPE.
                                  1 = 650 REFLECTION CARD
                                  2 = 650 FC CARD, 3 = BUSING TAPE
          24-25      $X         OUTPUT SCALING OF FREL DATA FROM TAPE.
                                  1 = USES FREL SCALE FACTOR ON TAPE
                                  2 = ALL SCALES SET EQUAL TO 1.0
                                  3 = USES FREL RESCALE FACTOR ON TAPE
                                  AN FC SCALE CARD MODIFIES THE SCALE
                                 FOR THE INDICATED GROUP ONLY.
          26-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.
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CELCON - CELL CONTENTS CARD
         FORMAT (A6,1XF3.0,A6)
           1- 6       CELCON
             7        $          BLANK
           8-10       XXX        NUMBER OF ATOMS OF SPECIFIED TYPE IN THE
                                   WHOLE UNIT CELL
          11-16                  BCD ATOM TYPE NAME (SYMBOL)
          17-72                  (IGNORED)

CELL   - CELL CONSTANT CARD.
         FORMAT (A6,1X,A6,3F8.3,3F9.5,F7.0)
           1- 6     CELL$$
             7      $          BLANK
           8-13                 SIX COLUMNS OF HOLLERITH PUNCHING OR
                                  BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                  (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                  NOT ALLOWED. THIS IDENTIFICATION IS
                                  CHECKED BY VARIOUS PROGRAMS FOR
                                  CONSTANCY, SO CHOOSE CAREFULLY AND
                                  REMEMBER YOUR CHOICE.     (A6)
          14-21     $AAA.AAA     A CELL DIMENSION  (F8.3)
          22-29     $AAA.AAA     B CELL DIMENSION  (F8.3)
          30-37     $AAA.AAA     C CELL DIMENSION  (F8.3)
          38-46     $+A.AAAAA    COS ALPHA  (F9.5)
          47-55     $+A.AAAAA    COS BETA (F9.5)
          56-64     $+A.AAAAA    COS GAMMA (F9.5)
          65-71     $AAAAA.      F(0,0,0)  (F7.0)

CELLSD - STANDARD DEVIATIONS OF CELL DIMENSIONS.
         FORMAT (A6,1X,A6,3F8.3,3F9.5)
           1- 6     CELLSD
             7      $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-21     $AAA.AAA     STANDARD DEVIATION OF =A= AXIAL LENGTH.
          22-29     $AAA.AAA     STANDARD DEVIATION OF =B= AXIAL LENGTH.
          30-37     $AAA.AAA     STANDARD DEVIATION OF =C= AXIAL LENGTH.
          38-46     $+A.AAAAA    STANDARD DEVIATION OF COS ALPHA.
          47-55     $+A.AAAAA    STANDARD DEVIATION OF COS BETA.
          56-64     $+A.AAAAA    STANDARD DEVIATION OF COS GAMMA.
          65-72                  BLANKS

CONDIT - CONDITION CARD.  SETS-UP CALCULATIONS CODES.
         FORMAT (A6,1X,A7,3F8.5,7I3,F8.5)
           1- 6     CONDIT
             7      $          BLANK
           8-13                 COMPOUND IDENTIFICATION (SEE COLS. 8-13
                                  OF THE CELL CARD).
          14-21     $X.XXXXX     WAVELENGTH  (F8.5)
          22-29     $X.XXXXX     SIN THETA (MAX).  (F8.5)
          30-37     $X.XXXXX     MINIMUM OBSERVED INTENSITY  (F8.5)
                                  (THE VALUE PUNCHED INTO THE SCALE CARD
                                  WILL SUPERCEDE THIS VALUE WHEN USING
                                  MULTIPLE LEVEL DATA.)
                    (THE NEXT SEVEN FIELDS ARE READ I3.)
          38-40     $$X          RADIATION TYPE (SWITCH LLL)
                                  (1)/(2) FOR (X-RAY)/(NEUTRON)
          41-43     $$X          CAMERA TYPE (SWITCH LL)
                                  (1)/(2)/(3)/(4)  FOR  (POWDER)/
                                  (SPECTROMETER)/EQUI-INCLINATION
                                  WEISSENBERG)/(PRECESSION)
          44-46     $$X          (1)/(2)  FOR  (APPLY 1/LP)/(BYPASS THE
                                 APPLICATION OF 1/LP)
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CONDIT - CONDITION CARD.  (CONTINUED)
          47-49     $$X          (1)/(2)  FOR  (CALCULATION OF THE SQUARE
                                 ROOT OF INTENSITY, FREL**2, EIC)/(BYPASS
                                 CALCULATION OF SQUARE ROOT)
          50-52     $$X          REFLECTION CARD FORMAT (SWITCH LLL8)
                                   (1)/(2)/(3) FOR (STANDARD FORMAT)/
                                   (MARK-SENSE FORMAT)/(FORMAT SPECIFIED
                                   IN =REFIN= AND =FORMAT= CARDS)
          53-55     $$X          JAX.  AXIS OF ROTATION FOR WEISSENBERG,
                                 AXIS CLOSEST TO HORIZONTAL FOR PRECESSION.
                                 (1)/(2)/(3) FOR (A)/(B)/(C) AXIS
          56-58     $$X          KAX.  AXIS PARALLEL TO THE BEAM FOR THE
                                 PRECESSION METHOD.
          59-66     $X.XXXXX     COS TAU 0.  ANGLE BETWEEN KAX AND THE
                                 HORIZONTAL FOR PRECESSION METHOD   (F8.5)
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

CONDIT - CONDITION CARD FOR CHANGE OF DATA.
         FORMAT (A6,1X,A7,3F8.5,7I3,F8.5)
           1- 6     CONDIT
             7      $
           8-13                  BLANK
                                 COMPOUND IDENTIFICATION (SEE COLS. 8-13
                                   OF THE CELL CARD).
          14-66     PUNCH ONLY THOSE APPLICABLE COLUMNS FOR WHICH THERE
                                 IS A CHANGE OF DATA. LEAVE ALL OTHER
                                 COLUMNS BLANK UNLESS CAMERA TYPE CHANGES
                                 THEN PUNCH IN FULL.
          67-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

CRYSET - CALLING CARD FOR DONNAY-TAKEDA TRANSFORMATION PROGRAM.
         FORMAT (A6)
           1- 6     CRYSET
           7-72                  (IGNORED)

CYCLES - NUMBER OF ITERATIONS AND CRITEREA
         FORMAT (A6,I3,3F5.3,3F8.4)
           1- 6       CYCLES
           7- 9       XXX       MAXIMUM NUMBER OF CYCLES (0 OR BLANK = 5)
          10-14       X.XXX     MAXIMUM ALLOWED VALUE OF R (DECIMAL FRACT)
                                  (0 OR BLANK = 1.0)
          15-19       X.XXX     MINIMUM IMPROVED CHANGE IN R TO CONTINUE
                                  CYCLING
          20-24       X.XXX     REJECTION RATIO FOR FC/FO LESS THAN THIS
                                  VALUE (0 OR BLANK = 0.001)
          25-32       XXX.XXXX  GRID INTERVAL IN X DIRECTION FOR FIRST
                                  CYCLE (THIS VALUE IS REDUCED ON EACH
                                  SUCCEEDING CYCLE FOR ATOMS WHICH ARE AT
                                  PEAKS)  (0 OR BLANK = 0.001*CELL EDGE)
          33-40       XXX.XXXX  INITIAL GRID INTERVAL FOR Y DIRECTION
          41-48       XXX.XXXX  INITIAL GRID INTERVAL FOR Z DIRECTION
          49-72                 (IGNORED)
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DATFIX - CALLING CARD FOR DATA MANIPULATION PROGRAM.
         FORMAT (A6,1XA6,1XI1,4F8.4)
           1- 6        DATFIX
             7         $          BLANK
           8-13                   COMPID - COMPOUND IDENTIFICATION CODE
            14         $          BLANK
            15         X          (0 OR BLANK)/(1) FOR (DO NOT)/(DO) LIST
                                    INDIVIDUAL REFLECTION INFORMATION
                                    H, K, L, F, AND E.
          16-23        XXX.XXXX    INITIAL VALUE OF B
                                    (0 OR BLANK = 3.0)
          24-31        XXX.XXXX    E(0.0,0) TO OVERRIDE CALCULATED VALUE
                                    (USUALLY LEFT BLANK)
          32-39        XXX.XXXX    F(0.0,0) TO OVERRIDE VALUE ON TAPE
                                    (USUALLY LEFT BLANK)
          40-47        XXX.XXXX    MINIMUM VALUE OF F FOR WHICH AN E IS TO
                                    BE CALCULATED  (BLANK = 0.0)
          48-72                   (IGNORED)

DATOMS - MOLECULE SHIFT CARD
         FORMAT (A6,3F8.0)
           1- 6        DATOMS
           7-14        XX.XXXXX    X DIRECTION SHIFT
          15-22        XX.XXXXX    Y DIRECTION SHIFT
          23-30        XX.XXXXX    Z DIRECTION SHIFT
          31-72                   (IGNORED)

DATRDN - CALLING CARD FOR DATA REDUCTION PROGRAM (LINK 10000)
         FORMAT (A6,1X,A6,6X)
           1- 6      DATRDN
             7                    BLANK
           8-13                   SIX COLUMNS OF HOLLERITH PUNCHING OR
                                    BLANKS TO IDENTIFY COMPOUND. MINUS ZERO
                                    (-0) OR ZERO (0) AS A LEADING SYMBOL IS
                                    NOT ALLOWED. THIS IDENTIFICATION IS
                                    CHECKED BY VARIOUS PROGRAMS FOR
                                    CONSTANCY, SO CHOOSE CAREFULLY AND
                                    REMEMBER YOUR CHOICE.    (A6)
          14-18                     BLANK
          19-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS

DELSIG - CALLING CARD FOR =DELSIG= PROGRAM (LINK 8000).
         FORMAT (A6,1X,A6,1X,A1,1X,A3,2(1X,I1),7X,2F10.4,(F10.4 OR I3))
           1- 6        DELSIG
             7         $          BLANK
           8-13                   COMPID, COMPOUND IDENTIFICATION CODE.
          14-15        $X         (A)/(B) FOR GROUPING F-OBSERVEDS BY EQUAL
                                    (NUMBERS)/(INTERVALS OF MAGNITUDE)(CIND)
          16-19        $XXX       (ORD)/(RMS) FOR (ARITHMETIC)/(ROOT-MEAN-
                                    SQUARE) AVERAGED DELTA-F  (RMSORD)
          20-21        $X         1=USE REFLECT. TAPE SCALE FACTORS  (ISCAL)
                                  2=MAKE ALL SCALE FACTORS = 1.0.
                                  3=USE RESCALE FACTORS ON REFLECT. TAPE.
          22-23        $X         1=NO GRAPH      (IGRAF)
                                  2=FOR GRAPH PLOTTED MODULO 100.
                                  3=FOR SCALED DELTA-F SO MAXIMUM = 100.
                                  4=BOTH GRAPHS 2 AND 3.
          31-40        XXXXX.XXXX MINIMUM FO TO BE CONSIDERED IN CALC.
          41-50        XXXXX.XXXX MAXIMUM FO TO BE CONSIDERED IN CALC.
          51-53        XXX       FOR COL 15 = A, NUMBER OF REFLECTIONS
                                    PER GROUP.
          51-60        XXXXX.XXXX FOR COL 15 = B, RANGE OF FO PER GROUP.
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DISPER - TEMPLETON DISPERSION CORRECTION CARD.
         FORMAT (A6,1X,A3,3X,2F10.3)
           1- 6     DISPER
             7      $              BLANK
           8-13                    ATOM TYPE NAME (SEE COLS. 8-13 OF FORMFX).
          14-21     $XXX.XXX       DELTA FJ PRIME  (F8.3)
          22-29     $XXX.XXX       DELTA FJ DOUBLE PRIME  (F8.3)
          30-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

EDIT   - EDIT CARD FOR MODIFYING REFLECTIONS AT FC TIME.
         FORMAT (A6,1X,5I5,2F10.5)
           1- 6     EDIT$$
             7      $              BLANK
           8-12     XXXXX          H OF REFLECTION NEEDING CHANGE.
          13-17     XXXXX          K OF REFLECTION NEEDING CHANGE.
          18-22     XXXXX          L OF REFLECTION NEEDING CHANGE.
                      NOTE= LEAVING ANY ONE OF FIELDS IN COLS. 23-52
                                BLANK WILL CAUSE FCALC TO USE OLD VALUES
          23-27     $$$$X          NEW JCODE STATUS (1)/(2)/(3) FOR
                                    (OBSERVED)/(UNOBSERVED)/(EXTINCT).
          28-32     $$$XX          NEW LEVEL INDICATOR (1 TO 64 ALLOWED)
          33-45     XXXX.XXXXX     NEW FRELATIVE AS (F10.5)
          43-52     XXXX.XXXXX     NEW LEAST SQUARES WEIGHT
          53-72     ANY LEGAL DESIRED PUNCHING, OR BLANKS.

END    - END CARD.
         FORMAT (A6)
           1- 6     END$$$
             7      $              BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

END-TRACE - END CARD TO INITIATE SNAPSHOT TRACE.
         FORMAT (A6,A5)
           1- 6       END$$$
           7-11       TRACE
          12-72       ANY LEGAL PUNCHING DESIRED, OR BLANKS.

ENDFIL - ENDFILE OUTPUT TAPE.  OPERATION CARD.  CAUSES ONE END-OF-FILE
         FORMAT (A6)
         TO BE WRITTEN ON THE BCD OUTPUT TAPE (NTOUT).
         USED IN ALL PROGRAMS WHENEVER DESIRED.
           1- 6     ENDFIL
           7-72                     (IGNORED)

ENDOBS - SIGNALS THAT FOLLOWING REFLECTIONS ARE SYSTEMATICALLY ABSENT.
         FORMAT (A6)
           1- 6     ENDOBS
           7-72                     (IGNORED)

ENDTAP - END OUTPUT TAPE.  OPERATION CARD.  WRITES MESSAGE =END OF
         OUTPUT TAPE= ON TAPE NTOUT.  WRITES 20 END-OF-TAPE MARKS ON
         TAPE NTOUT.  REWINDS TAPE NTOUT.  REDEFINES NTOUT TO NTOUTM
         (IF NTOUT = NTOUTM, ENDTAP CARD IS IGNORED.)
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (A6)
           1- 6     ENDTAP
           7-72                     (IGNORED)

EPSILON - ZONE WEIGHTS CARD
         FORMAT (A6,1X,6F3.0)
           1- 7       EPSILON
           8-10       XXX        EPSILON FOR H00 (BLANK = 1)
          11-13       XXX        0K0
          14-16       XXX        0L0
          17-19       XXX        0KL
          20-22       XXX        H0L
          23-25       XXX        HK0
          26-72                  (IGNORED)
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ESORT  - CALL THE UNITARY STRUCTURE FACTOR SORTING PROGRAM.
         FORMAT (A6,1X,A6,I1,F7.3)
           1- 6       ESORTS
             7        $          BLANK
           8-13                  COMPID, COMPOUND IDENTIFICATION CODE.
            14        X          (BLANK)/(1) FOR (YES)/(NO) LIST THREE-
                                   DIMENSIONAL E VALUES IN ORDER ON TAPE.
          15-21       XXX.XXX    MINIMUM VALUE OF E ON WHICH TO SORT.
          22-72                  (IGNORED)

FC     - SET-UP CARD FOR STRUCTURE FACTOR CALCULATION.
         FORMAT (A6,1X,A6,8X,8I4,F6.0,I4)
           1- 6     FCSSSS
             7      $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-21                 BLANK
          22-25     SSSX       RESCALE CODE.  (1)/(2) FOR USE (OLD)/(NEW)
                                 F RELATIVE SCALE FACTORS.
          26-29     SSSX       FIXAT.  (1)/(2)/(3)  FOR  (NO PARTIAL
                                 CONTRIBUTION)/(PARTIAL CONTRIBUTION)/
                                 (USE PREVIOUS FC AS PARTIAL CONTRIB.)
          30-33     SSSX       HI-FI.  (1)/(2)  FOR  (LO-FI)/(HI-FI) TRIG
                                 AND EXPONENTIAL FUNCTIONS.
          34-37     SSSX       DISPERSION CORRECTION.  (1)/(2)  FOR
                                 (DO NOT APPLY)/(APPLY WHERE NECESSARY)
          38-41     SSSX       USER PATCH. (1)/(2) FOR (BYPASS)/(APPLY)
          42-45     SSSX       (1)/(2) FOR (NORMAL)/(CRIPPLE AUTOMATIC
                                 SCALING OF ATOMS AT SYMMETRY CENTERS FOR
                                 CENTRIC ONLY)
          46-49     SSSX       FC SCALE FACTOR.  (1)/(2)  FOR  (NORMAL)/
                                 (SPECIAL).
          50-53     SSSX       FOR OVERALL T.F. ALWAYS COMPUTES CORRECT.
                                 TO OVERALL B.  (1)/(2) FOR (USE OLD)/
                                 (USE NEW) VALUE FOR B.
                                 FOR INDIVIDUAL T.F. (1)/(2)  FOR
                                 (DO NOT)/(DO) COMPUTE OVERALL B.
          54-59     SXXXX.     SPECIAL FC SCALE FACTOR.  (NUMBER OF
                                 ASYMMETRIC UNITS OR MOLES, IF OTHER
                                 THAN THAT DETERMINED BY LATTICE TYPE.)
          60-63     SSSI       BLANK, ZERO, OR ONE CAUSES PARAMETERS TO
                                 LIST ON BCD OUTPUT TAPE. TWO WILL CAUSE
                                 PARAMETERS AND FC TO LIST.  THREE
                                 SUPRESSES BOTH.  (IT IS BEST TO LIST FC
                                 AT FOURIER OR DIFFERENTIAL SYNTHESIS
                                 TIME BY CODING THE =FOURR= OR =DIFSYN=
                                 CARD TO LIST FC, THEREBY SAVING ABOUT
                                 1/3 OF CALCULATION TIME MOVING TAPES.)
          64-72                  ANY LEGAL PUNCHING DESIRED, OR BLANKS.

FILTER - FILTER CARD. FOR USE WITH SPECTROMETER DATA.
         FORMAT (A6,1X,I2,F10.8)
           1- 6     FILTER
           7- 9     $NN          ID NUMBER OF FILTER-- 1 TO 99     (I3)
          10-19     $.FFFFFFFF   TRANSMITTANCY OF FILTER  (F10.8)
          20-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

FINISH - =ABSOLUTE= TERMINATION CARD (NEVER USE AFTER AN =IGNORE= CARD
         OR IN THE MIDDLE OF A RUN).
         FORMAT (A6)
           1- 6     FINISH
           7-72                 (IGNORED)
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FORMAT - DEFINES BCD REFLECTION DATA.
         FORMAT (12A6)
           1- 6     FORMAT
           7-72                THE FORMAT OF THE BCD REFLECTION DATA, AS
                                 IF A STANDARD FORTRAN CARD (E.G.-
                                 =USUAL= FORMAT IS (7X,A6,4I4,F10.2))

FORMFN - ATOMIC FORM FACTORS FOR NEUTRONS.
         FORMAT (A6,1X,A6,F8.3,8A6,A1)
           1- 6     FORMFN
             7      $            BLANK
           8-13                  ATOM TYPE NAME (SEE COLS. 8-13 OF FORMFX).
          14-21     $FFF.FFF     COHERENT ATOMIC SCATTERING FACTOR (F8.3)
          22-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS

FORMFX - ATOMIC FORM FACTORS FOR X-RAYS.
         FORMAT (A6,1X,A6,F7.5,F8.3,6A6,A4)
           1- 6     FORMFX
             7      $            BLANK
           8-13                  UP TO SIX CHARACTERS, THE LAST OF WHICH
                                   MUST NOT BE A DIGIT, TO IDENTIFY THE
                                   ATOM-TYPE. BLANKS ARE IGNORED.
          14-20     $.XXXXX      SIN(THETA)/LAMBDA  (F7.5)
          21-28     $FFF.FFF     ATOMIC SCATTERING FACTOR  (F8.3)
             29     $            BLANK
          30-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

FOUREF - FOURIER REFINING PROGRAM CALLING CARD
         FORMAT (A6,1XA6,1X3I1,2I2)
           1- 6       FOUREF
             7        $          BLANK
           8-13                  COMPID - COMPOUND IDENTIFICATION CODE
             14                  BLANK
         (15-17)                 SUMMATION ORDER
             15         X        (1)/(2)/(3) IF H IS (FIRST)/(SECOND)/
                                   (THIRD) SUM INDEX
             16         X        (1)/(2)/(3) FOR K SUM INDEX
             17         X        (1)/(2)/(3) FOR SUM INDEX
                                   IT IS IMPORTANT FOR SPEED THAT (3) VARY
                                   LEAST RAPIDLY AND (1) MOST RAPIDLY.
          18-19         $X       (0 OR BLANK)/(1)/(2) FOR (SET ALL SCALES
                                   =1.0)/(USE SCALE FACTORS FROM TAPE)/(USE
                                   RESCALE FACTORS FROM TAPE)
          20-21         $X       (0 OR BLANK)/(1) FOR (READ NO ATOM PARAM.
                                   FROM TAPE)/(READ ATOM PARAM. FROM TAPE)
                                   WITH CODE=1 SOME OR ALL PARAMETERS MAY
                                   BE SUPERCEDED BY CARDS
          22-72                  (IGNORED)

FOURR  - CALLING CARD FOR FOURIER PROGRAM (LINK 4000)
         FORMAT (A6,1X,A6,3I3,F9.5,F4.2)
           1- 6     FOURR$
             7      $            BLANK
           8-13                  SIX COLUMNS OF HOLLERITH PUNCHING TO
                                   IDENTIFY COMPOUND,  COMPID.
          14-19                  BLANK
          20-22     $$X          (BLANK)/(1)  FOR (NO)/(YES) LIST FC.
          23-25     $XX          CALCULATION TYPE  (I3)   REFER TO
                                   SECT 1.40 FOR DETAILS.
                                   1=USER FUNCTION BY MEANS OF  PATPAT.
                                   2=PATTERSON  (A=FO**2)
                                   3=VECTOR MAP (SHARPENED,ORIGIN REMOVED
                                      PATTERSON).
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FOURR  - CALLING CARD FOR FOURIER PROGRAM (CONTINUED)
                                  4=FO FOURIER BY REJECTION TEST WITH
                                     (FO*RR-FC) WITH FMIN/2 FOR LESS-THANS
                                  5=FC FOURIER, FC CORRECTED FOR DISPERS.
                                     RATIO AND CRITERIA (4) USED.
                                  6=FO FOURIER, PHASE ANGLES DETERMINED
                                     FROM UNITARY STRUCTURE FACTORS.
                                  7=FC FOURIER, USES ALL REFLECTIONS.
                                  8=DELTA F, BY REJECTION TEST (FO*RR-FC)
                                     FOR OBSERVED, (FO-FC) FOR LESS-THANS.
                                  9=DELTA F, WITH LEAST SQUARES WEIGHT
                                     APPLIED TO DELTA F   W*(FO-FC).
                                     TEST LESS-THANS BY  (FMIN-FC).
                                 10=DELTA F, FO CORRECTED FOR DISPERSION
                                     RATIO AND CRITERIA (8) USED.
                                 11=DELTA F, OBSERVED REFLECTIONS ONLY.
                                 12=DELTA F, VARIABLE WEIGHTING W=(FC/FO)
                                     OR 1.0 WHICHEVER IS LESS AND REJECT
                                     LESS-THANS CALCULATING LESS-THAN.
                                 13=E MAP. PHASES FROM STATISTICS.
                                 14=E MAP. PHASES FROM FC.
          26-28     $$X         (BLANK)/(1)  USE (OLD)/(NEW) F RELATIVE
                                  SCALE FACTORS.
          29-37     XXX.XXXXX  ELECTRON DENSITY SCALE FACTOR.  BLANKS
                                  GIVES OUTPUT AS 10*(2/V)*SIGMA F. FACTOR
                                  PUNCHED REPLACES  10.
          38-41     X.XX       REJECTION RATIO USED BY CRITERIA TESTS OF
                                  (4) AND (8). IF LEFT BLANK RR SET EQUAL
                                  TO ZERO TO INCLUDE ALL REFLECTIONS.
          42-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

FUNCTN - FUNCTION SPECIFICTION CARD FOR ORFFE (SEE PAGES 2.61-BXX FOR DETAILS
         FORMAT(A6,1X,21I3,I2)
           1- 6      FUNCTN
             7       $          BLANK
           8-10      XXX        FUNCTION NUMBER
          11-70                 FUNCTION SPECIFICATION INTEGERS IN THREE
                                  COLUMN FIELDS  (20 FIELDS)
          74-72      $X         (BLANK)/(1) FOR (FUNCTION SPECIFICATION
                                  COMPLETE)/(CONTINUATION CARD FOLLOWS)

FUNCTN - FUNCTION CONTINUATION CARD - UP TO 10 ALLOWED PER FUNCTION
         FORMAT(A6,1X,21I3,I2)
           1- 6      FUNCTN
             7       $          BLANK
           8-70                 FUNCTION SPECIFICATION INTEGERS IN THREE
                                  COLUMN FIELDS  (21 FIELDS)
          71-72      $X         (BLANK)/(1) FOR (FUNCTION SPECIFICATION
                                  COMPLETE)/(ANOTHER CONTINUATION CARD
                                  FOLLOWS)

FZERO  - PUT IN ANY VALUE OF F(000) DESIRED.
         FORMAT (A6,7X,F9.5)
           1- 6     FZERO$
           7-13                 BLANKS
          14-22     XXX.XXXXX  VALUE OF F(000) DESIRED.
          23-72     ANY DESIRED LEGAL PUNCHING, OR BLANKS.

GRAFTL - PUTS A TITLE ON =DELSIG= GRAPHS.
         FORMAT (12A6)
           1- 6       GRAFTL
           7-72                 ANY DESIRED TITLE FOR GRAPH.

GRID   - FOURIER GRID CARD.
         FORMAT (A6,1X,A6,3I4)
           1- 6     GRID$$
             7      $          BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-17     $XXX       NUMBER OF GRID INTERVALS ALONG THE X
                                  AXIAL DIRECTION.
          18-21     $XXX       GRID INTERVALS ALONG Y AXIAL DIRECTION
          22-25     $XXX       GRID INTERVALS ALONG Z AXIAL DIRECTION
          26-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
HLIN    - GENERATE A LINEARLY-BONDED =HYDROGEN= ATOM.
          FORMAT (A6,2(1X,A6),8X,F6.3,1X,A6)
            1- 6        HLIN$$
              7         $          BLANK
            8-13                   ATOM ID OF FIRST DEFINING ATOM
             14         $          BLANK
           15-20                   ATOM ID OF SECOND DEFINING ATOM TO WHICH
                                     =HYDROGEN= IS TO BE =BONDED=.
           21-27                   BLANKS
           28-34        $XX.XXX    DISTANCE OF =HYDROGEN= FROM SECOND DEFIN-
                                     ING ATOM (MAY BE NEGATIVE, E.G.- FOR THE
                                     HYDROGEN-BOND CASE).  ZERO OR BLANK WILL
                                     USE 1.075 ANGSTROM UNITS.
             35         $          BLANK
           36-41                   ATOM ID FOR GENERATED =HYDROGEN= ATOMS.
                                     BLANK GIVES SERIALIZED IDENTIFICATION.
           42-72                   BLANKS.

HTERM   - GENERATE THREE TERMINAL TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS.
          FORMAT (A6,3(1X,A6),1X,F6.3,3(1X,A6))
            1- 6        HTERM$
              7         $          BLANK
            8-13                   ATOM ID OF FIRST ATOM DEFINING TETRAHEDRAL
                                     CHAIN FOR ORIENTATION OF =HYDROGEN=S.
             14         $          BLANK
           15-20                   ATOM ID OF SECOND ATOM DEFINING TETRAHED-
                                     RAL CHAIN FOR ORIENTATION OF =HYDROGEN=S
             21         $          BLANK
           22-27                   ATOM ID OF THIRD ATOM DEFINING TETRAHED-
                                     RAL CHAIN, AND TO WHICH THE =HYDROGENS=
                                     ARE ATTACHED.  THE FIRST =HYDROGEN= IS
                                     GENERATED FROM THE SAME VECTOR SENSE AS
                                     ATOMS 1 (COL 8-13) - 2 (COL 15-20).
                                     CHAIN, AND TO WHICH THE =HYDROGENS= ARE
                                     ATTACHED. THE FIRST =HYDROGEN= GENERATED
                                     FROM THE SAME VECTOR SENSE AS ATOMS
                                     1 (COL 8-13) AND 2 (COL 15-20).
             28         $          BLANK
           29-34        XX.XXX     BONDING DISTANCE. ZERO OR BLANK WILL USE
                                     1.075 ANGSTROM UNITS.
             35         $          BLANK
           36-41                   ATOM ID FOR FIRST GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
             42         $          BLANK
           43-48                   ATOM ID FOR SECOND GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
             49         $          BLANK
           50-55                   ATOM ID FOR THIRD GENERATED =HYDROGEN=
                                     ATOM.  BLANK GIVES SERIALIZED IDENT.
           56-72                   BLANKS.

HTET    - GENERATE TWO TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS.
          FORMAT (A6,3(1X,A6),1X,F6.3,2(1X,A6))
            1- 6        HTET$$
              7         $          BLANK
            8-13                   ATOM ID OF FIRST ATOM DEFINING BOND
             14         $          BLANK
            8-13                   ATOM ID IF TERMINAL ATOM TO WHICH THE
                                     THREE =HYDROGEN= ATOMS ARE BONDED.
           15-20                   ATOM ID OF SECOND ATOM DEFINING BOND, AND
                                     ATOM TO WHICH =HYDROGENS= ARE ATTACHED.
             21         $          BLANK
           22-27                   ATOM ID OF THIRD ATOM DEFINING BOND.
             28         $          BLANK
```

```
HTET    - GENERATE TWO TETRAHEDRALLY-BONDED =HYDROGEN= ATOMS. (CONTINUED)
           29-34        XX.XXX    BONDING DISTANCE. ZERO OR BLANK WILL USE
                                    1.075 ANGSTROM UNITS.
              35        $         BLANK
           36-41                  ATOM ID FOR FIRST GENERATED =HYDROGEN=
                                    ATOM.  BLANK GIVES SERIALIZED IDENT.
              42        $         BLANK
           43-48                  ATOM ID FOR SECOND GENERATED =HYDROGEN=
                                    ATOM.  BLANK GIVES SERIALIZED IDENT.
           49-72                  BLANKS.

HTRIG   - GENERATE A TRIGONALLY-BONDED =HYDROGEN= ATOM.
          FORMAT (A6,3(1X,A6),1X,F6.3,1X,A6)
            1- 6        HTRIG$
              7         $         BLANK
            8-13                  ATOM ID OF FIRST ATOM DEFINING BOND
             14         $         BLANK
           15-20                  ATOM ID OF SECOND ATOM DEFINING BOND, AND
                                    ATOM TO WHICH =HYDROGEN= IS ATTACHED.
             21         $         BLANK
           22-27                  ATOM ID OF THIRD ATOM DEFINING BOND.
             28         $         BLANK
           29-34        XX.XXX    BONDING DISTANCE. ZERO OR BLANK WILL USE
                                    1.075 ANGSTROM UNIT.
              35        $         BLANK
           36-41                  ATOM ID FOR GENERATED =HYDROGEN= ATOMS.
                                    BLANK GIVES SERIALIZED IDENTIFICATION.
           42-72                  BLANKS.

IGNORE  - IGNORE INPUT.  OPERATION CARD.  CAUSES FOLLOWING CARD TO BE
          IGNORED (SKIPPED UNCONDITIONALLY) AND SUBSEQUENT CARDS TO BE
          SKIPPED UNTIL A  *DATA  CARD IS REACHED.  (USED PRINCIPALLY
          JUST BEFORE A  *DATA  CARD).
          USED IN ALL PROGRAMS WHENEVER DESIRED.
          FORMAT (A6)
            1- 6      IGNORE
            7-72                  (IGNORED)

LABEL   - TAPE LABELING CARD. USED TO IDENTIFY BINARY TAPE.
          FORMAT (12A6)
            1- 6        LABEL$
            7-72      ALPHANUMERIC INFORMATION TO BE USED AS TAPE LABEL

LATICE  - CENTRICITY IDENTIFICATION CARD.
          FORMAT (A6,2X,A1,2X,A1)
            1- 6      LATICE    =LATTICE= SPELLING ALSO ACCEPTED
            7- 9      $$X       C = CENTRIC CELL,  A = ACENTRIC CELL.
           10-12      $$X       DESIGNATION OF LATTICE TYPE
                                  P,A,B,C,R,I,F   ONE OF THE
                                  FOREGOING MUST BE PUNCHED.
           13-72                ANY LEGAL PUNCHING DESIRED OR BLANKS.

LAYOUT  - DESCRIPTION OF MAP FOR FOURIER, PATTERSON, ETC..
          FORMAT (A6,1X,A6,9I4,1X,3I1,I4,I2)
            1- 6      LAYOUT        (A6)
              7           $       BLANK
            8-13                  COMPID, COMPOUND IDENTIFICATION CODE.

                      (THE NEXT NINE FIELDS ARE PUNCHED  (I4).)

           14-17      $XXX        NUMBER OF POINTS CALCULATED IN X DIRECTION
           18-21      $XXX        ORIGIN VALUE OF X (IN GRID COORDINATES).
           22-25      $XXX        INCREMENT ALONG X (IN GRID COORDINATES).
           26-29      $XXX        NUMBER OF POINTS CALCULATED IN Y DIRECTION
```

```
LAYOUT - DESCRIPTION OF MAP FOR FOURIER. (CONTINUED)
         30-33     $XXX        ORIGIN VALUE OF Y (IN GRID COORDINATES).
         34-37     $XXX        INCREMENT ALONG Y (IN GRID COORDINATES).
         38-41     $XXX        NUMBER OF POINTS CALCULATED IN Z DIRECTION
         42-45     $XXX        ORIGIN VALUE OF Z (IN GRID COORDINATES).
         46-49     $XXX        INCREMENT ALONG Z (IN GRID COORDINATES).
            50           $     BLANK
            51           X     SCANNING INDEX FOR X DIRECTION.  (I1)
            52           X     SCANNING INDEX FOR Y DIRECTION.  (I1)
            53           X     SCANNING INDEX FOR Z DIRECTION.  (I1)

                THE SCANNING INDEX FOR A GIVEN DIRECTION IS 1 IF THAT
         COORDINATE GOES FROM PAGE TO PAGE IN THE MAP (FIRST SUM), 2 IF
         IT IS DOWN THE PAGE (SECOND SUM), AND 3 IF IT IS ACROSS THE
         TOP OF THE PAGE (THIRD SUM).

         54-57       $$XX      LINE WIDTH.  (I4)

                LINE WIDTH W IS THE NUMBER OF POINTS ALONG X3 (THE
         THIRD SCANNING DIRECTION) TO APPEAR ON ONE PAGE.  IF THE
         NUMBER OF POINTS ALONG X3 IS GREATER THAN W + 1, W POINTS
         APPEAR ON THE FIRST PAGE AND THE NUMBER OF POINTS REMAINING
         TO BE PRINTED WILL BE DECREASED BY W. AS SOON AS THE NUMBER OF
         POINTS REMAINING ALONG X3 IS EQUAL TO OR LESS THAN W + 1, ALL
         REMAINING POINTS WILL BE PRINTED ON THIS PAGE. THE MAXIMUM
         PERMISSIBLE VALUE FOR W IS 30.
         (FOR LISTING ON A 120-CHAR. PRINTER (IBM 717), MAX. W IS 27.)
                AS AN EXAMPLE, IF THE NUMBER OF POINTS ALONG X3 IS
         21 AND W IS 20, ONE PAGE WILL BE LISTED WITH 21 POINTS PER
         LINE.  IF THERE ARE 61 POINTS ALONG X3 AND W IS 30, 30 POINTS
         WILL APPEAR ON THE FIRST PAGE AND 31 ON THE SECOND.
                IF THIS FIELD IS BLANK, OR W IS OUTSIDE THE RANGE
         10 TO 30, THE PROGRAM WILL COMPUTE AN OPTIMUM VALUE OF W.)

         58-59          $X     SPACE CONTROL INDEX.   (I2)

                THE SPACE CONTROL INDEX MAY BE 1, 2, 3, 4, FOR SINGLE
         DOUBLE, TRIPLE, OR QUADRUPLE SPACING, RESPECTIVELY. (TRIPLE
         OR QUADRUPLE SPACING REQUIRE EXTRA COMPUTING AND PRINTING
         TIME, AS BLANK LINES MUST BE PRINTED.)
         ANY NUMBER OTHER THAN ONE OF THESE WILL CAUSE DOUBLE SPACING.

         60-72          $      BLANK

LINK   - TO MARK BEGINNING OF A LINK.
         FORMAT (A6,I5)
           1- 6       LINK$$
           7-11       XXXXX    LINK NUMBER AS SPECIFIED IN =CALLER= (SEE
                                 APPENDIX V)
         12-72                (IGNORED)

LISTFC - CALLING CARD FOR =LISTFC= PROGRAM (LINK 11000).
         FORMAT (A6,1X,A6,3I1,I4,A1,I3,5I2,2A2,5I2)
           1- 6       LISTFC
             7        $        BLANK
           8-13                COMPID, COMPOUND IDENTIFICATION CODE.
            14        X        (1)/(2)/(3) FOR EACH INDEX DEPENDING UPON
                                 THE SORT., FOR (MINOR SORT INDEX THAT
                                 CHANGES MOST FREQUENTLY)/(INTERMEDIATE
                                 SORT)/(MAJOR SORT CHANGES LEAST IN
                                 FREQUENCY)  FOR H INDEX.
            15        X        SORTING FREQUENCY FOR  K  INDEX.
            16        X        SORTING FREQUENCY FOR  L  INDEX.
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LISTFC - CALLING CARD FOR =LISTFC= PROGRAM (CONTINUED)
          17-20        XXXX      EITHER THE NUMBER OF LINES/PAGE, OR ELSE
                                   THE TOTAL NUMBER OF PAGES TO BE LISTED.
             21        X         (L)/(P) IF COLS 17-20 IS (LINES)/(PAGES).
          22-24        XXX       NUMBER OF COLUMNS/PAGE
          25-26        XX        NUMBER OF BLANK SPACES BETWEEN COLUMNS.
          27-28        XX        NUMBER OF PRINT COLUMNS PER INDEX,
                                   (USUALLY 3)
          29-30        XX        NUMBER OF COLUMNS FOR F-OBSERVED.
          31-32        XX        NUMBER OF COLUMNS FOR F-CALCULATED
          33-34        XX        NUMBER OF COLUMNS FOR PHASE (IN CYCLES).
          35-36        XX        SPECIAL =LESS-THAN= FLAG (E.G.-   * ).
          37-38        XX        SPECIAL =EXTINCT= FLAG (E.G.-   E   ).
          39-40        $X        (BLANK)/(1) FOR (DO)/(DO NOT) PLACE MINUS
                                   SIGN IN FRONT OF THE F-OBSERVED THAT ARE
                                   LESS-THANS (THIS MAY THEN BE CONVERTED
                                   TO A LESS-THAN SIGN WITH PEN-AND-INK).
          41-42        $X        (BLANK)/(1) IF DESIRED TO (NOT PRINT)/
                                   (PRINT) THE PHASE ON FC IN THE CENTRIC
                                   CASE (LEAVE ZERO OR BLANK FOR ACENTRIC).
          43-44        $X        (BLANK)/(1) FOR (SINGLE)/(DOUBLE) SPACE.
          45-46        $X        (BLANK)/(1) FOR (DO NOT)/(DO) RESTORE
                                   PAGES AUTOMATICALLY.
          47-48        $X        (BLANK)/(1) FOR (PRINT)/(SUPRESS) PAGE
                                   TITLING.
          49-72                  BLANK.

LOADER - CALL SYSTEM UPDATE PROGRAM
         FORMAT (A6,1XA6,I4)
           1- 6       LOADER
             7        $         BLANK
           8-13                 NEW TAPE ID (E.G. =7MAY63=)
                                   USUALLY THE DATE OF TAPE PREPARATION.
          14-16       XXX       =LOGICAL= TAPE NUMBER UPON WHICH THE NEW
                                   SYSTEM TAPE IS TO BE GENERATED
          17-72                  (IGNORED)

LOADPC - DIRECTING INSTRUCTION FOR WRITING BINARY PATTERSON TAPE
         FORMAT (A6,1X,2I3,1X,2A6,2I4,F4.1,I4)
           1- 6     LOADPC                    (A6)
             7      $         BLANK
           8-13                 COMPID, COMPOUND IDENTIFICATION CODE.
          14-16        $TT     INPUT TAPE NUMBER (BCD). (I3)
                (BLANK OR 0 IN THIS FIELD CAUSES TAPE 5 TO BE USED)
          17-19        $TT     BINARY PATTERSON TAPE NUMBER. (I3)
             20      $         BLANK
          21-26      CCCCCC    TAPE CONTROL WORD.
                                   =SEARCH=  CAUSES TAPE TO BE SEARCHED FOR
                                      END OF LAST PATTERSON.
                                   =REWIND=  TO BEGIN NEW TAPE.   (A6)
          21-26      CCCCCC    TAPE CONTROL WORD--SEARCH TO CAUSE TAPE TO
                               BE SEARCHED FOR END OF LAST PATTERSON,
                               REWIND TO BEGIN NEW TAPE. (A6)
          27-30        $PPP    VALUE OF MAXIMUM POSITIVE PEAK IN PATTERSON
          31-34        $MMM    MINIMUM VALUE TO BE COUNTED AS SIGNIFICANT
          35-38        $R.R    RADIUS OF ORIGIN PEAK IN GRID UNITS (0 OR
                                   BLANK IMPLIES NO ORIGIN PEAK TO BE
                                   INSERTED)      (F4.1)
          39-42        $VVV    VALUE FOR ORIGIN PEAK. (I4)
          43-72          $     BLANK OR ANY DESIRED PUNCHING
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LSQPL  - CALLING CARD FOR LEAST-SQUARES LINES AND PLANES.
         FORMAT (A6,1X,A6,1X,I1,1X,I3,2(1X,I1))
           1- 6        LSQPL$
             7         $            BLANK
           8-13                     COMPID. COMPOUND IDENTIFICATION CODE.
          14-15        $X           (1)/(2) FOR L.S. (LINE)/(PLANE)  (LORP)
          16-19        $XXX         NUMBER OF ATOM CARDS OF ATOMS TO DEFINE
                                      (OR MAKE-UP) THE L.S. LINE OR PLANE (N1)
          20-21        $X           IGNORED IF = ZERO. IF NON-ZERO INTEGER
                                      CAUSES CALC. OF ANGLES BETWEEN THIS LINE
                                      OR PLANE AND ANY PRECEEDING LINES AND/OR
                                      PLANES CODED NON-ZERO.  (IANGLE)
          22-23        $X           IGNORED IF = ZERO. IF NON-ZERO INTEGER,
                                      CAUSES CALC. OF L.S. LINE OR PLANE WITH
                                      ATOMS PROVIDED AS INPUT PLUS THE ATOMS
                                      RELATED TO THE GIVEN ATOMS BUT GENERATED
                                      THRU THE ORIGIN AS A CENTER OF SYMMETRY.
          24-72                    (IGNORED)

MAP    - PRINT CONTROL CARD.
         FORMAT (A6,1X,3I4)
           1- 6      MAP$$$
             7       $            BLANK
           8-13                     COMPID. COMPOUND IDENTIFICATION CODE.
          14-17        $X           (1)/(2)/(3)  FOR (IGNORE CARD)/(SUPRESS THE
                                      PRINTING OF NUMBERS WITHIN THE RANGE
                                      SPECIFIED)/(WRITE MAP IN BINARY ON =NTAPEE=
                                      AS WELL AS FUNCTION 2)
          18-21        XX           ABSOLUTE UPPER LIMIT TO ESTABLISH PRINT
                                      SUPRESSION
          22-25        XX           ABSOLUTE LOWER LIMIT TO ESTABLISH PRINT
                                      SUPRESSION
          26-72                    (IGNORED)

MAXHKL - LIMITS FOR FOURIER SUMMATION.
         FORMAT (A6,1X,3I4,2F8.4)
           1- 6      MAXHKL
             7       $            BLANK
           8-13                     COMPID. COMPOUND IDENTIFICATION CODE.
          14-17      $XXX         MAXIMUM H TO BE USED    (I4)
          18-21      $XXX         MAXIMUM K TO BE USED
          22-25      $XXX         MAXIMUM L TO BE USED
          26-33      $X.XXXXX     MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                      NO LIMIT)    (F8.4)
          34-41      $X.XXXXX     MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS
                                      NO LIMIT)    (F8.4)
          42-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.

MODIFY - CALLING CARD FOR =MODIFY= PROGRAM.
         FORMAT (A6,1X,A6,3I3,I6,4F5.3,12I2)
           1- 6        MODIFY
             7         $            BLANK
           8-13                     COMPID. COMPOUND IDENTIFICATION CODE.
          14-16        $$X          1=REPLACE SPECIFIED WORD OF REFLECTION
                                      RECORD WITH QUANTITIES FROM CARDS
                                      SUPPLIED AND COPY REST OF TAPE.
                                    2=PLACE SPECIFIED PHASE ON REFLECTION
                                      (CENTROSYMMETRIC ONLY)
                                    3=REPLACE F-RELATIVE BY F-CALCULATED WITH
                                      A SPECIFIED GAUSSIAN ERROR FOR ALL
                                      REFLECTIONS.
                                    4=PLACE PHASE OF FC IN E FOR ALL REFLECT.
                                    5=RESCALE F-RELATIVE FOR ALL REFLECTIONS.
                                    6=TRANSFORM INDICES        (MODE3)
```

```
MODIFY - CALLING CARD FOR =MODIFY= PROGRAM. (CONTINUED)
          17-19        XXX        NUMBER BETWEEN 1-263 TO INDICATE WORD OF
                                    REFLECTION RECORD TO BE CHANGED (BLANK
                                    IF COL 16 GREATER THAN 2)     (MODEI)
          20-22        $$X        (1)/(2) FOR (FLOATING)/(FIXED) POINT DATA
                                    IN COLS 28-37 OF =MODREF= INPUT REFLEC-
                                    TION CARDS (BLANK IF COL 16 IS GREATER
                                    THAN 2)                       (MODEI)
          23-28        XXXXXX     NUMBER OF REFLECTIONS TO LIST (BLANK OR
                                    ZERO = 100)    (ILIST)
          29-33        X.XXX      MEAN RANDOM ERROR EXPRESSED AS A FRACTION
                                    BETWEEN 1 AND 0 (CODE 3 ONLY)  (ERROR)
          34-38        X.XXX      THRESHOLD VALUE OF INTENSITY FOR MANUFAC-
                                    TURED DATA (CODE 3 ONLY)    (FIMIN)
          39-43        X.XXX      MULTIPLICATIVE PARAMETER FOR ESTABLISHING
                                    WEIGHTS (CODE 3 ONLY)    (SLOP)
          44-48        X.XXX      ADDITIVE PARAMETER FOR ESTABLISHING
                                    WEIGHTS (CODE 3 ONLY)     (SEPT)
          49-72        XX         ROW-BY-ROW TRANSFORMATION MATRIX AND
                                    TRANSLATION VECTOR FOR PERMUTING THE
                                    INDICES (CODE 6 ONLY)     (MSYM)

MODREF - CARD TO MODIFY A REFLECTION RECORD.
         FORMAT (15X,3I4,F10.2)
           1- 6        MODREF
             7         $          BLANK
           8-15                   COMPID (OPTIONAL OR BLANK)
          16-19        XXXX       H INDEX
          20-23        XXXX       K INDEX
          24-27        XXXX       L INDEX
          28-37        XXXXXXX.XX QUANTITY TO BE INSERTED IN REFLECTION
                                    TAPE AS SPECIFIED ON =MODIFY= CARD.
          38-72                   (IGNORED)

NOREF  - DO NOT REFINE ON NAMED PARAMETER CARDS.
         FORMAT (A6,1X,A6,11A3)
           1- 6        NOREF$
             7         $          BLANK
           8-13                   ATOM ID (IF THIS FIELD IS LEFT BLANK THIS
                                    CARD ACTS ON ALL ATOMS).
         IF THE FOLLOWING FIELDS ARE ALL LEFT BLANK (OR NOT PUNCHED FROM
         THE FOLLOWING VALID LIST) THIS CARD ACTS ON THE NAMED ATOM.
         WITHIN ANY OF THESE ELEVEN FIELDS THE FOLLOWING SYMBOLS WILL
         HAVE MEANING=
           S     SCATTERING FACTOR
           M     MULTIPLICITY FACTOR
           X,Y,Z,   X,Y,Z ATOMIC PARAMETERS
           B     ISOTROPIC TEMPERATURE FACTOR
           B11,B22,B33,B12,B13,B23  ANISOTROPIC TEMPERATURE FACTORS
           (ALL SIX MUST BE PUNCHED)
          14-16        XXX        (SYMBOL FROM ABOVE LIST)
          17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43
          44-46        XXX        (SYMBOL FROM ABOVE LIST)
          47-72                   (IGNORED)

NOSCAL - CAUSES ALL SCALE FACTOR REFINEMENT TO BE SHUT OFF.
         FORMAT (A6)
           1- 6        NOSCAL     (OR =NOSCALE= IF IT WILL MAKE YOU HAPPY)
           7-72                   (IGNORED)

NOTEMP - CAUSES ALL TEMPERATURE FACTOR REFINEMENT TO BE SHUT OFF.
         FORMAT (A6)
           1- 6        NOTEMP
           7-72                   (IGNORED)
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OPRATR - OPERATOR INSTRUCTION CARD.  OPERATION CARD.  OCCURRANCE OF
         ONE OR MORE  OPRATR  CARDS CAUSES THE CONTENTS TO BE WRITTEN
         ON-LINE AS AN INSTRUCTION TO THE COMPUTER OPERATOR.  (THE
         INSTRUCTIONS ARE ALSO LISTED OFF-LINE LIKE  REMARK  CARD.)
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (12A6)
           1- 6     OPRATR
           7-72     INSTRUCTION TO COMPUTER OPERATOR  (11A6)

ORFLS  - CALLING CARD FOR BUSING-MARTIN-LEVY LEAST-SQUARES PROGRAM.
         FORMAT (A6,1X,A6,1I3, 3F4.3,I3)
           1- 6       ORFLS$
             7        $            BLANK
           8-13                    COMPID - COMPOUND IDENTIFICATION CODE
          14-16       $$X          NUMBER OF CYCLES TO BE CALC.  (NC)
          17-19       $$X          (1)/(2) FOR (ISOTROPIC)/(ANISOTROPIC)(ITF)
                                     PROGRAM CONVERTS IF REQUIRED. AVERAGE
                                     DIAGONAL ELEMENT USED IN ANISOTROPIC
                                     CONVERSION
          20-22       $$X          (BLANK)/(1)/(2) FOR REFINEMENT BASED ON
                                     (F)/(F**2)/(F CORRECTED FOR DISPERSION)
                                     (IFSQ)
          23-25       $$X          (BLANK)/(1) FOR USE (SCALE)/(RESCALE)
                                     FACTORS FROM TAPE     (IRESC)
          26-28       $$X          (BLANK)/(1) FOR (LO-FI)/(HI-FI) TRIG
                                     FUNCTIONS       (IFI)
          29-31       $$X          (BLANK)/(1) FOR (WEIGHTS FROM TAPE)/(ALL
                                     WEIGHTS EQUAL 1.0)      (IW)
          32-34       $$X          (BLANK)/(1)/(2)/(3) FOR (NO CARDS)/(PUNCH
                                     CARDS)/(PUNCH CARDS AND IGNORE NON
                                     POSITIVE DEFINITE TEST)/(SET BACK THE T.F.
                                     WHICH GO NON-POS-DEF)          (IT)
          35-37       $$X          (BLANK)/(1) FOR (DO NOT)/(DO) LIST THE
                                     REFLECT. INFO. DURING LAST CYCLE (ILIST)
          38-40       $$X          BLANK= DO NOT LIST.
                                     1 = LIST THE REFLECT. FOR WHICH WEIGHTED
                                         DELTA-F IS GREATER THAN  RR  (IREJ)
                                     2 = LIST REJECTED REFLECT. AND ALSO THE
                                         CORRELATION MATRIX FOR EACH CYCLE
          41-43       $$X          (BLANK)/(1)/(2) FOR (NO)/(USE)/(USE PREV-
                                     IOUS FC) FIXED ATOM CONTRIB. (IP)
          44-46       $$X          (BLANK)/(1) FOR (X-RAY)/(NEUTRON) (INEU)
          47-50       .XXX         DAMPING OR ENHANCING FACTOR FOR PARAMETER
                                     SHIFTS (BLANK OR 0.0 = 1.0)
          51-54       .XXX         RR TO CONTROL LIST (BLANK = 2.0)
          55-58       .XXX         REJECT FROM CONSIDERATION IN SHIFTS REFLECTIONS
                                   WHOSE WEIGHTED DELTA-F IS LARGER. (BLANK = 10**8
          59-61       $$X          (BLANK)/(1) (NO)/(SPECIAL) SYMMETRY PATCH
                                   REQUIRED.
          62-72                    (IGNORED)


PATSUP - DIRECTING INSTRUCTIONS FOR PATTERSON SUPERPOSITION
         FORMAT (A6,1X,A6,1X,I6,2I3,F9.3,2I4)
           1- 6     PATSUP       (A6)
             7      $            BLANK
           8-13                    COMPID, COMPOUND IDENTIFICATION CODE.
            14      $            BLANK
          15-20     FFFFFF       SUPERPOSITION FUNCTION INDICATOR. (I3)
                                 FUNCTIONS NOW AVAILABLE, $$$SUM, $$$MIN,
                                 $$$MIX, MIN(N) WHERE N = 2,3,...,9 . ANY
                                 OTHER NAME WILL CAUSE A USER-SUPPLIED
                                 SUBROUTINE TO BE CALLED
          21-23        $TT       TAPE NUMBER FOR BINARY PATTERSON TAPE (I3)
          24-26        $TT       TAPE NUMBER FOR BCD SUPERPOSITION OUTPUT. (I3)
                 (0 OR BLANK SIGNIFIES TAPE 6)
          27-35 FFFFFFFFF        OUTPUT SCALE FACTOR (0 OR BLANK MEANS NO
                                 SCALING) (F9.3)
          36-39       $MMM       MINIMUM NON-ZERO SUPERPOSITION FUNCTION
                                 VALUE) (IF ZERO OR BLANK, ALL VALUES ARE
                                 PRINTED.)  (I4)
          40-43       $SSS       MINIMUM VALUE TO BE COUNTED AS SIGNIFICANT
          44-72                  BLANK OR ANY DESIRED PUNCHING
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PAUSE  - STOP COMPUTER. OPERATION CARD. CAUSES COMPUTER TO WRITE ON-LINE
         MESSAGE =PRESS START TO CONTINUE= AND STOPS. USED PRINCIPALLY
         AFTER =OPRATR= CARDS TO WAIT FOR OPERATOR TO CARRY OUT INSTRUCT
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (A6)
           1- 6     PAUSE$
           7-72                    (IGNORED)

PEKPIK - CALLING CARD FOR PEAK SEARCHING PROGRAM(LINK 30600)
         FORMAT(13X2F10.5,4I5,F10.5)
           1- 6     PEKPIK
              7     $               BLANK
           8-13                     COMPID, THE COMPOUND IDENTIFICATION CODE.
          14-23     XXXX.XXXXX      UPPER AND LOWER LIMITS BETWEEN WHICH SEARCH IS T
          24-33     XXXX.XXXXX      BE SUPRESSED (TO AVOID RIPPELS) THIS IS THE
                                    SAME FUNCTION AS THE =MAP= CARD OF =FOURR= SO
                                    THAT IF THESE FEILDS ARE LEFT BLANK VALUES FROM
                                    THE =MAP= CARD WILL BE USED (FROM =NTAPED=)
         34-38      XXXXX           NUMBER OF PEAKS OF HIGHEST DENSITY EXPECTED
                                    TO BE LOCATED IN THE ASSYMETRIC UNIT
          39-43     XXXXX           MAXIMUM NUMBER OF PEAKS TO BE SOUGHT
                                    BLANK OR 0 = 100
          44-48     XXXXX           (BLANK)/(1) - (DO NOT)/(DO)  PUNCH =ATOM= CARDS
                                    FOR PEAKS LOCATED DURING SEARCH.
          49-53     XXXXX           (BLANK)/(1) - (DO NOT)/(DO) SEARCH FOR HOLES AS
                                    WELL AS PEAKS
          54-63     XXXX.XXXXX      DESIRED RESOLUTION IN TERMS OF GRID COORDINATES
                                    SQUARED  (BLANK OR 0 = 3.0)
          64-72                     MUST BE BLANK

PLANE  - DESIGNATES PLANE TO BE TREATED
         FORMAT (A6,1XA4,I2,6F8.4)
           1- 6       PLANE$
              7       $             BLANK
           8-11       A$A$          X$Y$, Y$X$, X$Z$, Z$X$, Y$Z$, OR Z$Y$
                                      TO DESIGNATE THE PLANE DESIRED
          12-13       $X            (0)/(1) TO (SEARCH WHOLE TAPE)/(QUIT WHEN
                                      FIRST NON-ZONE REFLECTION IS FOUND)
          14-21       XXX.XXXX      BEGINNING POINT OF FIRST COORDINATE DIRECT
                                      (IN FRACTIONAL COORDINATES)
          22-29       XXX.XXXX      FINAL POINT OF FIRST COORDINATE DIRECTION
          30-37       XXX.XXXX      INTERVAL IN FIRST DIRECTION
          38-45       XXX.XXXX      BEGINNING POINT OF SECOND COORDINATE
                                      DIRECTION (IN FRACTIONAL COORDINATES)
          46-51       XXX.XXXX      FINAL POINT OF SECOND COORDINATE DIRECTION
          52-59       XXX.XXXX      INTERVAL IN SECOND DIRECTION
          60-72                     (IGNORED)

PRINTR - PRINTER INSTRUCTION CARD.  OPERATION CARD.  OCCURENCE OF ONE
         OR MORE =PRINTR= CARDS CAUSES THE CONTENTS TO BE WRITTEN OFF-
         LINE AS AN INSTRUCTION TO THE PRINTER OPERATOR AND CAUSES THE
         PRINTER TO BE STOPPED.  THE PRINTER WILL ALSO STOP AGAIN,
         INDICATING THE END OF THE JOB AND TO RETURN THE PRINTER TO
         ITS NORMAL CONDITION.
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (12A6)
           1- 6     PRINTR      (A6)
           7-72     INSTRUCTION TO OFF-LINE PRINTER OPERATOR. (11A6)

RADIUS - SPECIFIES SIZE OF PATTERSON SHELL TO BE CALCULATED.
         FORMAT (A6,2X10F6.0)
           1- 6       RADIUS
              7       $             BLANK
           8-13       XXXXX.        STARTING VALUE OF THETA(1) IN DEGREES
                                      (THE EQUATORIAL ANGLE, LONGITUDE)
          14-19       XXXXX.        FINAL VALUE OF THETA(1) IN DEGREES
          20-25       XXXXX.        GRID INTERVAL FOR BOTH LONGITUDE AND
                                      LATITUDE IN DEGREES
          26-31       XXXXX.        FIRST RADIUS (MUST NOT BE ZERO OR BLANK)
          32-37       XXXXX.        SECOND (AND SUBSEQUENT) RADII IF DESIRED
                                      (FIRST BLANK OR ZERO MARKS END)
          38-43       XXXXX.        THIRD RADIUS
          44-49       XXXXX.        FOURTH RADIUS
          50-55       XXXXX.        FIFTH RADIUS
          56-61       XXXXX.        SIXTH RADIUS
          62-67       XXXXX.        SEVENTH RADIUS
          68-72       $$$$$         BLANKS
```

```
REF     - REFINE ON NAMED PARAMETER CARDS.
          FORMAT (A6,1X,A6,11A3)
            1- 6        REF$$$
                7       $           BLANK
            8-13                    ATOM ID (IF THIS FIELD IS LEFT BLANK THIS
                                      CARD ACTS ON ALL ATOMS).
          IF THE FOLLOWING FIELDS ARE ALL LEFT BLANK (OR NOT PUNCHED FROM
          THE FOLLOWING VALID LIST) THIS CARD ACTS ON THE NAMED ATOM.
          WITHIN ANY OF THESE ELEVEN FIELDS THE FOLLOWING SYMBOLS WILL
          HAVE MEANING=
            S     SCATTERING FACTOR
            M     MULTIPLICITY FACTOR
            X,Y,Z,   X,Y,Z ATOMIC PARAMETERS
            B     ISOTROPIC TEMPERATURE FACTOR
            B11,B22,B33,B12,B13,B23  ANISOTROPIC TEMPERATURE FACTORS
                (ALL SIX MUST BE PUNCHED)
           14-16        XXX         (SYMBOL FROM ABOVE LIST)
           17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43
           44-46        XXX         (SYMBOL FROM ABOVE LIST)
           47-72                    (IGNORED)

REFLECTION CARD - FOR INPUT INTENSITY DATA FROM FILMS OR COUNTER.
          FORMAT (A6,1X,A6,I2,3I4,F10.2,F10.4)
            1- 6      $$$$$$        BLANKS  (A6)
                7      $            BLANK
            8-13                    COMPOUND IDENTIFICATION, OPTIONAL OR BLANK
           14-15     $X            LESS-THAN INDICATOR--   1, OR 9 MEANS THAT
                                      REFLECTION OBSERVED, ANY OTHER NUMBER
                                      MEANS REFLECTION WAS LESS-THAN MINIMUM
                                      OBSERVABLE. A BLANK OR ZERO COMPARES
                                      PUNCHED INTENSITY WITH MINIMUM OBSERVED
                                      INTENSITY.   (I2).
           16-19      $XXX          H INDEX  (I4)
           20-23      $XXX          K INDEX  (I4)
           24-27      $XXX          L INDEX  (I4)
           28-37      $XXXXXX.XX     INTENSITY/FREL/FREL**2   (F10.2)
                                      OR PEAK DEKACOUNTS FOR SPECTROMETER.
           38-47      XXXXX.XXXX SIGMA. STANDARD DEVIATION OF MEASUREMENT
                                      (F10.4.  (OPTIONAL OR BLANK)
           48-72      ANY LEGAL PUNCHING DESIRED OR BLANKS (FOR FILM ONLY).
          FOLLOWING FOR SPECTROMETER DATA ONLY- FORMAT FOR ENTIRE CARD
          FORMAT (A6,1X,A6,I2,3I4,F10.2,F10.4,I3,F6.1,F10.2,I3,F6.1)
           48-50      XXX           PEAK FILTER CODE (I3)
           51-56      XXXX.X        PEAK SCAN TIME (DECISECONDS). (F6.1)
           57-66      XXXXXXX.XX BACKGROUND DECACOUNTS.  (F10.2)
           67-69      XXX           BACKGROUND FILTER CODE (I3).
           70-75      XXXX.X        BACKGROUND SCAN TIME (DECISECONDS).
                                      MAY NOT BE LESS THAN 0.1.

REFLECTION CARD - MARK SENSE CARD FOR COUNTER DATA (650 CARD FORMAT).
          FORMAT (A6,2A1,A5,A4,A1,A5,A4,3A3)
            1- 6      $$$$$$        BLANK.
               11      X            MEASUREMENT TYPE (A1)
               12      X            PEAK FILTER CODE (A1)
           13-17      XXXXX         PEAK DEKACOUNTS (A5)
           18-21      XXXX          PEAK SCAN TIME (DECISECONDS) (A4)
               22      X            BACKGROUND FILTER CODE (A1)
           23-27      XXXXX         BACKGROUND DEKACOUNTS (A5)
           28-31      XXXX          BACKGROUND SCAN TIME (DECISECONDS). MUST
                                      NOT BE LESS THAN ONE SECOND. (A4)
           72-74      XXX           H INDEX (A3)
           75-77      XXX           K INDEX (A3)
           78-80      XXX           L INDEX (A3)
           NOTE - ALL FIELDS ARE READ ALPHANUMERIC, THEN CONSIDERED AS
                    DECIMAL INTEGERS WITH LEADING ZEROS REQUIRED. SIGNS
                    PUNCHED OVER UNITS POSITION.
```

```
REFIN  - INSTRUCTION CARD FOR UNUSUAL REFLECTION INPUT.
         FORMAT (A6,I3,2I6,3I3,14(1X,A2))
           1- 6     REFIN$
           7- 9     $$X          (1)/(2)/(3) FOR (BIN TAPE)/(BCD TAPE)/
                                   (BCD CARD)
          10-15     XXXXXX       NUMBER OF REFLECTIONS TO SKIP BEFORE
                                   PROCESSING FIRST REFLECTION RECORD
          16-21     XXXXXX       MAXIMUM NUMBER OF REFLECTIONS TO PROCESS
                                   USING INFORMATION FROM THE LAST
                                 PRECEEDING =SCALE= CARD
          22-24     XXX          VALUE OF H FOR LAST REFLECTION TO BE
                                   PROCESSED USING INFORMATION FROM LAST
                                   PRECEEDING =SCALE= CARD
          25-27     XXX          VALUE OF K FOR LAST REFLECTION
          28-30     XXX          VALUE OF L FOR LAST REFLECTION

                    NOTE - THERE ARE TWO WAYS TO TERMINATE USE OF INFOR-
                    MATION FROM THE PRECEEDING =SCALE= CARD- THE NUMBER
                    OF REFLECTIONS OR THE VALUES OF H, K, L FOR THE LAST
                    REFLECTION. EITHER MAY BE USED OR BOTH. IF BOTH ARE
                    SPECIFIED THE FIRST TO BE SATISFIED WILL TERMINATE
                    TREATMENT OF THAT REFLECTION  GROUP.

          31-72     $XX            FOURTEEN FIELDS FOR SPECIFICATIONS OF
                                   REFLECTION DATA

                    THIS SERVES TO SPECIFY THE ORDER AND MODE (WHETHER
                    FIXED OR FLOATING) OF THE ITEMS TO BE READ AS REFLEC-
                    TION DATA. IT ALSO INDICATES WHICH WORDS OF A RECORD
                    ARE TO BE IGNORED. TREAT EACH FIELD AS REPRESENTING
                    FROM 1 TO 9 WORDS IN A REFLECTION RECORD. IF A WORD
                    OR GROUP OF WORDS IS TO BE SKIPPED, PUNCH =XB= WHERE
                    X IS AN INTEGER FROM 1 TO 9 DEPENDING ON HOW MANY
                    CONSECUTIVE WORDS ARE TO BE SKIPPED. IF X IS ZERO ONE
                    WORD WILL BE SKIPPED.

                    IN FIELDS CORRESPONDING TO USEFUL INFORMATION PUNCH-
                      FH OR IH FOR FLOATING OR FIXED H
                      FK OR IK FOR FLOATING OR FIXED K
                      FL OR IL FOR FLOATING OR FIXED L
                      FR OR IR FOR FLOAT. OR FIXED FUNCTION OF INTENSITY
                      FW OR IW FOR FLOATING OR FIXED WEIGHT
                      FO OR IO FOR FLOAT. OR FIXED LESS-THAN INDICATOR
                      FI OR II FOR FLOAT. OR FIXED LEVEL INDICATOR
                    THESE FIELDS MUST BE PUNCHED IN THE SAME ORDER AS
                    THEY APPEAR IN YOUR REFLECTION DATA RECORDS. A BLANK
                    IN ANY OF THESE FIELDS CAUSES IMMEDIATE TERMINATION
                    OF READING THIS CARD.

REMARK - REMARK CARD.  OPERATION CARD.  A REMARK CARD IS USED TO INSERT
         A REMARK ONTO THE BCD OUTPUT TAPE AT ANY TIME FOR INCLUSION ON
         THE OFF/LINE LISTING.
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (12A6)
           1- 6     REMARK       (A6)
           7-72     ALPHANUMERIC INFORMATION FOR REMARK  (11A6)

RLIST - CALLING CARD FOR RLIST PROGRAM(LINK 12200)
         FORMAT (7XAL,2XA1,I3,2F3.3)
           1 - 6    RLIST$
             7      $            BLANK
           8 - 13                COMPID - COMPOUND IDENTIFICATION CODE
           14 - 15  $            BLANK
           16       X            (H)/(K)/(L)/(A) FOR LIST LEVEL BY LEVELS
                                 OF H, K, L, OR A = ALL LEVELS.
           17-19    $$X          (0 OR BLANK)/(1)/(2)/ FOR (USE SCALE
                                 FACTORS)/(USE RESCALE FACTORS)/(SET SCALES
                                 =1).SCALES WILL BE SUPERCEEDED BY ANY
                                 SCALE CARDS WHICH MAY BE SUPPLIED.
           20-24    .XXX         EQUAL DIVISIONS OF SIN THETA /LAMBDA FOR
                                 GROUPING REFLECTIONS. BLANK OR ZERO = 0.09
                                 PER ANGSTROM.
           25-28    .XXX         FRACTION OF TOTAL REFLECTIONS TO BE
                                 INCLUDED IN APPROXIMATELY EQUAL GROUPS OF
                                 INCREASING SIN THETA /LAMBDA (BLANK OR
                                 ZERO , OR LESS THAN 0.01) = 0.1.
           29-72                 ANY LEGAL PUNCHING DESIRED OR BLANKS
```

```
RPLANE - CALLING CARD FOR PROJECTION OF MOLECULE ON PLANE
         FORMAT (A6,1XA6,2I2)
           1- 6        RPLANE
             7         $          BLANK
           8-13                   COMPID - COMPOUND IDENTIFICATION CODE
          14-15        $X         (0)/(1)/(2) FOR SCALES BY (1.0)/(SCALE)/
                                    (RESCALE) FACTOR
          16-17        $X         (0)/(1) FOR (DO NOT)/(DO) READ THE ATOMS
                                    FROM TAPE. SOME OR ALL MAY BE SUPERCEDED
                                    BY =ATOM= CARDS.
          18-72                   (IGNORED)

SAVE   - SAVE CARD.  REWIND AND UNLOAD (7090,7094) FUNCTION CARD.  THIS CARD
         IS USED TO PREVENT THE LOSS OF A NEWLEY GENERATED TAPE.  IT CAUSES
         THE SPECIFIED LOGICAL TAPE TO BE MECHANICALLY REMOVED FROM THE
         COMPUTOR.
         FORMAT (A6,12I3)
           1- 6      SAVE$$
           7- 9
          10-12
          ....
          40-42
                     NUMBERS OF THE LOGICAL TAPES TO BE UNLOADED.  THE
                     FIRST BLANK FEILD TERMINATES THE SCAN OF THE CARD.

SCALE  - SCALE CARD FOR INTENSITY DATA.
         FORMAT (A6,F10.4,I4,F10.4,I2,5F5.3)
           1- 6      SCALE$
           7-16      $XXXX.XXXX SCALE FACTOR TO APPLY TO INPUT INTENSITY,
                                FREL, OR FREL**2    (F10.4)
          17-20        $$XX       GROUP IDENTIFICATION  (ONE NUMBER PER
                                    GROUP FROM 01 TO MAX OF 64).    (I4)
          21-30      $XXXX.XXXX MINIMUM OBSERVED INTENSITY  (F10.4)
          31-32      $W         WEIGHT ROUTINE SWITCH  (1)/(2)/(3)
                                  FOR (ALL WEIGHTS=1.0)/(APPLY U. OF W.
                                  WEIGHTING SCHEME)/(APPLY USER SUPPLIED
                                  WEIGHTING SCHEME).    (I2)
                                  U.W. SCHEME IS  (WEIGHT = Q1/MAX1F
                                    (SIGMA,Q2*FREL+Q3,Q4*FRELM+Q5)
                       (REFER TO SECTION 1.100 FOR EXPLANATION OF NEXT
                         FIVE FIELDS, F5.3)
          33-37        X.XXX     Q1
          38-42        X.XXX     Q2
          43-47        X.XXX     Q3
          48-52        X.XXX     Q4
          53-57        X.XXX     Q5
          58-72        ANY LEGAL PUNCHING DESIRED, OR BLANKS.

SCALE  - SCALE CARD FOR F RELATIVE DATA.
         FORMAT (A6,F10.4,I4)
           1- 6      SCALE$
           7-16      $XXXX.XXXX SCALE FACTOR TO APPLY TO F REL (F10.4)
          17-20      $$XX       GROUP IDENTIFICATION (1-64)    (I4)
                                  A GROUP IDENTITY OF ZERO WILL APPLY
                                  OVERALL F-RELATIVE SCALE TO STORED
                                  VALUES OF SCALE FACTORS. SCALE CARDS
                                  LOADED AFTER GROUP=ZERO WILL NOT BE
                                  AFFECTED.
          21-72      ANY LEGAL PUNCHING DESIRED, OR BLANKS.

SHLPAT - CALLING CARD FOR SHELL PATTERSON PROGRAM
         FORMAT (A6,2XA6,1X3I1,2I2,F10.5)
           1- 6        SHLPAT
             7         $          BLANK
           8-13                   COMPID - COMPOUND IDENTIFICATION CODE
             14        $          BLANK
       (15-17)                    SUMMATION ORDER
             15        X          (1)/(2)/(3) IF H IS (FIRST)/(SECOND)/
                                    (THIRD) SUMMATION INDEX
             16        X          (1)/(2)/(3) FOR K SUMMATION INDEX
             17        X          (1)/(2)/(3) FOR L SUMMATION INDEX
                                    IT IS VERY IMPORTANT WHERE SPEED IS A
                                    CONSIDERATION THAT THE INDEX DESIGNATED
                                    (3) VARY LEAST RAPIDLY AND THE INDEX
                                    MARKED (1) VARY MOST FREQUENTLY.
```

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SHLPAT - CALLING CARD FOR SHELL PATTERSON PROGRAM (CONTINUED)
          18-19        $X          (0)/(1)/(2) FOR (PATTERSON F**2.0,SHARP.
                                     PATTERSON E**2)/(SHARP. PATTERSON WITH
                                     ORIGIN REMOVED (E**2)-I) AS COEFFICIENTS
          20-21        $X          (0)/(1)/(2) FOR SCALE OF (1.0)0(SCALE)/
                                     (RESCALE). RELEVANT ONLY FOR F**2.
          22-31        XXXX.XXXXX    SCALING OF RESULTS
          32-72                    (IGNORED)

STARTT - CARD TO START CONTINUATION REFLECTION TAPE.
         USED IF THE BCD TAPE TO DATA REDUCTION MUST BE SPLIT.
         FORMAT (A6)
           1- 6     STARTT
             7      $           BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

SYMTRY - SYMMETRY OPERATION CARD.
         THE SYMMETRY OF THE SPACE GROUP IS INDICATED BY SUPPLYING THE
         SET OF GENERAL EQUIVALENT POSITIONS. EACH EQUIVALENT POSITION
         IS SPECIFIED ON A SEPARATE SYMTRY CARD.
                  A SIMPLE RULE IS THAT ANY GENERAL EQUIVALENT POSITION
         IN THE INTERNATIONAL TABLES MAY BE WRITTEN VERBATIM WITH THE
         FOLLOWING CONVENTIONS, (1) MINUS SIGNS PRECEDE THE NEGATIVE
         QUANTITY, E.G. -X FOR X-BAR,  (2) FRACTIONS ARE WRITTEN WITH
         THE SLASH, E.G. 1/2 FOR ONE-HALF,  (3) BLANKS ARE IGNORED.
         NOTE-  1/2-X  OR  -X+1/2  ARE BOTH ACCEPTABLE FORMATS.
                  AS AN EXAMPLE SPACE GROUP C2/M COULD HAVE THE
         FOLLOWING FOUR CARDS.
         SYMTRY     X,     Y,     Z
         SYMTRY     X + 1/2,     -Y + 1/2,     Z
         SYMTRY     X + 1/2,     Y + 1/2,     Z
         SYMTRY     X,     -Y,     Z
         FORMAT (12A6)
         1 - 6      SYMTRY
         7 - 72     GENERAL EQUIVALENT POSITION

TAPES  - TAPE ASSIGNMENT CARD. OPERATION CARD. A BLANK FIELD OR ZEROS IN
         COLS 7-42 IMPLIES NO CHANGE IN ASSIGNMENT FOR THE TAPE WHICH IS
         DESIGNATED BY THAT FIELD.
         USED IN ALL PROGRAMS WHENEVER DESIRED.
         FORMAT (A6,12I3)
           1- 6     TAPES$
                    NEW LOGICAL TAPE NUMBER FOR ----
           7- 9     $XX         NTIN     BCD INPUT TAPE (FROM CARD READER)
          10-12     $XX         NTOUT    BCD OUTPUT TAPE (TO PRINTER)
          13-15     $XX         NTAPEA   BINARY DATA TAPE (REFLECTIONS)
          16-18     $XX         NTAPEB   BINARY DATA TAPE (STRUCT.FACTORS)
          19-21     $XX         NTAPEC   BCD CARD OUTPUT (TO PUNCH)
          22-24     $XX         NTAPED   SPECIAL BCD OUTPUT (OPTIONAL PRNT)
          25-27     $XX         NTAPEE   SPECIAL UTILITY OUTPUT TAPE
          28-30     $XX         NTAPEF   SPECIAL UTILITY INPUT TAPE
          31-33     $XX         NTAPEG   UNDESIGNATED INPUT-OUTPUT
          34-36     $XX         NTAPEH   UNDESIGNATED INPUT-OUTPUT
          37-39     $XX         NTAPEI   UNDESIGNATED INPUT-OUTPUT
          40-42     $XX         NTAPEJ   UNDESIGNATED INPUT-OUTPUT
          43-72                 (IGNORED)

TAPFUL - CARD TO INDICATE FILLED REFLECTION TAPE.
         USED IF THE BCD TAPE TO DATA REDUCTION MUST BE SPLIT.
         FORMAT (A6)
           1- 6     TAPFUL
             7      $           BLANK
           8-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.
```

```
TITLE - TITLE CARD.  OPERATION CARD.  PRINTS TITLE ON EACH PAGE OF
        OFF-LINE OUTPUT.
        USED IN ALL PROGRAMS WHENEVER DESIRED.
        FORMAT (12A6)
          1- 6     TITLE$      (A6)
          7-72     ALPHANUMERIC INFORMATION FOR PAGE TITLE.

UIJ   - ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRAT.
        SEE D.W.J.CRUICKSHANK, ACTA CRYST., VOL 9, 747-758 (1956).
        FORMAT (A6,1X,A6,6F8.4)
          1- 6     UIJ$$$
          7-61     FORMAT IDENTICAL WITH BIJ CARD.
         62-72     ANY LEGAL PUNCHING DESIRED, OR BLANKS.

WEBSTE - SORT REFLECTIONS ON THEIR INDICES IN ANY ORDER.
         FORMAT (
           1- 6       WEBSTE
           7-13                  BLANK
             14       X           (2)/(3) FOR (ONE AND TWO DIMENSIONALS)/
                                    (THREE DIMENSIONALS)
             15       X           (1)/(2)/(3) FOR SORT (FIRST)/(SECOND)/
                                    (THIRD) ON THE H INDEX.
             16       X           (1)/(2)/(3) FOR K INDEX SORT.
             17       X           (1)/(2)/(3) FOR L INDEX SORT.
          18-72                   (IGNORED)

XLIMIT - LIMITS X VALUE TO GIVE BETTER FIT IN E
         FORMAT (A6,1X3F6.3)
           1- 6       XLIMIT
              7       $           BLANK
           8-13       XX.XXX      PERMISSIBLE MAXIMUM ERROR IN ESTIMATED X
                                    (BLANK = 0.2) WHERE X IS POWER OF
                                    (SIN THETA)/LAMBDA. USED TO GIVE BETTER
                                    EMPIRICAL FIT OF E,S.
          14-19       XX.XXX      MINIMUM PERMISSIBLE RATIO FOR AN ESTIMATED
                                    LEVEL SCALE FACTOR TO THE OVERALL
                                    ESTIMATED SCALE FACTOR (BLANK = 1.0, I.E
                                    NO VARIATION)
          20-25       XX.XXX      MAXIMUM PERMISSIBLE RATIO FOR A LEVEL
                                    SCALE FACTOR TO THE OVERALL SCALE FACTOR
                                    (BLANK = 1.0)
          26-72                   (IGNORED)
```

APPENDIX III

DESCRIPTION OF CALCULATION CONTROL INDICATORS .. CALLED CALCOS(J).

EACH CALCOS(J) IS USED TO CONTROL SOME ASPECT OF PROGRAM FLOW. THE ARRAY IS CARRIED IN RECORD 5 OF THE BINARY REFLECTION TAPE. THIS RECORD IS INITIALIZED BY THE DATA REDUCTION PROGRAM BUT THE CONTROLLERS ARE MODIFIED BY OTHER PROGRAMS. MOST MODIFICATIONS ARE PERFORMED BY THE PARAMETER LOADING PROGRAM AT FC TIME.

THE FOLLOWING TABLE SERVES TO SHOW THE FUNCTION OF EACH OF THE CALCOS.

J	CALCOS(J) NON-ZERO (USUALLY FLOATING 1.0)	CALCOS(J) IDENTICALLY ZERO
1	(NOT YET USED)	
2	(NOT YET USED)	
3	(NOT YET USED)	
* 4	REFINE OVERALL T.F.	CALCULATE OV.T.F. BUT DONT APPLY IT
* 5	CAUSE GENRAT TO BY-PASS SCALING ATOMS ON CENTERS	AUTOMATIC SCALING FOR ATOMS AT CENTERS
* 6	APPLY NEWEST FREL SCALE	LEAVE FREL SCALE FROZEN
* 7	CALL USER PATCH TO FC	BYPASS USER PATCH
8	EDIT UP TO 25 REFLCTIONS	NO EDITING NEEDED
9	SOME ATOMS HAVE INDIVIDUAL SCALING	NO INDIVIDUAL ATOM SCALE FACTORS
* 10	SOME ATOMS HAVE DISPERSION CORRECTION	NO DISPERSION CORRECTION
* 11	FC SCALING (NUMBER OF ASYMMETRIC UNITS) IS SPECIAL AND SUPPLIED BY USER IN THE FC CARD	USUAL FC SCALING DETERMINED BY LATTICE TYPE
* 12	HI-FI FUNCTIONS	LO-FI FUNCTIONS
13	GENERAL TEMP. FACTOR	ONLY ISOTROPIC TEMPERATURE FACT
* 14	USE PREVIOUS FC AS PARTIAL CONTRIB. (CALCOS(14) IS TESTED ONLY IF CALCOS(15) IS NON-ZERO)	USE PREV. PART. CONTRIB. AS PARTIAL CONTRIBUTION
* 15	PARTIAL CONTRIBUTION (I.E. A SET OF ATOMS MAY BE TREATED AS **FIXED** BY STORING THEIR CONTRIBUTION TO FC AS THE BASIS FOR FC AS EACH REFLECTION IS PROCESSED)	NO PARTIAL CONTRIBUTION
16	INDIVIDUAL ATOM T.F. (SEE CALCOS(13) TO NOTE THAT THESE MAY BE ISO ONLY OR MIXED)	OVERALL TEMP. FACT.
17	ACENTRIC	CENTRIC

* CALCOS(J) SET DIRECTLY BY USER AT FC TIME ON THE FC CARD. OTHERS ARE SET AT DATA REDUCTION TIME OR INDIRECTLY BY THE PROGRAM.

APPENDIX IV

BINARY TAPE FORMAT FOR =X-RAY 63= SYSTEM REFLECTION TAPE

RECORD 1 63 WORDS. COMPOUND AND TAPE ID AND CELL CONSTANTS.

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 010101000000
2	COMPOUND ID	COMPDN (A6) -0 OR 0 NOT ALLOWED
3	CELL VOLUME	FLT. PT.
4	AO	*
5	BO	*
6	CO	*
7	COS ALPHA	*
8	COS BETA	*
9	COS GAMMA	*
10	A*	*
11	B*	*
12	C*	*
13	COS AL*	*
14	COS BET*	*
15	COS GAM*	*
16	A SQUARED	BEGINING OF THE METRIC TENSOR IN FLT. PT.
17	ABCOSG	
18	ACCOSB	
19	ABCOSG	
20	B SQUARED	
21	BCCOSA	
22	ACCOSB	
23	BCCOSA	
24	C SQUARED	END OF METRIC TENSOR
25	A* SQUARED	BEGIN INVERSE METRIC TENSOR IN FLT. PT.
26	A*B*COSG*	
27	A*C*COSB*	
28	A*B*COSG*	
29	B* SQUARED	
30	B*C*COSA*	
31	A*C*COSB*	
32	B*C*COSA*	
33	C* SQUARED	END OF INVERSE METRIC TENSOR
34	A* SQUARED/4	
35	B* SQUARED/4	
36	C* SQUARED/4	
37	A*B*COSG*/2	
38	A*C*COSB*/2	
39	B*C*COSA*/2	
40	A*B*/2	
41	A*C*/2	
42	B*C*/2	
43	FOOO	IN FLOATING POINT
44	TAPE REWRITE COUNT	817 INTEGER = ZERO AT DATA RUN TIME
45 TO 55	TAPHED	11 A6 WORDS FOR TAPE IDENTIFICATION
56 TO 63	A6 RECORDS WITH HISTORY OF REWRITES	

THIS RECORD IS ENDED WITH BLANK TAPE AFTER END OF RECORD MARK. (FOR REWRITE AFTER REFINEMENT).

RECORD 2 — 3 TO 18 WORDS — BCD EQUIVALENCE TABLE OF ATOM TYPE CODES. (DICTIONARY OF ATOM TYPE SYMBOLS)

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 020202000000
2	NO. OF KINDS FORM F.	817 INTEGER
3 TO 18	BCD EQUIVALENT OF ATOM TYPE NAME (E.G.- OCT 236060606060 FOR CARBON).	

EACH SYMBOL IS LEFT-JUSTIFIED - NO TRAILING CHARACTER MAY BE A NUMBER
RECORD ONLY AS LONG AS NECESSARY FOR NUMBER OF DIFFERENT ATOM TYPES

RECORD 3 — 33 WORDS — DISPERSION CORRECTIONS FOR ATOMS NEEDING THEM.

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 030303000000
2 TO 17	FJP	REAL PART OF DISPERSION CORRECTION.
18 TO 33	FJPP	IMAGINARY PART OF DISPERSION CORRECTION.

DISPERSION CORRECTIONS STORED IN ORDER ACCORDING TO TABLE OF REC 2

RECORD 4 — 15 TO 578 WORDS — SYMMETRY OPERATIONS FOR SPACE GROUP.

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 040404000000
2	JSYM	817 COUNT OF NUMBER OF SYM OPS
3	JJSYM	12*JSYM .. TO FACILITATE READ IN.
4 TO 579		MATRICES OF SYMMETRY OPERATIONS (48 MAX).
LAST	LATTICE	A CODE TO TELL IF SPACE GROUP IS CENTERED I.E. P,A,B,C,R,I, OR F)

RECORD 5 — 149 WORDS — F-RELATIVE SCALE FACTORS.

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 050505000000
2 TO 65		SCALE FACTORS TO BE APPLIED TO F RELATIVE. THEY ARE TAGGED BY SCALE FACTOR ID NUMBERS DESIGNATED FOR EACH REFLECTION IN GROUP CODE STORED IN EACH REFLECTION RECORD.
66		NROT, THE NUMBER OF ROTATION MATRICES.
67		NATOMS, A FUNCTION OF THE NUMBER OF ATOMS STORED IN THE FOLLOWING RECORD 6.
68 TO 84		CALCOS(J), CALCULATION CONTROL INDICATORS. SEE APPENDIX III, SECT. 3.3 FOR DETAILS.
85		BCHNG, THE CHANGE IN OVERALL ISOTROPIC T.F. AS CALCULATED BY PREVIOUS FC.
86 TO 149		RESCALE CONSTANTS TO APPLY TO F-RELATIVE ON NEXT CYCLE IN PLACE OF WORDS 2 TO 65, IF SO CODED BY PROGRAM.

THIS RECORD IS ENDED WITH BLANK TAPE AFTER END OF RECORD MARK. (FOR REWRITE AFTER REFINEMENT).

RECORD 6 — 19 TO LOTS AND LOTS OF WORDS — ATOM PARAMETERS

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 060606000000
2		(DUMMY WORD)
3	FCMULT	TELLS FC HOW TO SCALE ITSELF FOR LATTICE CENTERING. IT IS SET BY DATA REDUCTION.
4	MOLES	ESSENTIALLY A B17 FC OVERALL SCALE FACTOR.
5	NATOM	THE NUMBER OF WORDS IN THE RECORD BEGINNING WITH WORD 7.
6	INDXC	NUMBER OF WORDS DESCRIBING EACH ATOM 14 = GENERAL TEMP. FACTOR. 8 = INDIVIDUAL ISOTROPIC TEMP. FACTOR. 6 = OVERALL ISOTROPIC TEMP. FACTOR. (REPEAT UNIT STARTS WITH WORD 21)
7	B11	TEMPERATURE FACTORS AS FLOATING POINT.
8	B22	
9	B33	
10	B12	
11	B13	
12	B23	
13	B	ISOTROPIC TEMPERATURE FACTOR.
14	TTAG	TEMP. FACTOR TAG TO IDENTIFY ISOTROPIC OR ANISOTROPIC INDIVID. TEMP. FACTOR
15	NAMEAT	BCD ATOM IDENTIFICATION
16	ATN	ATOM TYPE NUMBER
17	JKSF	INDIVIDUAL ATOM SCALE FACTOR
18	X	PARAMETERS IN FLOATING POINT.
19	Y	
20	Z	

FROM THIS POINT ONWARDS-
REPEAT IN UNITS OF 14 (WORDS 7-20) FOR INDIVID. GENERAL TEMP. FACTORS.
REPEAT IN UNITS OF 8 (WORDS 13-20) FOR INDIVID. ISOTROPIC T. F.
REPEAT IN UNITS OF 6 (WORDS 15-20) FOR OVERALL TEMP. FACTOR.
THIS RECORD IS ENDED WITH BLANK TAPE AFTER END OF RECORD MARK. (FOR REWRITE AFTER REFINEMENT).

RECORD 7 — TEN WORDS OF SUMMARY DATA FOLLOWED BY ERROR INFORMATION

WORD	CONTENTS	DESCRIPTION
1	RECORD ID	OCT 070707000000 TO INDICATE THAT THE FOLLOWING RECORDS CONTAIN REFLECT. DATA
2	MAXACH	MAXIMUM H ON TAPE
3	MAXKAY	MAXIMUM K ON TAPE
4	MAXELL	MAXIMUM L ON TAPE
5	EZRO	E(000) (AFTER DATAFIX)
6	NREF	NUMBER OF REFLECTIONS ON TAPE
7	MAXLEV	MAXIMUM VALUE OF LEVEL INDICATOR (WORD 7 OF REFLECTION RECORD)
8	IGRID1	X GRID (STORED AFTER FC WITH GRID CARD)
9	IGRID2	Y GRID (STORED AFTER FC WITH GRID CARD)
10	IGRID3	Z GRID (STORED AFTER FC WITH GRID CARD) (WORDS 8, 9, AND 10 ARE INITIALIZED BY DATA REDUCTION TO 777000)
11	ITF	TEMPERATURE FACTOR MODE AT LAST LEAST SQUARES CYCLE. 0 = ISOTROPIC 1 = ANISOTROPIC
12	NQ	NUMBER OF DIFFERENT SCALE GROUPS
13	NP	TOTAL NUMBER OF PARAMETERS INCLUDING THOSE TO BE VARIED AS WELL AS THOSE TO BE HELD CONSTANT
14	NV	NUMBER OF PARAMETERS VARIED IN CYCLE WHICH WAS CARRIED OUT WHEN TAPE WAS WRITTEN
15	NM	THE NUMBER OF ELEMENTS IN THE MATRIX
16 TO 15+NP	KI(I)	THE INDICATOR TELLING WHICH PARAMETERS WERE VARIED DURING THE GIVEN REFINEMENT CYCLE
16+NP TO 16+NM+NP	AM(I)	THE INVERSE MATRIX FROM THE FINAL CYCLE

RECORD 8 36 TO 41 WORDS. ONE RECORD OF THIS TYPE FOR EVERY REFLECTION.

WORD	CONTENTS	DESCRIPTION
1	H	B17 FORTRAN INTEGERS
2	K	
3	L	
4	FREL	F RELATIVE.
5	ORT	SIN(THETA)/LAMBDA
6	JCODE	B17 INTEGER LESS-THAN EXTINCT CODES.
7	LEVEL	B17 INTEGER GROUP SCALE FACTOR.
8	WEIGHT	LEAST SQUARES WEIGHTING FACTOR. (IF NO WEIGHTS ARE CALCULATED, F REL MIN IS STORED FOR LATER CALC. OF WEIGHTS)
9	E1	UNITARY STRUCTURE FACTOR DATA.
10	E2	UNITARY STRUCTURE FACTOR DATA.
11	PARTA	PARTIAL CONTRIBUTION TO A.
12	PARTB	PARTIAL CONTRIBUTION TO B.
13	PARTAR	PARTIAL CONTRIBUTION TO THE REAL PART OF THE DISPERSION CORRECTION.
14	PARTAI	PARTIAL CONTRIBUTION TO THE IMAGINARY PART OF THE DISPERSION CORRECTION. (WORD CONTAINS 1/LP IMMEDIATELY AFTER DATA REDUCTION, UNTIL SUCH TIME AS A FIXED ATOM WITH DISPERSION CORRECTION CALCULATION IS MADE)
15	FC	STRUCTURE FACTOR.
16	ATAPE	A
17	BTAPE	B
18	AR	REAL PART OF FC WITH DISPERSION CORRECTION
19	AI	IMAG PART OF FC WITH DISPERSION CORRECTION
20	SFDCR	RATIO OF FC WITHOUT DISPERSION CORRECTION TO FC WITH DISPERSION CORRECTION.
21 TO 35	FJ	UP TO 16 ATOMIC SCATTERING FACTORS.
(22-36) TO (36-253)		FOURIER CODES.
	JGEN	NUMBER OF WORDS WHICH FOLLOW.
	JGENER(1)	-1 SIGNAL
	JGENER(2)	ABSOLUTE VALUE OF H
	JGENER(3)	ABSOLUTE VALUE OF K
	JGENER(4)	ABSOLUTE VALUE OF L
	JGENER(5)	INDICES SIGN INDICATOR AS 1 = H,K,L 2 = -H,K,L 3 = H,-K,L 4 = H,K,-L 5 = -H,-K,-L 6 = H,-K,-L 7 = -H,K,-L 8 = -H,-K,L
	JGENER(6)	FRINGE FUNCTION RELATIONSHIP INDICATOR AS 1 = SAME PHASE 3 = PHASE CHANGE OF PI/3 4 = PHASE CHANGE OF PI/2 5 = PHASE CHANGE OF 2*PI/3 7 = PHASE CHANGE OF PI 9 = PHASE CHANGE OF 4*PI/3 10 = PHASE CHANGE OF 3*PI/2 11 = PHASE CHANGE OF 5*PI/3
	JGENER(7)	EITHER ANOTHER PAIR AS ABOVE IF SAME
	JGENER(8)	MAG(H,K,L) OR -1 IF MAG OF (H,K,L) CHANGES OR -2 IF ALL SYMOPS HANDLED IF -1, NEW MAG(H,K,L) AND PROPER SYMMETRY RELATIONS FOLLOWS
	JGENER(JGEN)	THE MULTIPLICITY FOR UNIQUE REFLECTION

SEE COMMENTS IN FCFUN AND GEN FOR MORE DETAILS.

RECORD (8+N) FOR THE N-TH REFLECTION IN THIS FILE.

RECORD (9+N) SIGNALS END-OF-TAPE.

RECORD UP TO 41 WORDS LONG TO IMITATE REFLECTION RECORDS.

WORD 1	OCT 101010000000
WORDS 2 TO 20	NUMBER OF REFLECTIONS TO THIS POINT IN THIS FILE (REPEATED IN EACH WORD) AS B17 INTEGERS.
WORDS 21 TO 36	VALUES OF THE SCATTERING FACTORS FOR (SIN THETA)/LAMBDA = ZERO.
LAST 5 WORDS	DUMMY RECORDS SIMULATING FOURIER CODES, EACH WORD CONTAINS INTEGER ONE.

RECORD (10+N) SIGNALS END-OF-REFLECTIONS FOR THIS COMPOUND.

RECORD UP TO 41 WORDS LONG TO IMITATE REFLECTION RECORDS.

WORD 1	OCT 111111000000
WORDS 2 TO 41	IDENTICAL WITH RECORD (9+N).

RECORD A MARKS THE BEGINNING OF CONTINUATION TAPES.

WORD 1 CONTAINS OCT 212121000000.
WORD 2 CONTAINS A B17 INTEGER WHICH TELLS WHICH SEGMENT THIS IS.
WORDS 3 TO 23 HAVE BCD COMPOUND IDENTIFICATION COPIED FROM RECORD 1.

APPENDIX V

SYSTEM LINK LABELS AND CALLING CARDS FOR PROGRAM SYSTEM

THIS LIST IS THE TABLE OF LIBRARY PROGRAMS IN THE =X-RAY 63= CRYSTALLOGRAPHY PROGRAM SYSTEM. THIS LIST WILL BE UP-DATED FROM TIME TO TIME AS ADDITIONAL PROGRAMS ARE ADDED TO THE SYSTEM. WHEN LOADING THE PROGRAMS, THE ORDER OF PROGRAM DECKS MUST BE IN THE ORDER OF INCREASING LINK LABEL NUMBERS. REFER TO THE TABLE OF CONTENTS FOR THE LIST OF PROGRAMS WHICH ARE CURENTLY INCLUDED IN THE WORKING SYSTEM TAPE.

LINK LABEL	CALLING CARD	PROGRAM
100	LOADER	BEGINNING PROGRAM (BSS LOADER AND TAPE GENERATOR)
1000	FC	PARAMETER LOADER FOR FC (FCONE)
1001	(CALLED BY FCONE)	FC AND STATISTICS PROGRAM (FCTWO)
2000	DIFSYN	DIFFERENTIAL SYNTHESIS
2100	DFSYNA	MODIFIED DIFFERENTIAL SYNTHESIS
3000	LSQFM	FULL-MATRIX LEAST SQUARES
3500	LSQBD	BLOCK-DIAGONAL LEAST SQUARES
3600	ORFLS	BUSING-MARTIN-LEVY FULL-MATRIX LEAST-SQUARES
4000	FOURR	FOURIER SYNTHESIS
5000	FOUREF	FOURIER REFINEMENT (SHIFTS ATOMS TO FOURIER PEAK)
5500	SHLPAT	SHELL PATTERSON
6000	BONDLA	BOND LENGTHS AND ANGLES
6300	PROJCT	PROJECTION OF A MOLECULE ON A PLANE
6500	LSQPL	LEAST SQUARES PLANE AND LINE
7000	SUPTAP	PREPARATION OF SUPERPOSITION BINARY TAPE
7100	SUPERA	PATTERSON SUPERPOSITION PROGRAM =A=
7200	SUPERB	PATTERSON SUPERPOSITION PROGRAM =B=
7300	SUPERC	PATTERSON SUPERPOSITION PROGRAM =C=
7400	SUPROT	ROTATION PROGRAM TO FIT MODEL TO PATTERSON
8000	DELSIG	DELTA F VS FO PLOT FOR SIGMA FOR DATA REDUCTION
9000	PHASE	CALCULATION OF KARLE-HAUPTMAN PHASES

LINK LABEL	CALLING CARD	PROGRAM
10000	DATRDN	DATA REDUCTION
10300	DATCOR	DATA CORRELATION FOR FILMS
10500	DATFIX	CALCULATION OF SCALED UNITARY STRUCTURE FACTORS
10600	MODIFY	SEARCH AND MODIFY REFLECTION TAPE
10700	WEIGHT	PREPARE WEIGHTS FOR LEAST-SQUARES
10800	ESORT	SORT FOR KARLE-HAUPTMAN PHASE DETERMINATION
11000	LISTFC	FINAL STRUCTURE FACTOR LISTING
11100	CRYSET	CONNAY-TAKEDA CRYSTAL TRANSFORMATIONS
12000	RPLANE	CALC. R OVER A PROJECTION FOR MOVED MOLECULE
12200	RLIST	CALC. R FOR SPECIAL CLASSES OF REFLECTION
12500	PARAM	LEAST-SQUARES REFINEMENT OF LATTICE PARAMETERS
15000	TFINFO	CALCULATES TEMPERATURE FACTOR STATISTICS
20000	GESET	GENERAT. OF REFLECT. AND CRYSTAL SET FOR GE XRD-5
27000	REFPAK	INTERCONVERTS REFLECTION TAPE AND BINARY DECK
28000	REFSOR	REFLECTION SORTING FROM TAPE
29000	TAPCOP	GENERAL TAPE COPYING ROUTINE
30000	PATCON	PATTERSON CONVOLUTION PROGRAM
31000	BYEBYE	CONVERT SYSTEM REFLECT. TAPE TO NON-SYSTEM FORMATS
31100	NRLA	SPARE ENTRY =A= FOR EXPERIMENTAL PURPOSES
31200	NRLB	SPARE ENTRY =B= FOR EXPERIMENTAL PURPOSES
32700	(CALLED BY EXEMW)	EXECUTION ERROR DIAGNOSTICS

APPENDIX VI

SAMPLE CARD ORDERS FOR JOBS SUBMITTED TO THE RESEARCH COMPUTER LABORATORY AT THE UNIVERSITY OF WASHINGTON

EXAMPLE ONE. THIS EXAMPLE HAS THE INTENSITY DATA FOR 9-METHYL ADENINE (WHICH HAS BEEN ASSIGNED THE MNEMONIC =9-MEAD=). THE DATA IS REDUCED AND THE REFLECTION TAPE GENERATED IS THEN USED TO CALCULATE STRUCTURE FACTORS BASED ON A SET OF TRIAL PARAMETERS. THE STRUCTURE FACTORS ARE THEN USED AS THE COEFFICIENTS FOR AN ELECTRON-DENSITY FOURIER IN WHICH THE LAYOUT IS 25THS ALONG A (1ST SUM), 1/2 OF 50THS ALONG B (2ND SUM), AND 25THS ALONG C (3RD SUM).

```
*0310045 STEWART, ROBERT                SPECIAL
*      XEQ
*      MAX TIME (030)
                 5000
                EL H31 TAPE  B5, (10)        ) FILE PROTECTED
                EEL H02 TAPE  A6, (11)   500 ) NOT FILE PROTECTED
*      TA[illegible]EL      TAPE  B6, (12)   500 ) SCRATCH
*      PRINTER
*      OVERFLOW OFF
*      END PRINTER
*****  INSERT THE BINARY DECK FOR =85FORT=.  *****
*      DATA
TITLE   9-METHYL ADENINE  JULY 29, 1963
TAPES          11 12
DATRON 9-MEAD
LABEL    DATA REDUCTION  9-METHYL ADENINE
CELL    9-MEAD    7.670  12.240   8.470  0.0      -0.55097  0.0          308
FORMFX N        0.00      7.000 NITROGEN INTL.  TABLE VOL. 3'202,1961
FORMFX N        0.05      6.781
FORMFX N        0.10      6.203
FORMFX N        0.15      5.420
FORMFX N        0.20      4.600
*****  INSERT REMAINDER OF NITROGEN SCATTERING FACTORS.  *****
FORMFX C          0.00   06.000 CARBON
FORMFX C          0.05   05.764 J. BERGHUIS
FORMFX C          0.10   05.141 00 ACTA CRYST. (1955).
FORMFX C          0.15   04.362 00 VOL. 8, 478-483.
FORMFX C          0.20   03.612
*****  INSERT REMAINDER OF CARBON SCATTERING FACTORS.  *****
FORMFX H        0.0000   01.000 HYDROGEN
FORMFX H        0.0473   00.952 R. MCWEENY
FORMFX H        0.0947   00.829 00 ACTA CRYST. (1951).
FORMFX H        0.1420   00.664 00 VOL. 4, 513-519.
FORMFX H        0.1893   00.514
*****  INSERT REMAINDER OF HYDROGEN SCATTERING FACTORS.  *****
```

```
SYMTRY   X, Y, Z
SYMTRY   X, 1/2 - Y, 1/2 + Z
CONDIT 9-MEAD 1.5418  1.00     0.80      1  3  1  1  1  1
SCALE     20.4135    1          1
        9-MEAD 9  00  00  02  00005.20
        9-MEAD 9  00  00  04  00066.80
        9-MEAD 9  00  00  06  00007.60
        9-MEAD 9  00  01  01  00595.30
        9-MEAD 9  00  01  02  00073.80
        9-MEAD 9  00  01  04  00018.50
        9-MEAD 9  00  01  05  00003.40
        9-MEAD 9  00  01  07  00003.20
        9-MEAD 9  00  02  00  00375.50
        9-MEAD 9  00  02  01  00068.20
        9-MEAD 9  00  02  02  00227.30
        9-MEAD 9  00  02  03  00008.50
*****   INSERT REMAINDER OF THE INTENSITY DECK (REFLECTION CARDS).  *****
END
FC      9-MEAD            1   1   2   1   1   1   1   2     1
GRID    9-MEAD  25  50  25
ATOM    N 1     .2469    .1292    .7327    2.000
ATOM    N 2     .2715    -.0630   .6904    2.000
ATOM    N 3     .2257    .0684    .2967    2.000
ATOM    N 4     .2525    -.0993   .3937    2.000
ATOM    N 5     .2218    .2611    .5313    2.000
ATOM    C 1     .2654    .0235    .7759    2.000
ATOM    C 2     .2615    -.0339   .5308    2.000
ATOM    C 3     .2250    .0721    .4597    2.000
ATOM    C 4     .2383    .1559    .5761    2.000
ATOM    C 5     .2440    -.0350   .2657    2.000
ATOM    C 6     .2672    -.2185   .4058    2.000
END
FOURR   9-MEAD          1  4
LAYOUT          26   0   1  26   0   1  26   0   1 123  26 2
END
```

EXAMPLE TWO. THIS EXAMPLE IS BASED ON THE SAMPLE CALCULATION FOR ALPHA QUARTZ GIVEN BY BUSING, MARTIN, AND LEVY IN THE OAK RIDGE FORTRAN ORFLS PROGRAM. THESE DATA LISTED IN THIS EXAMPLE CAN BE PUNCHED INTO CARDS TO BE USED AS A TEST CASE FOR THE X-RAY PROGRAM SYSTEM. IT SHOULD BE EMPHASIZED THAT THE BUSING-MARTIN-LEVY PROGRAM USES A LINEAR INTERPOLATION TO OBTAIN THE SCATTERING FACTORS AND A SERIES EXPANSION TO OBTAIN THE COSINE AND SINE ARGUMENTS. THE X-RAY SYSTEM USES A FOUR-POINT INTERPOLATION OF SCATTERING FACTORS AND A TABLE-LOOK-UP METHOD FOR OBTAINING THE COSINE AND SINE FUNCTIONS. THE RESULTS OF THE SYSTEM CALCULATION WILL VARY SLIGHTLY FROM THE RESULTS OF BUSING-MARTIN-LEVY. THE INITIAL INTENSITIES ARE REDUCED, AND THE TRIAL PARAMETERS ARE USED TO CALCULATE STRUCTURE FACTORS FOR ALPHA QUARTZ (ASSIGNED THE MNEMONIC =ALQTZ=). AN ELECTRON-DENSITY MAP IS CALCULATED WITH 25THS ALONG A, 25THS ALONG B, AND 9THS ALONG C. THE PARAMETERS, STORED ON THE REFLECTION TAPE, ARE USED AS INPUT TO =ORFLS= FOR FOUR CYCLES OF LEAST-SQUARES REFINING. AFTER EACH CYCLE, PARAMETER CARDS WILL BE PUNCHED BY =ORFLS=.

```
*****  FOLLOWING ARE THE THREE SPECIAL POSITION PATCHES AS FORTRAN
*****    ROUTINES.  THESE MUST BE ASSEMBLED AND INSERTED IN THE DECK
*****    AS BINARY CARDS WHERE INDICATED. THIS EXAMPLE USES THE =LOADER=
*****    FEATURE TO GENERATE A NEW =COMPOUND SPECIFIC= SYSTEM TAPE WITH
*****    THE REQUIRED =ORFLS= PATCHES INCORPORATED.  THIS NEW =SYSTEM=
*****    TAPE CAN THEN BE RETAINED FOR THIS COMPOUND AND THEN RELEASED.


*      LABEL
CALPAT    EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.
      SUBROUTINE PATCH(INSYM,I,TJ,HJ,HHJ,IREJKT,ATOM)
      DIMENSION HJ(3),HHJ(6)

C     BY-PASS MODIFICATION FOR FIRST ATOM
      IF(I-1)2,2,1
    1    HJ(1)=HJ(1)+HJ(2)
         HJ(2)=0.0
         HHJ(1)=HHJ(1)+HHJ(2)
         HHJ(2)=0.0
         HHJ(5)=HHJ(5)-HHJ(6)
         HHJ(6)=0.0
    2 RETURN
      END
```

```
*       LABEL
CALRES    EXAMPLE. HYPOTHETICAL PROBLEM BASED ON ALPHA QUARTZ.
        SUBROUTINE RESETX(XYZ,ATOM,NA)
        DIMENSION XYZ(3,2)
        XYZ(2,2)=XYZ(1,2)
        RETURN
        END


*       LABEL
CALBET     EXAMPLE. HYPOTHETICAL PROBLEM BASED ON 1LP81 QU1RTZ=
        SUBROUTINE RESETB(BETA,ATOM,NA)
        DIMENSION BETA(6,2)
        BETA(2,2)=BETA(1,2)
        BETA(6,2)=-BETA(5,2)
        RETURN
        END


*****  FOLLOWING IS THE CARD DECK FOR ALPHA QUARTZ TEST CASE.  *****


********* RUN SEQUENCE NUMBER *****  24600   ***************************
*0310053 STEWART, JAMES M.
*       XEQ
*       MAX TIME (020)
*       CARDS BCD (      FORM NO.      ,                    )
*       OUTPUT     2000
*       TAPE (REEL H31 TAPE B5 , (10)       ) FILE PROTECTED
*       TAPE (REEL     TAPE A5 , ( 9)       ) SCRATCH
*       TAPE (REEL     TAPE A6 , (11)       ) SCRATCH
*       TAPE (REEL     TAPE B6 , (12)       ) SCRATCH
*****   INSERT BINARY DECK FOR =B5FORT=.  *****
*       DATA
TITLE   ALPHA QUARTZ TEST DECK (SEE ORNL ORFLS WRITE-UP)
TAPES          11 12
DATRON  ALQTZ
LABEL   ALPHA QUARTZ TEST DECK (SEE ORNL ORFLS WRITE-UP)
CELL    ALQTZ     4.913    4.913    5.404  0.0      0.0       -0.500    90.0
FORMFX  O--      .000     10.000   OXYGEN (-II) FOR ALPHA QUARTZ TEST CASE
FORMFX  O--      .05       9.551
FORMFX  O--      .100      8.475
FORMFX  O--      .150      7.159
FORMFX  O--      .200      5.908
FORMFX  O--      .250      4.857
FORMFX  O--      .300      4.028
FORMFX  O--      .350      3.394
FORMFX  O--      .400      2.916
FORMFX  O--      .450      2.568
FORMFX  O--      .500      2.287
FORMFX  O--      .550      2.106
FORMFX  O--      .600      1.929
FORMFX  O--      .700      1.714
FORMFX  O--      .800      1.574
FORMFX  O--      .900      1.469
FORMFX  O--     1.00       1.381
FORMFX  O--     1.10       1.299
FORMFX  O--     1.20       1.220
```

```
FORMFX SI      .000     10.000   SILICON +4     TEST CASE   FOR ALPHA QUARTZ
FORMFX SI      .050      9.950
FORMFX SI      .100      9.790
FORMFX SI      .150      9.540
FORMFX SI      .200      9.200
FORMFX SI      .250      8.790
FORMFX SI      .300      8.330
FORMFX SI      .350     07.830
FORMFX SI      .400      7.310
FORMFX SI      .450      6.780
FORMFX SI      .500      6.260
FORMFX SI      .550      5.770
FORMFX SI      .600      5.280
FORMFX SI      .700      4.420
FORMFX SI      .800      3.710
FORMFX SI      .900      3.130
FORMFX SI     1.00       2.680
FORMFX SI     1.10       2.330
FORMFX SI     1.20       2.060
LATICE   A   P
SYMTRY      X,Y,Z
SYMTRY    X-Y,-Y,-Z
SYMTRY    Y-X,-X,1/3+Z
SYMTRY    -X,Y-X,1/3-Z
SYMTRY    -Y,X-Y,2/3+Z
SYMTRY    Y,X,2/3-Z
CONDIT ALQTZ   0.707    1.0      0.1       1  2  2  1  1
       ALQTZ       1    0   0     234.6
       ALQTZ       1    1   0     317.5
       ALQTZ       6    1   0      76.0
       ALQTZ       5    3   0      27.9
       ALQTZ       4    0   1     308.2
       ALQTZ       3    1   1      56.5
       ALQTZ       3    2   1       1.5
       ALQTZ       4    4   1       6.7
       ALQTZ       3    1  -1     199.8
       ALQTZ       5    2  -1     145.6
       ALQTZ       2    0   2      78.7
       ALQTZ       6    1   2      11.5
       ALQTZ       5    3   2      38.0
       ALQTZ       1    0  -2      80.1
       ALQTZ       5    1  -2      45.2
       ALQTZ       3    2  -2       9.0
       ALQTZ       3    0   3      74.1
       ALQTZ       2    2   3     212.0
       ALQTZ       3    0  -3      12.5
       ALQTZ       4    1  -3     231.3
       ALQTZ       6    0   4      44.4
       ALQTZ       6    2   4      32.0
       ALQTZ       5    0  -4     180.2
       ALQTZ       4    2  -4      33.3
       ALQTZ       1    1   5     162.5
       ALQTZ       3    0  -5       8.2
       ALQTZ       2    2   6      85.9
       ALQTZ       4    0  -6     110.5
       ALQTZ       4    1   7      10.6
       ALQTZ       1    1  -7      78.0
       ALQTZ       3    0   8     134.9
       ALQTZ       2    1  -8      37.2
       ALQTZ       2    0  -9      10.8
END
```

```
FC      ALQTZ                          2            2                    2
GRID    ALQTZ    25  25    9
ATOM    O--     0.4100  0.2700  0.1200  0.38
ATOM    SI      0.5200  0.5200 0.333333 0.43
END
FOURR   ALQTZ          1  4
LAYOUT  ALQTZ    26    0    1  26    0    1  10    0    1 231   26 2
END
LOADER  ORTEST   9
LINK    3600
*****   INSERT BINARY DECK =ORFLS=
*****   INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =ALBET=
*****   INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =ALPAT=
*****   INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =ALRES=
*****   INSERT BINARY DECKS FOR ALL REQUIRED ORFLS SUBROUTINES, ATNUM,
*****   BSTUW, ERASE, EXPUW, ORCAL, ORFUN, ORIN,  OROUT, ORPRE, ORPT,
*****   ORSBT, ORSMI, ORTES, ORWT, SLIUW, SLOUW, ORTRIG, SQRUW, TIME.
END
TAPES          12 11
ORFLS   ALQTZ    4   2   1      1   1   1   1
ATOM    O--     0.4100  0.2700  0.1200  0.38
ATOM    SI      0.5200  0.5200 0.333333 0.43  0.5
NOREF   SI     Y   Z   822    823
END
```

EXAMPLE THREE. THIS EXAMPLE IS BASED ON THE STRUCTURE OF GUANIDINIUM ALUMINUM SULFATE HEXAHYDRATE (MNEMONIC =GUANAL=). THE SPACE-GROUP REQUIRES PATCHING OF THE X-RAY SYSTEM VERSION OF THE BUSING-MARTIN-LEVY =ORFLS= FULL-MATRIX LEAST-SQUARES PROGRAM. IN THIS EXAMPLE, CODING OF THE PATCHES WAS DONE UTILIZING THE =IFFW= ENTRY OF THE =CALLER= SUB-ROUTINE OF THE UTILITY PACKAGE, WHOSE CALLING SEQUENCE IS-

```
        CALL  IFFW (WORD, K, ARG1, ARG2, ... , ARGN)
```

=IFFW= SETS K TO 1, 2, ..., N IF =WORD= EXACTLY MATCHES ARG1, ARG2, ..., ARGN, RESPECTIVELY, OR TO N+1 IF IT MATCHES NONE.

THIS EXAMPLE UPDATES THE X-RAY SYSTEM PROGRAM TAPE WITH THE PATCHES REQUIRED BY =GUANAL= FOR =ORFLS=. THE DATA IS REDUCED USING AN OLD BINARY REFLECTION TAPE AS INPUT TO GET F-RELATIVE, H, K, AND L. THE =MODIFY= PROGRAM IS THEN CALLED TO COPY FC TO F-REL, SO THAT THE FOURIER WILL BE, IN EFFECT, AN FC FOURIER IN ORDER TO CHECK THE =ORFLS= PATCHES FOR PROPER SYMMETRY. FINALLY, ONE CYCLE OF FULL-MATRIX LEAST-SQUARES REFINEMENT IS DONE WITH =ORFLS=. SPACE GROUP = P 3 1 M.

(NOTE - THIS IS A TEST CASE OF =GUANAL= WHICH HAS BEEN LABELED =FONAL2=)

***** FOLLOWING ARE THE SPECIAL POSITION PATCHES AS FORTRAN SUBROUTINE.
****** THE BINARY CARDS FROM THE ASSEMBLED PATCHES ARE INSERTED IN THE
***** =ORFLS= BINARY CARD DECK AS DESCRIBED UNDER EXAMPLE TWO, P 3.6-3

```
*       LABEL
CGUANREX      RESET X,Y, AND Z
C
        SUBROUTINE RESETX (XYZ, ATOM, NA)
C
C       FOR GUANAL THERE IS NO NEED TO RESET X, Y, AND Z AS LONG AS NO
C       REFINEMENT IS ATTEMPTED ON  PARAMETERS SET TO ZERO, 1/3, OR 2/3 AT
C       START.
        RETURN
        END
```

```
*     LABEL
CGUANPA   ORFLS PATCH FOR GUANIDINIUM AL SULFATE
C
      SUBROUTINE PATCH(INSYM,I,TS,HJ,HHJ,IREJKT,ATOM)
      DIMENSION HJ(3), HHJ(6)
C
C     WHEN IREJKT IS SET EQUAL TO ONE THE GENERATED ATOM WILL BE
C     ACCEPTED
      IREJKT=1
      CALL IFFW(ATOM,KATM,6HAL+++1,2HC1,6HAL+++2,2HC2,2HS1,2HS2,2HO1,
     12HO2,2HO3,2HO4,2HO7,2HO8,2HN1)
C
      GO TO (1,1,2,2,3,3,3,3,3,3,3,3,3,40),KATM
C
C     IF ATOM IN ONEFOLD POSITION CALCULATE ONLY FIRST TIME
 1    IF(INSYM-1) 40,40,39
C
C     IF ATOM IN TWO-FOLD POSITION CALCULATE ONLY FIRST TWO TIMES
 2    IF (INSYM-2) 40,40,39
C
C     IF ATOM IN 3-FOLD POSITION CALCULATE ONLY ON 1ST, 4TH, AND 5TH
 3    IF (INSYM - 1) 33,40,33
 33   IF (INSYM - 4) 39,40,34
 34   IF (INSYM - 5) 39, 40, 39
C
C     THE ABOVE DEPENDS UPON THE SYMOPS BEING STORED AT DATA REDUCTION
C     TIME IN THE ORDER
C     X,Y,Z,
C     -X,Y-X,Z
C     X-Y,-Y,Z
C     Y-X,-X,Z
C     -Y,X-Y,Z
C     Y,X,Z
C
C     WHEN IREJKT IS SET EQUAL TO TWO THE ORCAL CALLING SUBROUTINE WILL
C     SKIP THIS GENERATED ATOM
 39   IREJKT=2
 40   RETURN
      END

*     LABEL
CGUANBET  ORFLS PATCH TO RESET BETAS FOR GUANIDINIUM AL SULFATE
C
      SUBROUTINE RESETB (BETA, ATOM, NA)
C
      DIMENSION BETA(6,1), ATOM(1)
C
C     SCAN THE TABLE OF ATOMS LOOKING FOR THOSE IN SPECIAL POSITIONS
C
      DO 40 I=1,NA
C
      CALL IFFW(ATOM(I),KATM,6HAL+++1,2HC1,6HAL+++2,2HC2,2HS1,2HS2,2HO1,
     12HO2,2HO3,2HO4,2HO7,2HO8,2HN1)
      GO TO (1,1,2,2,2,2,2,2,2,2,2,2,2,40),KATM
C
C     IF ATOM IS IN ONE FOLD POSITION FORCE BETA(1,3) AND (2,3) TO ZERO
C     FORCE BETA(1,2) TO BE 1/2 OF BETA(1,1)
C     SET BETA(2,2) EQUAL TO BETA(1,1)
 1    BETA (2,I) = BETA (1,I)
C
C     FOR THE ONE-FOLD, TWO-FOLD, AND THREE-FOLD BETA(1,2) =
C     BETA(2,2)/2,  AND BETA(1,3. AND BETA(2,3) ARE ZERO
C
C
 2    BETA(4,I) = BETA(2,I)/2.0
 40   CONTINUE
      RETURN
      END
```

```
*****  FOLLOWING IS THE CARD DECK FOR  =GUANAL=.  *****


********* RUN SEQUENCE NUMBER *****  26810   ***************************
*0310053 STEWART,BOSCO                SPECIAL
*      XEQ
*      MAX TIME (120)
*      OUTPUT   10000
*      TAPE (REEL H31 TAPE B5 , (10)       ) FILE PROTECTED
*      TAPE (REEL 0593TAPE B1 , ( 8)       ) NOT FILE PROTECTED
*      TAPE (REEL 65  TAPE B6 , (12)       ) FILE PROTECTED
*      TAPE (REEL     TAPE  A5, ( 9)       ) SCRATCH
*      TAPE (REEL     TAPE A6 , (11)       ) SCRATCH
*****  INSERT BINARY DECK FOR  =B5FORT=.  *****
*      DATA
TITLE PERFECT DATA FOR FONAL2 USING X-RAY 63  7/8/63
LOADER GUTEST  9
LINK   3600
*****  INSERT BINARY DECK =ORFLS=
*****  INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =GUANBE=
*****  INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =GUANPA=
*****  INSERT BINARY DECK FOR ASSEMBLED ORFLS PATCH =GUANRE=
*****  INSERT BINARY DECKS FOR ALL REQUIRED ORFLS SUBROUTINES, ATNUM,
*****  BSTUW, ERASE, EXPUW, ORCAL, ORFUN, ORIN,  OROUT, ORPRE, ORPT,
*****  ORSBT, ORSMI, ORTES, ORWT, SLIUW, SLOUW, ORTRIG, SQRUW, TIME.
END
TAPES          11 12
DATRON FONAL2
LABEL PERFECT DATA FOR FONAL2  USING NEW X-RAY 63  7/8/63
CELL   FONAL2  11.75   11.75    8.94                    -0.5        606.
FORMFX S      0.00000  16.000 SULFUR
FORMFX S      0.07960  14.240 H. VIERVOLL AND O. OGRIM
FORMFX S      0.15920  11.500 OO ACTA CRYST. (1949).
FORMFX S      0.23870  09.630 OO VOL. 2, 277-279.
FORMFX S      0.31830  08.500
*****  INSERT REMAINDER OF SULFUR SCATTERING FACTORS.  *****
FORMFX AL+++     0.00  10.00  ALUMINUM (3+)
FORMFX AL+++     0.05  09.93  J. BERGHUIS
FORMFX AL+++     0.10  09.72  OO ACTA CRYST. (1955).
FORMFX AL+++     0.15  09.38  OO VOL. 8, 478-483.
FORMFX AL+++     0.20  08.94
*****  INSERT REMAINDER OF ALUMINUM(III) SCATTERING FACTORS.  *****
FORMFX O         0.00  08.000 OXYGEN
FORMFX O         0.05  07.796 J. BERGHUIS
FORMFX O         0.10  07.250 OO ACTA CRYST. (1955).
FORMFX O         0.15  06.482 OO VOL. 8, 478-483.
FORMFX O         0.20  05.634
*****  INSERT REMAINDER OF OXYGEN SCATTERING FACTORS.  *****
FORMFX N         0.00  07.000 NITROGEN
FORMFX N         0.05  06.781 J. BERGUIS
FORMFX N         0.10  06.203 OO ACTA CRYST. (1955).
FORMFX N         0.15  05.420 VOL. 8, 478-483.
FORMFX N         0.20  04.600
*****  INSERT REMAINDER OF NITROGEN SCATTERING FACTORS.  *****
FORMFX C         0.00  06.000 CARBON
FORMFX C         0.05  05.764 J. BERGHUIS
FORMFX C         0.10  05.141 OO ACTA CRYST. (1955).
FORMFX C         0.15  04.362 OO VOL. 8, 478-483.
FORMFX C         0.20  03.612
*****  INSERT REMAINDER OF CARBON SCATTERING FACTORS.  *****
```

```
FORMFX H        0.0000  01.000 HYDROGEN
FORMFX H        0.0473  00.952 R. MCWEENY
FORMFX H        0.0947  00.829 00 ACTA CRYST. (1951).
FORMFX H        0.1420  00.664 00 VOL. 4, 513-519.
FORMFX H        0.1893  00.514
*****  INSERT REMAINDER OF HYDROGEN SCATTERING FACTORS.  *****
LATICE  A  P
SYMTRY  X,Y,Z
SYMTRY  Y,X,Z
SYMTRY -X,Y-X,Z
SYMTRY -Y,X-Y,Z
SYMTRY X-Y,-Y,Z
SYMTRY Y-X,-X,Z
CONDIT FONAL2 1.5418  1.0                1  3  1  2  3  3
REFIN   1      7   842          IH IK IL FR 18 ID II
END
TAPES          11  8
FC      FONAL2                    2
GRID    FONAL2  10  10   9
REMARK *GUANAL* USING FINAL COORDINATES (CYCLE 23 D OUT (R=8.4 USING
REMARK ANISOTROPIC TEMP FACTORS)). THIS CALC USED ISOTROPIC TEMP FACTOR
REMARK B=2.0. LATER CALC WILL USE ANISOTROPIC TEMP FACTORS
REMARK FONAL2 USING NEW X-RAY 63
B       FONAL2  2.0
ATOM    S1      +.34733 +.00000 +.75861
ATOM    S2      +.68162 +.00000 +.31535
ATOM    AL+++1  +.00000 +.00000 +.00000
ATOM    AL+++2  +.33333 +.66667 +.05733
ATOM    O1      +.45654 +.00000 +.83754
ATOM    O2      +.55758 +.00000 +.28350
ATOM    O3      +.37241 +.00000 +.60481
ATOM    O4      +.70396 +.00000 +.47600
ATOM    O5      +.88133 +.22407 +.79884
ATOM    O6      +.79186 +.11512 +.24119
ATOM    O7      +.87010 +.00000 +.88350
ATOM    O8      +.13473 +.00000 +.11785
ATOM    O9      +.53120 +.32677 +.94361
ATOM    O10     +.53443 +.19616 +.17700
ATOM    N1      +.11590 +.00000 +.50556
ATOM    N2      +.55741 +.34218 +.55382
ATOM    C1      +.00000 +.00000 +.50319
ATOM    C2      +.33333 +.66667 +.55004
ATOM    H1       +.9167  +.1155  +.5033 2.500
ATOM    H2       +.5833  +.1583  +.5497 2.500
ATOM    H3       +.7417  +.2083  +.5497 2.500
ATOM    H4       +.8750  +.0750  +.8333 2.500
ATOM    H5       +.9417  +.1417  +.1667 2.500
ATOM    H6       +.7200  +.1800  +.8889 2.500
ATOM    H7       +.5917  +.1417  +.9000 2.500
ATOM    H8       +.8000  +.2750  +.2378 2.500
ATOM    H9       +.8833  +.3917  +.2000 2.500
END
TAPES          8 11
MODIFY FONAL2  3              0.0  0.1  0.0  1.0
END
FOURR  FONAL2          1  4  1
LAYOUT FONAL2  11   0   1  11   0   1  10   0   1 231  11 2
END
```

```
TAPES          11  8
ORFLS   FONAL2  1  1                1  1  1  2
ATOM    N2      .553000 .333000 .520000 1.5
ATOM    O5      .880000 .222000 .780000 1.5
ATOM    O6      .806000 .120000 .258000 1.5
ATOM    O9      .523000 .333000 .934000 1.5
ATOM    O10     .524000 .188000 .174000 1.5
ATOM    S1      .351000 .000000 .750000 1.5
ATOM    S2      .682000 .000000 .306000 1.5
ATOM    N1      .113000 .000000 .500000 1.5
ATOM    O1      .455000 .000000 .844000 1.5
ATOM    O2      .567000 .000000 .238000 1.5
ATOM    O3      .386000 .000000 .591000 1.5
ATOM    O4      .672000 .000000 .470000 1.5
ATOM    O7      .856000 .000000 .865000 1.5
ATOM    O8      .140000 .000000 .130000 1.5
ATOM    AL+++2  .333300 .666700 .059000 1.5
ATOM    C2      .333300 .666700 .520000 1.5
ATOM    C1      .000000 .000000 .500000 1.5
ATOM    AL+++1  .000000 .000000 .000000 1.5
B                1.5
NOREF   S1      Y
NOREF   S2      Y
NOREF   N1      Y
NOREF   O1      Y
NOREF   O2      Y
NOREF   O3      Y
NOREF   O4      Y
NOREF   O7      Y
NOREF   O8      Y
NOREF   AL+++2  X   Y
NOREF   C2      X   Y
NOREF   C1      X   Y
NOREF   AL+++1  X   Y   Z
NOSCALE
END
```

EXAMPLE FOUR. THIS EXAMPLE IS BASED ON THE STRUCTURE OF A SUBSTITUTED TRIS-PHOSPHINE COMPLEX OF PALLADIUM(II) BROMIDE (MNEMONIC =REDBRM= FOR =RED BROMIDE=). THE DATA IS REDUCED AND STRUCTURE FACTORS CALCULATED ON A TRIAL STRUCTURE. A FOURIER IS CALCULATED ON A GRID OF 12 X 12 X 12 TO CHECK THE SYMMETRY AND TWO CYCLES OF =ORFLS= LEAST-SQUARES ARE RUN. THE SPACE-GROUP IS P 21 21 21.

```
********* RUN SEQUENCE NUMBER *****  26810   ***************************
=0310053 WATSON, DAVID
*      XEQ
*      MAX TIME (020)
*      CARDS BCD (      FORM NO.      ,                    )
*      OUTPUT    10000
*      TAPE (REEL H31 TAPE B5 , (10)        ) FILE PROTECTED
*      TAPE (REEL     TAPE  A6, (11)        ) SCRATCH
*      TAPE (REEL     TAPE  B6, (12)        ) SCRATCH
*      PRINTER
*      OVERFLOW OFF
*****  INSERT BINARY DECK FOR  =B5FORT=.  *****
*      DATA
TAPES        11 12
TITLE    REDBRM LS TEST   HEAVY ATOMS  7 AUGUST 1963
DATRON REDBRM
LABEL    REDBRM LS TEST   HEAVY ATOMS  7 AUGUST 1963
CELL    REDBRM  11.70   16.28   20.63  +0.0     +0.0     +0.0      1908.
FORMFX PD        0.00   46.00
FORMFX PD        0.05   45.07
FORMFX PD        0.10   42.67
FORMFX PD        0.15   39.65
FORMFX PD        0.20   36.70
*****  INSERT REMAINING PALLADIUM SCATTERING FACTORS.  *****
FORMFX BR        0.00   35.00
FORMFX BR        0.05   34.22
FORMFX BR        0.10   32.21
FORMFX BR        0.15   29.70
FORMFX BR        0.20   27.27
*****  INSERT REMAINING BROMINE SCATTERING FACTORS.  *****
FORMFX P         0.00   15.00
FORMFX P         0.05   14.47
FORMFX P         0.10   13.17
FORMFX P         0.15   11.66
FORMFX P         0.20   10.34
*****  INSERT REMAINING PHOSPHORUS SCATTERING FACTORS.  * ** **
FORMFX C         0.00   06.000 CARBON
FORMFX C         0.05   05.764 J. BERGHUIS
FORMFX C         0.10   05.141 OO ACTA CRYST. (1955).
FORMFX C         0.15   04.362 OO VOL. 8, 478-483.
FORMFX C         0.20   03.916
*****  INSERT REMAINING CARBON SCATTERING FACTORS.  *****
FORMFX H       0.0000   01.000 HYDROGEN
FORMFX H       0.0473   00.952 R. MCWEENY
FORMFX H       0.0947   00.829 OO ACTA CRYST. (1951).
FORMFX H       0.1420   00.664 OO VOL. 4, 513-519.
FORMFX H       0.1893   00.514
*****  INSERT REMAINING HYDROGEN SCATTERING FACTORS.  *****
```

```
LATICE   A  P
SYMTRY    X,     Y,    Z
SYMTRY     -X+1/2,    -Y,     Z+1/2
SYMTRY     X+1/2,     -Y+1/2,    -Z
SYMTRY      -X,    Y+1/2,     -Z+1/2
CONDIT REDBRM 1.5418  0.99999 3.2        1  3  2  2  1  1
SCALE      1.8914   1     3.2     212.800.0000.0000.00012.80
       REDBRM 9  02  00  00     000.81
       REDBRM 9  04  00  00     009.43
       REDBRM 9  06  00  00     002.15
       REDBRM 9  08  00  00     001.67
       REDBRM 9  10  00  00     002.87
       REDBRM 9  14  00  00     000.63
       REDBRM 9  01  01  00     001.45
       REDBRM 9  02  01  00     006.72
       REDBRM 9  03  01  00     001.18
       REDBRM 9  04  01  00     000.95
*****  INSERT REMAINING =REDBRM= REFLECTION CARDS.  *****
END
FC     REDBRM              1   1   1   1   1   1   1   1    1.
GRID   REDBRM  12  12  12
ATOM   PD   1  -.096   0.193   0.179  2.5
ATOM   BR   2  -.113   0.055   0.233  2.5
ATOM   BR   3  0.099   0.178   0.091  2.5
ATOM    P   4  0.022   0.230   0.263  2.5
ATOM    P   5  -.118   0.323   0.155  2.5
ATOM    P   6  -.198   0.141   0.094  2.5
END
FOURR  REDBRM        1  4  1 10.0    0.1
LAYOUT REDBRM  13   0   1  13   0   1  13   0   1 312     2
END
TAPES        12 11
ORFLS  REDBRM  2  1                1  1  2
END
```

APPENDIX VIII

SYSTEM COMMON ALLOCATION FOR =X-RAY 63=

```
* SYSTEM COMMON ALLOCATION FOR =X-RAY 63=
CARD    COMMON  12                  BCD CARD RECORD (FORTRAN ARRAY) FILLED
        REM                           BY IFFC
NTIN    COMMON  1                   BCD INPUT TAPE (FROM CARD READER)
NTOUT   COMMON  1                   BCD OUTPUT TAPE (TO PRINTER)
NTAPEA  COMMON  1                   BINARY DATA TAPE (REFLECTIONS)
NTAPEB  COMMON  1                   BINARY DATA TAPE (STRUCTURE FACTORS)
NTAPEC  COMMON  1                   BCD CARD OUTPUT (TO PUNCH)
NTAPED  COMMON  1                   SPECIAL BCD OUTPUT (OPTIONALLY TO PRINT)
NTAPEE  COMMON  1                   SPECIAL UTILITY OUTPUT TAPE
NTAPEF  COMMON  1                   SPECIAL UTILITY INPUT TAPE
NTAPEG  COMMON  1                   UNDESIGNATED INPUT-OUTPUT
NTAPEH  COMMON  1                   UNDESIGNATED INPUT-OUTPUT
NTAPEI  COMMON  1                   UNDESIGNATED INPUT-OUTPUT
NTAPEJ  COMMON  1                   UNDESIGNATED INPUT-OUTPUT
NTPROG  COMMON  1                   PROGRAM TAPE NUMBER
NTINM   COMMON  1                   MONITOR INPUT TAPE (USUAL NTIN)
NTOUTM  COMMON  1                   MONITOR OUTPUT TAPE (USUAL NTOUT)
NTAU    COMMON  1                   USUAL VALUE OF NTAPEA
NTBU    COMMON  1                   ETC
NTCU    COMMON  1
NTDU    COMMON  1
NTEU    COMMON  1
NTFU    COMMON  1
NTGU    COMMON  1
NTHU    COMMON  1
NTIU    COMMON  1
NTJU    COMMON  1
IOU     COMMON  49                  IO UNIT TABLE
QUIT    COMMON  1                   SYSTEM EXIT ROUTINE
        REM                         (IOU AND QUIT SHARE THOSE FIFTY CELLS,
        REM                          STARTING AT OPPOSITE ENDS AND NOT
        REM                          MEETING IN THE MIDDLE (WE HOPE).)
PRFLG   COMMON  1                   FLAG TO CAUSE PRINTER STOP AT QUIT TIME
LINKNO  COMMON  1                   LINK NUMBER (LABEL) OF PROGRAM IN CORE
        COMMON  6
IDPROG  COMMON  1                   PROGRAM ID FOR LISTING PURPOSES
TITLE   COMMON  11                  PAGE TITLE
IDCOMP  COMMON  1                   COMPOUND ID
NPAGE   COMMON  1                   PAGE NUMBER
LINCT   COMMON  1                   LINES LEFT ON PAGE
LINMX   COMMON  1                   MAXIMUM LINES PER PAGE (BESIDES HEADING)
NCROS   COMMON  1                   NUMBER OF INPUT CARDS READ SINCE *DATA
```

```
C       SYSTEM COMMON ALLOCATION FOR =X-RAY 63=
        DIMENSION CARD(12), SPASE(58), TITLE(11)
        COMMON CARD,NTIN, NTOUT, NTAPEA,NTAPEB,NTAPEC,NTAPED,NTAPEE,
      1  NTAPEF,NTAPEG,NTAPEH,NTAPEI,NTAPEJ,NTPROG,NTINM,NTOUTM,NTAU,
      2  NTBU,NTCU,NTDU,NTEU,NTFU,NTGU,NTHU,NTIU,NTJU,SPASE,IDPROG,
      3  TITLE,IDCOMP,NPAGE,LINCT,LINMX,NCROS
```

APPENDIX IX

EXPLANATION OF APPENDIX IX

THE X-RAY SYSTEM IS DESIGNED TO BE RUN IN CONJUNCTION WITH, OR INDEPENDENTLY OF, OTHER MONITORS WITH AS FEW CHANGES AS POSSIBLE. THE SUBROUTINE =SYSCOM= (FOR FORTRAN OR IBSYS MONITORS) OR =SYSBEL= (FOR BELL MONITOR) INITIALIZES THE TAPE ASSIGNMENT STORAGE, LINE COUNTING, AND OTHER NECESSARY X-RAY FUNCTIONS. IT ASSUMES A CLEARED-TO-ZERO CORE CONDITION FOR THE STORAGE OF VALUES SET WITHIN ITSELF. THUS, IF AN OPERATOR CLEARS-AND-LOADS THE CALLING CARD WITH THE APPROPRIATE START CARD (=IBSCARD= WITH =SYSCOM= OR =IBSBEL= WITH =SYSBEL=) AND WITH THE X-RAY SYSTEM TAPE MOUNTED ON UNIT 85, EXECUTION WILL COMMENCE AND =SYSCOM= OR =SYSBEL= WILL GIVE INITIALIZATION FOR THE TAPE-UNIT DESIGNATION AS GIVEN IN SECTION 1.0-8.

WHEN IT IS DESIRED TO RUN THE X-RAY SYSTEM AS A SUB-SYSTEM OF SOME OTHER MONITOR, A PROGRAM MAY BE PREPARED WHICH STARTS EACH EXECUTION UNDER THAT MONITOR THEN TRANSFERS CONTROL TO THE X-RAY SYSTEM. WHEN THIS EXECUTION IS FINISHED THE X-RAY SYSTEM MUST THEN PROPERLY RESTORE THE CALLING MONITOR TO CONTROL FOR ACCOUNTING, ETC. STUDYING THE LISTINGS OF =85FORT= (WHICH IS DESIGNED FOR EXECUTION UNDER THE FORTRAN (II) MONITOR), =85BELL= (FOR THE BELL LABORATORY MONITOR), AND =85IBSY= (FOR THE IBM SYSTEM MONITOR) IS THE BEST WAY TO SEE ALL THE DETAILS OF THE PROCEDURE. HOWEVER, THE FOLLOWING SUMMARY MAY BE MADE-

(1) THE CALLING SYSTEM TRAPPING ABILITY (IF ANY) MUST BE DISABLED.

(2) HIGH CORE MUST BE ZEROED (IF NOT ALREADY DONE BY THE CALLING MONITOR).

(3) A PROPER EXIT ROUTINE (I.E.- ONE THAT WILL RESTORE THE CALLING MONITOR) MUST BE MOVED TO HIGH CORE AT =QUIT=.

(4) ALL TAPE SPECIFICATIONS (LOGICAL TAPE NUMBERS) AND PAGINATION CONSTANTS WHICH =SYSCOM= OR =SYSBEL= WOULD INITIALIZE TO VALUES NOT SUITABLE TO THE CALLING MONITOR MUST BE STORED.

(5) THE X-RAY LOADER MUST BE MOVED TO UPPER MEMORY AND EXECUTED.

AT THE END OF EXECUTION THE X-RAY SYSTEM TRANSFERS UNCONDITIONALLY TO =QUIT=, THUS RESTORING THE CALLING MONITOR IN THE MANNER SPECIFIED.

SYMBOLIC LISTING OF =185CARD=

```
*       LABEL
*        ROW
*        FAP
*185CARD - ON-LINE START CARD FOR X-RAY SYSTEM ON 85))
         COUNT    30
         TTL VERSION OF 2 JAN 63
* THIS CARD WILL INITIATE THE XRAY SYSTEM ON 85.  PUT CARD IN ON-LINE
* CARD READER. PUT PROGRAM TAPE ON 85. CLEAR, LOAD CARDS.
* PROVISION IS MADE FOR REDEFINING NTINM AND NTOUTM AT STUFF+2 AND
* STUFF+1, RESPECTIVELY.
         FUL
         ORG      0
P        TAPENO   85
*
         IOCT     3,,STUFF-3
         LCHA     LOS
         TCOA     *
*
ST       AXT      5,4
         TRA      RD
         TRA      RD
RD       REWP
         RTBP
         RCHP     IO
         TCOP     *
         RTBP
         RCHP     1
         TCOP     *
         TRCP     NG
         TRA      2
NG       TIX      RD,4,1
         HTR      ST
IO       IORT     0,,4
*
LOS      IOCP     QUIT,,1
         IOCD     NTPROG-2,,3
*
STUFF    HTR      QUIT                PROGRAM EXIT
         PZE      ,,                  NTOUTM
         PZE      ,,                  NTINM
         PZE      ,,10                NTPROG
*
NTPROG   BOOL     77431
QUIT     BOOL     77333
         END
*ENDIN
```

SYMBOLIC LISTING OF =185BEL=

```
*       LABEL
*        ROW
*        FAP
*185BEL - ON-LINE START CARD FOR X-RAY SYSTEM ON B5 UNDER BELL MONITOR
         COUNT    30
         TTL  VERSION OF 6 JUNE 1963
* THIS CARD WILL INITIATE THE XRAY SYSTEM ON B5.  PUT CARD IN ON-LINE
* CARD READER, PUT PROGRAM TAPE ON B5, CLEAR, LOAD CARDS.
* STUFF+1, RESPECTIVELY.
*    $$$REQUIRES IOUBE VERSION OF IO TABLE$$$
         FUL
         ORG      0
P        TAPENO   B5
*
         IOCT     3,,STUFF-3
         LCHA     LDS
         TCOA     *
*
ST       AXT      5,4
         TRA      RD
         TRA      RD
RD       REWP
         RTBP
         RCHP     IO
         TCOP     *
         RTBP
         RCHP     1
         TCOP     *
         TRCP     NG
         TRA      2
NG       TIX      RD,4,1
         HTR      ST
IO       IORT     0,,4
*
LDS      IOCP     QUIT,,1
         IOCD     NTPROG-2,,3
*
STUFF    HTR      QUIT                PROGRAM EXIT
         PZE      ,,                  NTOUTM
         PZE      ,,                  NTINM
         PZE      ,,15               NTPROG
*
NTPROG   BOOL     77431
QUIT     BOOL     77333
         END
```

SYMBOLIC LISTING OF =SYSCOM=

```
*       LABEL
*       FAP
*SYSCOM - SUBROUTINE TO INITIALIZE SYSTEM COMMON
        COUNT   100
        TTL VERSION OF NOV 62
        ENTRY   SYSCOM
SYSCOM  SXA     X4,4
        SXA     X2,2
*
* FOR ANY UNDEFINED SYSTEM TAPE, ETC., USE THE USUAL VALUE
        AXT     13,4
        CLA     NT,4
        NZT     NTPROG+1,4
        STO     NTPROG+1,4
        TIX     *-3,4,1
        CLA     NLINU
        NZT     LINMX
        STO     LINMX
*
        ZET     NTIN                IF THIS IS THE FIRST TIME SYSCOM HAS
        TRA     I1                    BEEN CALLED, COMPLETE INITIALIZATION
        AXT     12,4                SET WORKING TAPES
        CLA     NTINM+1,4
        STO     NTIN+1,4
        TIX     *-2,4,1
        AXT     12,4                RESET PAGE HEADING
        CLA     =H
        STO     TITLE+1,4
        TIX     *-1,4,1
        STZ     NPAGE
        STZ     NCROS
*
* UNLESS ONE IS ALREADY SUPPLIED, PUT MONITOR EXIT ROUTINE INTO QUIT
I1      ZET     QUIT
        TRA     I2
        AXT     QL,4
        CLA     QR+QL,4
        STO     QUIT+QL,4
        TIX     *-2,4,1
*
* DITTO FOR IOU TABLE
I2      ZET     IOU
        TRA     X2
        LAC     $(IOU),4
        CLA     0,4                 GET NUMBER OF ENTRIES
        ALS     18                    MOVE TO DECREMENT
        ORA     =020                  PUT ON BINARY-TAPE DESIGNATOR
        STO     IOU                   SAVE LARGEST LEGAL LOGICAL UNIT
        REM                             FOR COMPARISON IN IOSW
        STO     TXL
        AXT     12,2
        CLA     1,4                 MOVE TAPE TABLE TO COMMON
        STO     IOU,2                 IN INVERTED ORDER
        TXI     *+1,4,-1
        TXI     *+1,2,1
TXL     TXL     *-4,2,**
```

```
*
X2      AXT     **,2
X4      AXT     **,4
        TRA     1,4
*
* TABLE OF STANDARD TAPE ASSIGNMENTS
                ,,0                     USUAL NTJU
                ,,0                               I
                ,,0                               H
                ,,0                               G
                ,,4                     F
                ,,2                     E
                ,,6                               D
                ,,7                               C
                ,,12                    B
                ,,11                    A
                ,,6                           NTOUTM
                ,,5                           NTINM
                ,,3                           NTPROG
NT      BES     0
NLINU   PZE     ,,57                    USUAL MAXIMUM LINES/PAGE
        REM                               (EXCLUSIVE OF HEADING)
*
* THE FOLLOWING ROUTINE IS TO BE EXECUTED AT QUIT TO RETURN CONTROL
* TO THE FORTRAN MONITOR.
QR      AXT     MXL,4                   MOVE MONEX ROUTINE BACK WHERE IT
        CLA     QUIT+QL,4                 CAME FROM, SO 1-TO-CS WILL NOT
        STO     QR+QL,4                   TRAMPLE ALL OVER IT ON THE WAY IN.
        TIX     QUIT+1,4,1
        TRA     MONEX                   BYE BYE
* THE FOLLOWING STEPS PERFORM THE NORMAL FORTRAN-MONITOR EXIT FUNCTION.
MONEX   AXT     5,1                     INITIALIZE TRIAL COUNT
        REWA    1                       REWIND THE SYSTEM TAPE
        RTBA    1                       LOAD 1-TO-CS
        RCHA    LD1CS
        LCHA    0
        RTBA    1                       SKIP DOWN TO SIGN-ON RECORD
        RTBA    1
        TCOA    *
        TRCA    MXER
        TRA*    2                       EXIT TO MONITOR
MXER    TIX     MONEX+1,1,1             REDUNDANCY CHECK.  TRY AGAIN, OR ...
        HPR     -1,7                    GIVE UP
        TRA     MONEX                     AND MAYBE TRY LATER
LD1CS   ICCT    0,,3
MXL     EQU     *-MONEX
QL      EQU     *-QR
*
* SYSTEM COMMON ALLOCATION
CARD    COMMON  12                      BCD CARD RECORD (FORTRAN ARRAY) FILLED
        REM                               BY IFFC
NTIN    COMMON  1                       BCD INPUT TAPE (FROM CARD READER)
NTOUT   COMMON  1                       BCD OUTPUT TAPE (TO PRINTER)
NTAPEA  COMMON  1                       BINARY DATA TAPE (REFLECTIONS)
NTAPEB  COMMON  1                       BINARY DATA TAPE (STRUCTURE FACTORS)
NTAPEC  COMMON  1                       BCD CARD OUTPUT (TO PUNCH)
NTAPED  COMMON  1                       SPECIAL BCD OUTPUT (OPTIONALLY TO PRINT)
NTAPEE  COMMON  1                       SPECIAL UTILITY OUTPUT
NTAPEF  COMMON  1                       SPECIAL UTILITY INPUT
NTAPEG  COMMON  1                       UNDESIGNATED INPUT-OUTPUT
NTAPEH  COMMON  1                       UNDESIGNATED INPUT-OUTPUT
NTAPEI  COMMON  1                       UNDESIGNATED INPUT-OUTPUT
NTAPEJ  COMMON  1                       UNDESIGNATED INPUT-OUTPUT
```

```
NTPROG  COMMON   1          PROGRAM TAPE NUMBER
NTINM   COMMON   1          MONITOR INPUT TAPE (USUAL NTIN)
NTOUTM  COMMON   1          MONITOR OUTPUT TAPE (USUAL NTOUT)
NTAU    COMMON   1          USUAL VALUE OF NTAPEA
NTBU    COMMON   1          ETC
NTCU    COMMON   1
NTDU    COMMON   1
NTEU    COMMON   1
NTFU    COMMON   1
NTGU    COMMON   1
NTHU    COMMON   1
NTIU    COMMON   1
NTJU    COMMON   1
IOU     COMMON  49          IO UNIT TABLE
QUIT    COMMON   1          SYSTEM EXIT ROUTINE
        REM                 (IOU AND QUIT SHARE THOSE FIFTY CELLS,
        REM                  STARTING AT OPPOSITE ENDS AND NOT
        REM                  MEETING IN THE MIDDLE (WE HOPE).)
PRFLG   COMMON   1          FLAG TO CAUSE PRINTER STOP AT QUIT TIME
LINKNO  COMMON   1          LINK NUMBER (LABEL) OF PROGRAM IN CORE
        COMMON   6
IDPROG  COMMON   1          PROGRAM ID FOR LISTING PURPOSES
TITLE   COMMON  11          PAGE TITLE
IDCOMP  COMMON   1          COMPOUND ID
NPAGE   COMMON   1          PAGE NUMBER
LINCT   COMMON   1          LINES LEFT ON PAGE
LINMX   COMMON   1          MAXIMUM LINES PER PAGE (BESIDES HEADING)
NCRDS   COMMON   1          NUMBER OF INPUT CARDS READ SINCE *DATA
        END
```

SYMBOLIC LISTING OF =SYSBEL=

```
*       LABEL
*        FAP
*SYSBEL - SUBROUTINE TO INITIALIZE SYSTEM COMMON. BELL IOU TABLE.
        COUNT    100
        TTL VERSION OF NOV 62
        ENTRY    SYSCOM
SYSCOM  SXA      X4,4
        SXA      X2,2
*
* FOR ANY UNDEFINED SYSTEM TAPE, ETC., USE THE USUAL VALUE
        AXT      13,4
        CLA      NT,4
        NZT      NTPROG+1,4
        STO      NTPROG+1,4
        TIX      *-3,4,1
        CLA      NLINU
        NZT      LINMX
        STO      LINMX
*
        ZET      NTIN                IF THIS IS THE FIRST TIME SYSCOM HAS
        TRA      I1                    BEEN CALLED, COMPLETE INITIALIZATION
        AXT      12,4                SET WORKING TAPES
        CLA      NTINM+1,4
        STO      NTIN+1,4
        TIX      *-2,4,1
        AXT      12,4                RESET PAGE HEADING
        CLA      =H
        STO      TITLE+1,4
        TIX      *-1,4,1
        STZ      NPAGE
        STZ      NCRDS
*
* UNLESS ONE IS ALREADY SUPPLIED, PUT MONITOR EXIT ROUTINE INTO QUIT
I1      ZET      QUIT
        TRA      I2
        AXT      QL,4
        CLA      QR+QL,4
        STO      QUIT+QL,4
        TIX      *-2,4,1
*
* DITTO FOR IOU TABLE
I2      ZET      IOU
        TRA      X2
        LAC      $(IOU),4
        CLA      0,4                 GET NUMBER OF ENTRIES
        ALS      18                    MOVE TO DECREMENT
        ORA      =020                  PUT ON BINARY-TAPE DESIGNATOR
        STO      IOU                   SAVE LARGEST LEGAL LOGICAL UNIT
        REM                              FOR COMPARISON IN IOSW
        STO      TXL
        AXT      12,4
        CLA      1,4                 MOVE TAPE TABLE TO COMMON
        STO      IOU,2                 IN INVERTED ORDER
        TXI      *+1,4,-1
        TXI      *+1,2,1
TXL     TXL      *-4,2,**
```

```
*
X2      AXT     **,2
X4      AXT     **,4
        TRA     1,4
*
* TABLE OF STANDARD TAPE ASSIGNMENTS
                ,,0                     USUAL NTJU
                ,,0                             I
                ,,0                             H
                ,,0                             G
                ,,0                             F
                ,,0                             E
                ,,3                       D
                ,,14                    C
                ,,16                      B
                ,,6                       A
                ,,3                     NTOUTM
                ,,2                     NTINM
                ,,15                    NTPROG
NT      BES     0
NLINU   PZE     ,,52                  USUAL NOL MAXIMUM LINES/PAGE
        REM                             (EXCLUSIVE OF HEADING)
*
* THE FOLLOWING ROUTINE IS TO BE EXECUTED AT QUIT TO RETURN CONTROL
* TO THE FORTRAN MONITOR.
QR      AXT     MXL,4                 MOVE MONEX ROUTINE BACK WHERE IT
        CLA     QUIT+QL,4               CAME FROM, SO 1-TO-CS WILL NOT
        STO     QR+QL,4                 TRAMPLE ALL OVER IT ON THE WAY IN.
        TIX     QUIT+1,4,1
        TRA     MONEX                 BYE BYE
* THE FOLLOWING STEPS PERFORM THE NORMAL FORTRAN-MONITOR EXIT FUNCTION.
MONEX   AXT     5,1                   INITIALIZE TRIAL COUNT
        REWA    1                     REWIND THE SYSTEM TAPE
        RTBA    1                     LOAD 1-TO-CS
        RCHA    LO1CS
        LCHA    0
        RTBA    1                     SKIP DOWN TO SIGN-ON RECORD
        RTBA    1
        TCOA    *
        TRCA    MXER
        TRA*    2                     EXIT TO MONITOR
MXER    TIX     MONEX+1,1,1           REDUNDANCY CHECK.  TRY AGAIN, OR ...
        HPR     -1,7                  GIVE UP
        TRA     MONEX                   AND MAYBE TRY LATER
LO1CS   IOCT    0,,3
MXL     EQU     *-MONEX
QL      EQU     *-QR
*
* SYSTEM COMMON ALLOCATION
CARD    COMMON  12                    BCD CARD RECORD (FORTRAN ARRAY) FILLED
        REM                             BY IFFC
NTIN    COMMON  1                     BCD INPUT TAPE (FROM CARD READER)
NTOUT   COMMON  1                     BCD OUTPUT TAPE (TO PRINTER)
NTAPEA  COMMON  1                     BINARY DATA TAPE (REFLECTIONS)
NTAPEB  COMMON  1                     BINARY DATA TAPE (STRUCTURE FACTORS)
NTAPEC  COMMON  1                     BCD CARD OUTPUT (TO PUNCH)
NTAPED  COMMON  1                     SPECIAL BCD OUTPUT (OPTIONALLY TO PRINT)
NTAPEE  COMMON  1                     SPECIAL UTILITY OUTPUT
NTAPEF  COMMON  1                     SPECIAL UTILITY INPUT
NTAPEG  COMMON  1                     UNDESIGNATED INPUT-OUTPUT
NTAPEH  COMMON  1                     UNDESIGNATED INPUT-OUTPUT
NTAPEI  COMMON  1                     UNDESIGNATED INPUT-OUTPUT
NTAPEJ  COMMON  1                     UNDESIGNATED INPUT-OUTPUT
```

```
NTPROG  COMMON  1          PROGRAM TAPE NUMBER
NTINM   COMMON  1          MONITOR INPUT TAPE (USUAL NTIN)
NTOUTM  COMMON  1          MONITOR OUTPUT TAPE (USUAL NTOUT)
NTAU    COMMON  1          USUAL VALUE OF NTAPEA
NTBU    COMMON  1          ETC
NTCU    COMMON  1
NTDU    COMMON  1
NTEU    COMMON  1
NTFU    COMMON  1
NTGU    COMMON  1
NTHU    COMMON  1
NTIU    COMMON  1
NTJU    COMMON  1
IOU     COMMON  49         IO UNIT TABLE
QUIT    COMMON  1          SYSTEM EXIT ROUTINE
        REM                (IOU AND QUIT SHARE THOSE FIFTY CELLS,
        REM                 STARTING AT OPPOSITE ENDS AND NOT
        REM                 MEETING IN THE MIDDLE (WE HOPE).)
PRFLG   COMMON  1          FLAG TO CAUSE PRINTER STOP AT QUIT TIME
LINKNO  COMMON  1          LINK NUMBER (LABEL) OF PROGRAM IN CORE
        COMMON  6
IDPROG  COMMON  1          PROGRAM ID FOR LISTING PURPOSES
TITLE   COMMON  11         PAGE TITLE
IDCOMP  COMMON  1          COMPOUND ID
NPAGE   COMMON  1          PAGE NUMBER
LINCT   COMMON  1          LINES LEFT ON PAGE
LINMX   COMMON  1          MAXIMUM LINES PER PAGE (BESIDES HEADING)
NCRDS   COMMON  1          NUMBER OF INPUT CARDS READ SINCE *DATA
        END
```

SYMBOLIC LISTING OF *BSFORT*

```
*       LABEL
*       FAP
*BSFOR     PROGRAM TO CALL X-RAY SYSTEM FROM BS
        COUNT   100
        TTL VERSION OF 1 JAN 63
*
P       TAPENO  BS
        CLA     *10817              SET PROGRAM TAPE NUMBER
*
        AXT     NX,2                MOVE LOADER TO UPPER MEMORY
        CLA     XLA+NX,2
        STO     .XLA+NX,2
        TIX     *-2,2,1
*
        TEFP    *+1
        REWP
 CHC    AXT     5,1
        RTBP                        READ AND CHECK LINK LABEL
        RCHP    CHSEL1
        TCOP    *
        TRCP    CHD
        TEFP    CHD
        AXT     5,1                 GO TO LOADER
        TRA     .XLC
CHD     BSRP                        REDUNDANCY - TRY AGAIN
        TIX     CHC+1,1,1
        TRA     .XXA
CHSEL1  IORT    .XLZ,,4             READ IN LABEL
*
* LINK LOADER (EXECUTED FROM UPPER MEMORY)     ENTER AT .XLC
XLA     BSRP                        REDUNDANCY - TRY AGAIN
        IOT
        NOP
        TIX     .XLC,1,1
XXA     WPDA                        COMMENT BAD TAPE
        AXT     12,1
        RCHA    .XCIL
        TRA     .XXA1
        LCHA    .XCIL
 XXA1   LCHA    .XCIL+1
        LXA     .XCIL,2
        TXI     .XXA2,2,1
 XXA2   SXA     .XCIL,2
        TIX     .XXA1-1,1,1
 XXA3   HTR     .XXA3
XLC     RTBP                        READ IN LINK
        RCHP    .XLZ+1
XLD     TCOP    .XLD                DELAY
        TRCP    .XLA
        TEFP    .XXA
        TRA     .XLZ+2              OK, GO TO THE LINK (SEE NOTE BELOW)
        REM
XCI     OCT     041100020000   9L   X-RAY PROGRAM TAPE UNREADABLE
        OCT     010000000000   8L
        OCT     202201000000   7L
```

```
        OCT     000400000000   6L
        OCT     000000450100   5L
        OCT     000020102000   4L
        OCT     000004000200   3L
        OCT     000000000400   2L
        OCT     020042005000   1L
        OCT     210004100000   0L
        OCT     143521060200  11L
        OCT     020242417500  12L
        REM
 XCIL   IOCT    .XCI,,1
        IOCT    .XL(0),,1
XLZ             ,,**                LABEL
        IOCP    **,,**              IO COMMAND FOR FIRST SEGMENT
        IORT    **,,**              IO COMMAND FOR SECOND SEGMENT OF LINK
        TRA     **                  STARTING INSTRUCTION
        REM IF THE TAPE WAS PREPARED BY MONITOR CHAIN, THERE WILL BE
        REM A SINGLE IORT AT .XLZ+1 AND THE TRA AT .XLZ+2.  TO RETAIN
        REM COMPATIBILITY, WE TRANSFER TO .XLZ+2, WHICH IS EITHER A TRA
        REM OR AN IORT, WHICH IS THE SAME THING AS A (TAGLESS) TXH WHICH
        REM IS THE SAME AS A NOP FOR PRESENT PURPOSES.
 XL(0)  PZE
NX      EQU     *-XLA
        REM
 .X     COMMON  0
 .XLA   EQU     .X+2
 .XXA   EQU     .XLA+4
 .XXA1  EQU     .XXA+5
 .XXA2  EQU     .XXA1+3
 .XXA3  EQU     .XXA2+2
 .XLC   EQU     .XXA3+1
 .XLO   EQU     .XLC+2
 .XCI   EQU     .XLO+4
 .XCIL  EQU     .XCI+12
 .XLZ   EQU     .XCIL+2
.XL(0)  EQU     .XLZ+4
        COMMON  24
NTPROG  COMMON  1
        END
```

SYMBOLIC LISTING OF =B5IBSY=

```
*       LABEL                                                           B5IB000
*       FAP                                                             B5IB001
*B5IBSY      PROGRAM TO USE X-RAY SYSTEM UNDER THE IBSYS MONITOR....    B5IB002
        COUNT   150                                                     B5IB003
        SST                     LETS HAVE A LOOK AT IBSYS SYMBOL TBL    B5IB004
        LTM                                                             B5IB005
        LFTM                    GIVE UP FLOATING TRAP                   B5IB006
        STZ     KILL            SHUT OFF TRAPPING MODE                  B5IB007
        ENB     KILL            KILL ALL DATA CHANNEL TRAPS             B5IB008
        LSNM                    GIVE UP BEING A 704(IF ANY)             B5IB009
TRICKY  TCOA    *               MAKE SHURE CHAN A QUIET                 B5IB010
        TCOB    *               DITTO B                                 B5IB011
        TRCA    *+1             SHUT OFF ALL IO CHECKS                  B5IB012
        TRCB    *+1                                                     B5IB013
        TEFA    *+1                                                     B5IB014
        TEFB    *+1                                                     B5IB015
        DCT                     FORGET ABOUT DIVIDE OVERFLOWS           B5IB016
        NOP                                                             B5IB017
        BTT     1000            SHUT OFF THOSE POSITION INDICATORS      B5IB018
        NOP                                                             B5IB019
        BTT     2000                                                    B5IB020
        NOP                                                             B5IB021
        ETT     1000                                                    B5IB022
        NOP                                                             B5IB023
        ETT     2000                                                    B5IB024
        NOP                                                             B5IB025
        SLF                     TO HELL WITH SENSE LIGHTS               B5IB026
        TOV     *+1             WHO CARES IF THERE WAS AN OVERFLOW      B5IB027
BURP    AXT     5,1             GET SET TO MAKE 5 TRIES                 B5IB028
        REWB    5               REWIND THE X-RAY SYSTEM TAPE            B5IB029
        RTBB    5               SKIP DOWN THE X-RAY TAPE                B5IB030
        TCOB    *                                                       B5IB031
        TEFB    *+2             TILL AN END OF FILE IS FOUND            B5IB032
        TRA     *-3             KEEP TRYING                             B5IB033
        WTBB    5               PUT IBSYSES GOODIES ON THE TAIL END OF B5IB034
        RCHB    DUMPY           FIVE                                    B5IB035
        LCHB    DUMPY+1                                                 B5IB036
        TCOB    *               WAIT                                    B5IB037
        TRCB    CHDDR           AND HOPE THERE ARE NO REDUNDANCIES...   B5IB038
        TRA     MADEIT          WHEW....                                B5IB039
CHDDR   TIX     BURP+1,1,1      TRY FIVE TIMES BEFORE QUITTING          B5IB040
        WPDA                    THEN GIVE UP WITH A BAD TAPE COMMENT    B5IB041
        AXT     12,1                                                    B5IB042
        RCHA    STUFF                                                   B5IB043
        TRA     PRINT                                                   B5IB044
        LCHA    STUFF                                                   B5IB045
PRINT   LCHA    STUFF+1                                                 B5IB046
        LXA     STUFF,2                                                 B5IB047
        TXI     *+1,2,1                                                 B5IB048
        SXA     STUFF,2                                                 B5IB049
        TIX     PRINT-1,1,1                                             B5IB050
        TCOA    *                                                       B5IB051
        TTR*    SYSRET          AS LONG AS WE CANT GET ON LETS GET OFF..B5IB052
```

```
DUMPY   IOCT    0,,5                                                    85I8053
        IOCD    6,,1996                                                 85I8054
STUFF   IOCT    XCI,,1                                                  85I8055
        IOCT    XL(0),,1                                                85I8056
*  THE FOLLOWING STEPS CLEAR THE MEMORY TO ZERO IN A FAIR IMITATION OF  85I8057
*  THE STANDARD FORTRAN MONITOR AND ASSURE THAT SYSCOM WILL BE HAPPY....85I8058
        AXC     NNEND,4         INITIALIZE CORE TO ZERO                 85I8059
        TXI     *+1,4,32767                                             85I8060
        STZ     32767,4                                                 85I8061
        TIX     *-1,4,1                                                 85I8062
*  THE FOLLOWING STEPS JAM A WAY OF RESTORING IBSYS INTO QUIT WHICH IS  85I8063
*       WHERE FINAL, TERMINAL, DONE FOR, I GIVE UP, TYPE TRANSFERS GO TO 85I8064
MADEIT  CLA     SYSIOR          GET LOC OF IBSYS CLOCK OUT              85I8065
        STA     HIBSYS          STORE IT IN EXIT ROUTINE                85I8066
        CLA     SYSRET          GET THE ADDRESS ON SYSTEM RETURN        85I8067
        ALS     18              DECREMENTIZE IT                         85I8068
        STO     HIBSYS+1        FIX UP CLOCK OUT CALLING SEQUENCE       85I8069
        REWB    5               REWIND X-RAY SYSTEM TAPE                85I8070
        AXT     MXL,4                                                   85I8071
        CLA     MONEX+MXL,4     PICK UP EXIT COMMANDS                   85I8072
        STO     QUIT+MXL,4      AND STUFF THEM IN QUIT                  85I8073
        TIX     *-2,4,1         REGION IN COMMON STORAGE                85I8074
        TRA     LINFIX                                                  85I8075
MONEX   AXT     5,1             GIVE FIVE TRIES AT RESTORING IBSYS      85I8076
        BSRB    5               BACK OFF                                85I8077
        TEFB    QUIT+3          AND LOOK FOR  END OF FILE               85I8078
        RTBB    5               READ UNTIL EOF DETECTED                 85I8079
        TCOB    QUIT+4          WAIT FOR QUIET CHANNEL                  85I8080
        TEFB    QUIT+7          IS EOF REACHED...                       85I8081
        TRA     QUIT+3          NO    TRY AGAIN                         85I8082
        TRCB    QUIT+7          DONT WORRY ABOUT REDUNDANCIES HERE.     85I8083
        RTBB    5               LETS TRY TO GET IBSYS BACK ON THE AIR   85I8084
        RCHB    QUIT+21         BRING BACK IBNUC ET. AL. ......         85I8085
        LCHB    QUIT+22                                                 85I8086
        TCOB    QUIT+11         LET IT GET IN ----STEADY NOW-----       85I8087
        TRCB    QUIT+18         REDUNDANCY HERE COULD REALLY SHOOT US UP85I8088
        RUNB    5               REWIND AND UNLOAD X-RAY SYSTEM          85I8089
        WEFB    2               END OFF THE IBSYS PUNCH TAPE SO THAT    85I8090
        WEFB    2                 THE NEXT MANS JOB WILL RUN*******     85I8091
HIBSYS  TSX     **,4            CALL CLOCKOUT                           85I8092
        FIVE    ,,**            CALLING SEQUENCE OF CLOCKING OPERATION  85I8093
        BSRB    5               NUTS****** $ = * . ( . )//              85I8094
        TIX     QUIT+8,1,1      TRY IT FOUR MORE TIMES FOR KICKS        85I8095
        TRA     QUIT+13         HAVING FAILED THAT ...PRAY THAT ENOUGH  85I8096
        IOCT    0,,5            IS RESTORED TO COMPLETELY BAFFEL THE    85I8097
        IOCD    6,,1996         OPERATOR.... (DONT CRY THINGS CANT GET  85I8098
        REM                     MUCH WORSE..... CAN THEY.......         85I8099
MXL     EQU     *-MONEX                                                 85I8100
KILL    PZE     0,0,0                                                   85I8101
*  INITIALIZE OUR SYSTEM TAPES TO AGREE WITH THE USUAL U. MD. SET UP    85I8102
*  THE FOLLOWING STEPS DEFINE TAPES DIFFERENTLY THAN U.W. STANDARD      85I8103
*  AS SET BY SYSTEM INITIALIZING SUBROUTINE SYSCOM                      85I8104
*  FINAL VERSION OF BSIBSYS WILL HAVE TO BE MUCH SMARTER....            85I8105
LINFIX  CLA     =10B17          DEFINE PROGRAM TAPE TO BE B5            85I8106
        STO     NTPROG                                                  85I8107
        CLA     =8B17           SET PRINT TAPE TO B1                    85I8108
        STO     NTPROG-2          STO INPUT IS STILL ON A2              85I8109
        STO     NTPROG-6        FOURIER OUTPUT IS ALSO ON B1            85I8110
        CLA     =2B17           SET OFFLINE PUNCH TAPE TO BE B2         85I8111
        STO     NTPROG-5                                                85I8112
        CLA     =6B17           SET  SET NTAPEE                         85I8113
        STO     NTPROG-7                                                85I8114
*                                                                       85I8115
        AXT     NX,2            MOVE LOADER TO UPPER MEMORY             85I8116
        CLA     XLA+NX,2                                                85I8117
        STO     .XLA+NX,2                                               85I8118
        TIX     *-2,2,1                                                 85I8119
*                                                                       85I8120
        TEFB    *+1                                                     85I8121
        REWB    5                                                       85I8122
```

```
 CHC    AXT     5,1
        RTBB    5                       READ AND CHECK LINK LABEL
        RCHB    CHSEL1
        TCOB    *
        TRCB    CHD
        TEFB    CHD
        AXT     5,1                     GO TO LOADER
        TRA     .XLC
CHD     BSRB    5                       REDUNDANCY TRY AGAIN
        TIX     CHC+1,1,1
        TRA     .XXA
CHSEL1  IORT    .XLZ,,4                 READ IN LABEL
*
* LINK  LOADER (EXECUTED FROM UPPER MEMORY)      ENTER AT .XLC
XLA     BSRB    5                       REDUNDANCY TRY AGAIN
        IOT
        NOP
        TIX     .XLC,1,1
XXA     WPDA                            COMMENT BAD TAPE
        AXT     12,1
        RCHA    .XCIL
        TRA     .XXA1
        LCHA    .XCIL
 XXA1   LCHA    .XCIL+1
        LXA     .XCIL,2
        TXI     .XXA2,2,1
 XXA2   SXA     .XCIL,2
        TIX     .XXA1-1,1,1
        TCOA    .XXA2+2
        WPDA
        RCHA    .FUDGE
        AXT     100,1
        LCHA    .FUDGE
        TIX     .XXA3-2,1,1
 XXA3   TRA     QUIT                    AS LONG AS WE CANT GET ON THE AIR LETS
        REM                               TRY TO PUT MAMA B. BACK ON AND LET
        REM                               SOMEONE ELSE PAY THE TAB.....  $$$$$
XLC     RTBB    5                       READ IN LINK
        RCHB    .XLZ+1
XLD     TCOB    .XLD                    DELAY
        TRCB    .XLA
        TEFB    .XXA
        TRA     .XLZ+2                  OK, GO TO THE LINK (SEE NOTE BELOW)
        REM
XCI     OCT     041100020000   9L       X-RAY PROGRAM TAPE UNREADABLE
        OCT     010000000000   8L
        OCT     202201000000   7L
        OCT     000400000000   6L
        OCT     000000450100   5L
        OCT     000020102000   4L
        OCT     000004000200   3L
        OCT     000000000400   2L
        OCT     020042005000   1L
        OCT     210004100000   0L
        OCT     143521060200  11L
        OCT     020242417500  12L
FUDGE   IOCT    NTIN,,1                 FUDGE A FEW EXTRA LINES SO OPERATOR WILL
        REM                               SEE COMMENTS
        REM
 XCIL   IOCT    .XCI,,1
        IOCT    .XL(0),,1
XLZ             ,,**                    LABEL
        IOCP    **,,**                  IO COMMAND FOR FIRST SEGMENT
```

```
         IORT     **,,**              IO COMMAND FOR SECOND SEGMENT OF LINK   85I8186
         TRA      **                  STARTING INSTRUCTION                    85I8187
         REM IF THE TAPE WAS PREPARED BY MONITOR CHAIN, THERE WILL BE        85I8188
         REM A SINGLE IORT AT .XLZ+1 AND THE TRA AT .XLZ+2.  IO RETAIN       85I8189
         REM COMPATIBILITY, WE TRANSFER TO .XLZ+2, WHICH IS EITHER A TRA     85I8190
         REM OR AN IORT, WHICH IS THE SAME THING AS A (TAGLESS) TXH WHICH    85I8191
         REM IS THE SAME AS A NOP FOR PRESENT PURPOSES.                      85I8192
 XL(0)   PZE                                                                 85I8193
NX       EQU      *-XLA                                                      85I8194
NNEND    EQU      *                   TO DEFINE LAST LOCATION OF PROGRAM     85I8195
         REM                                                                 85I8196
.X       EQU      32561                                                      85I8197
 .XLA    EQU      .X+2                                                       85I8198
 .XXA    EQU      .XLA+4                                                     85I8199
 .XXA1   EQU      .XXA+5                                                     85I8200
 .XXA2   EQU      .XXA1+3                                                    85I8201
 .XXA3   EQU      .XXA2+8                                                    85I8202
 .XLC    EQU      .XXA3+1                                                    85I8203
 .XLO    EQU      .XLC+2                                                     85I8204
 .XCI    EQU      .XLO+4                                                     85I8205
.FUDGE   EQU      .XCI+12                                                    85I8206
.XCIL    EQU      .FUDGE+1                                                   85I8207
 .XLZ    EQU      .XCIL+2                                                    85I8208
.XL(0)   EQU      .XLZ+4                                                     85I8209
NTIN     EQU      32549                                                      85I8210
NTPROG   EQU      32537                                                      85I8211
QUIT     EQU      32475                                                      85I8212
LINMX    EQU      32451                                                      85I8213
         END                                                                 85I8214
```

SYMBOLIC LISTING OF =B5BELL=

```
*       LABEL
*       FAP
*B5BELL     PROGRAM TO USE X-RAY SYSTEM UNDER THE BELL MONITOR
*
        COUNT   150
        CALL    FOOL8E
        LTM
        LFTM                        GIVE UP FLOATING TRAP
        STZ     KILL                SHUT OFF TRAPPING MODE
        ENB     KILL                KILL ALL DATA CHANNEL TRAPS
        CLA     TRICK1
        STO     11
        STO     13
        LSNM                        GIVE UP BEING A 704(IF ANY)
TRICKY  TCOA    *                   MAKE SHURE CHAN A QUIET
        TCOB    *                   DITTO B
        TRCA    *+1                 SHUT OFF ALL IO CHECKS
        TRCB    *+1
        TEFA    *+1
        TEFB    *+1
        DCT                         FORGET ABOUT DIVIDE OVERFLOWS
        NOP
        BTT     1000                SHUT OFF THOSE POSITION INDICATORS
        NOP
        BTT     2000
        NOP
        ETT     1000
        NOP
        ETT     2000
        NOP
        SLF                         TO HELL WITH SENSE LIGHTS
        TOV     *+1                 WHO CARES IF THERE WAS AN OVERFLOW
*  THE FOLLOWING STEPS CLEAR THE MEMORY TO ZERO IN A FAIR IMITATION OF
*  THE STANDARD FORTRAN MONITOR AND ASSURE THAT SYSCOM WILL BE HAPPY....
        AXC     NNEND,4            INITIALIZE CORE TO ZERO
        TXI     *+1,4,32767
        STZ     32767,4
        TIX     *-1,4,1
*       THE FOLLOWING STEPS JAM A PROPER BELL EXIT INTO QUIT WHICH IS
*       WHERE FINAL, TERMINAL, DONE FOR, I GIVE UP, TYPE TRANSFERS GO TO
        AXT     MXL,4
        CLA     MONEX+MXL,4         PICK UP EXIT COMMANDS
        STO     QUIT+MXL,4          AND STUFF THEM IN QUIT
        TIX     *-2,4,1             REGION IN COMMON STORAGE
        TRA     LINFIX
MONEX   REWA    1                   REWIND SYSTEM TAPE
        RTBA    1                   LOAD THE FIRST RECORD OF
        REM                         THE BELL MONITOR BY SIMULATION
        REM                         PUSH LOAD TAPE BUTTON
        RCHA    QUIT+5              RESET AND LOAD CHANNEL A
        REM                         WITH A COMMAND TO BRING IN THE
        REM                         FIRST THREE WORDS OF THE FIRST RECORD
        LCHA    0                   LOAD DATA CHANNEL WITH FIRST WORD OF
        REM                         BOOT STRAP AND PULL UP ON SAID STRAP
        TRA     1                   THE LOAD TAPE BUTTON IS NOW PUSHED...
        REM                         GOOD LUCK MOTHER BELL ... AND HAPPY
        REM                         LANDINGS
```

```
LDICS   IOCT    0,,3            TRANSMIT THREE WORDS STARTING AT
        REM                     LOCATION ZERO AND TRANSFER BACK WITHOUT
        REM                     DISCONNECTING
MXL     EQU     *-MONEX
KILL    PZE     0,0,0
TRICK1  TTR     TRICKY
*  THE  FOLLOWING TWO CONSTS DEFINE THE SYSTEM PROG TAPE AND MAX LINES.
PROGTP  PZE     0,0,15
LINES   PZE     0,0,52
*       SET THE MAXIMUM LINES/PAGE (BESIDES HEADING) FOR BELL LIST TAPE
LINFIX  CLA     LINES
        STO     LINMX
        CLA     PROGTP
        STO     NTPROG
*
        AXT     NX,2            MOVE LOADER TO UPPER MEMORY
        CLA     XLA+NX,2
        STO     .XLA+NX,2
        TIX     *-2,2,1
*
        TEFB    *+1
        REWB    5
 CHC    AXT     5,1
        RTBB    5               READ AND CHECK LINK LABEL
        RCHB    CHSEL1
        TCOB    *
        TRCB    CHD
        TEFB    CHD
        AXT     5,1             GO TO LOADER
        TRA     .XLC
CHD     BSRB    5               REDUNDANCY TRY AGAIN
        TIX     CHC+1,1,1
        TRA     .XXA
CHSEL1  IORT    .XLZ,,4         READ IN LABEL
*
* LINK  LOADER (EXECUTED FROM UPPER MEMORY)     ENTER AT .XLC
XLA     BSRB    5               REDUNDANCY TRY AGAIN
        IOT
        NOP
        TIX     .XLC,1,1
XXA     WPDA                    COMMENT BAD TAPE
        AXT     12,1
        RCHA    .XCIL
        TRA     .XXA1
        LCHA    .XCIL
 XXA1   LCHA    .XCIL+1
        LXA     .XCIL,2
        TXI     .XXA2,2,1
 XXA2   SXA     .XCIL,2
        TIX     .XXA1-1,1,1
        TCOA    .XXA2+2
        WPDA
        RCHA    .FUDGE
        AXT     100,1
        LCHA    .FUDGE
        TIX     .XXA3-2,1,1
 XXA3   TRA     QUIT            AS LONG AS WE CANT GET ON THE AIR LETS
        REM                       TRY TO PUT MAMA B. BACK ON AND LET
        REM                       SOMEONE ELSE PAY THE TAB.....  $$$$$
XLC     RTBB    5               READ IN LINK
        RCHB    .XLZ+1
XLD     TCOB    .XLD            DELAY
        TRCB    .XLA
```

```
         TEFB     .XXA
         TRA      .XLZ+2                OK, GO TO THE LINK (SEE NOTE BELOW)
         REM
XCI      OCT      041100020000   9L X-RAY PROGRAM TAPE UNREADABLE
         OCT      010000000000   8L
         OCT      202201000000   7L
         OCT      000400000000   6L
         OCT      000000450100   5L
         OCT      000020102000   4L
         OCT      000004000200   3L
         OCT      000000000400   2L
         OCT      020042005000   1L
         OCT      210004100000   0L
         OCT      143521060200  11L
         OCT      020242417500  12L
FUDGE    IOCT     NTIN,,1               FUDGE A FEW EXTRA LINES SO OPERATOR WILL
         REM                              SEE COMMENTS
         REM
 XCIL    IOCT     .XCI,,1
         IOCT     .XL(0),,1
XLZ               ,,**                  LABEL
         IOCP     **,,**                IO COMMAND FOR FIRST SEGMENT
         IORT     **,,**                IO COMMAND FOR SECOND SEGMENT OF LINK
         TRA      **                    STARTING INSTRUCTION
         REM  IF THE TAPE WAS PREPARED BY MONITOR CHAIN, THERE WILL BE
         REM  A SINGLE IORT AT .XLZ+1 AND THE TRA AT .XLZ+2.  TO RETAIN
         REM  COMPATIBILITY, WE TRANSFER TO .XLZ+2, WHICH IS EITHER A TRA
         REM  OR AN IORT, WHICH IS THE SAME THING AS A (TAGLESS) TXH WHICH
         REM  IS THE SAME AS A NOP FOR PRESENT PURPOSES.
 XL(0)   PZE
NX       EQU      *-XLA
NNEND    EQU      *                     TO DEFINE LAST LOCATION OF PROGRAM
         REM
.X       EQU      32561
 .XLA    EQU      .X+2
 .XXA    EQU      .XLA+4
 .XXA1   EQU      .XXA+5
 .XXA2   EQU      .XXA1+3
 .XXA3   EQU      .XXA2+8
 .XLC    EQU      .XXA3+1
 .XLD    EQU      .XLC+2
 .XCI    EQU      .XLD+4
.FUDGE   EQU      .XCI+12
.XCIL    EQU      .FUDGE+1
 .XLZ    EQU      .XCIL+2
.XL(0)   EQU      .XLZ+4
NTIN     EQU      32549
NTPROG   EQU      32537
QUIT     EQU      32475
LINMX    EQU      32451
         END
```

APPENDIX X

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APPENDIX XI

=LISTUP= - A NON-SYSTEM LISTING UPDATE PROGRAM

=LISTUP= IS A PROGRAM TO UPDATE A SYMBOLIC LISTING TAPE BY ADDING, REPLACING, OR DELETING LISTINGS FROM A MASTER TAPE. ALTHOUGH WRITTEN FOR, AND INCLUDED WITH, THE =X-RAY 63= SYSTEM, THIS PROGRAM RUNS INDEPENDENTLY AND IS NOT A PART OF NOR DOES IT RUN IN THAT SYSTEM. THE PROGRAM WAS WRITTEN BY DARRELL F. HIGH.

A. PREPARATION OF THE SOURCE TAPE.

THE INPUT TAPES TO THIS PROGRAM ARE EITHER THE OUTPUT OF PREVIOUS RUNS OF THE PROGRAM, OR ELSE LISTING OUTPUTS OF THE FORTRAN COMPILER AND FAP ASSEMBLER IN THE FORTRAN MONITOR SYSTEM. THERE ARE ONLY THREE RULES FOR THE PREPARATION OF THESE TAPES.

RULE 1 - MANDATORY. THE SYMBOLIC DECK FOR EACH PROGRAM SHALL HAVE AS ITS FIRST CARD THE MONITOR CONTROL CARD =*LABEL=, CONTAINING =*= IN COLUMN 1, =LABEL= IN COLUMNS 7-11 OR COLUMNS 8-12, AND SERIAL INDENTIFICATION IN COLUMNS 73-78. (COLUMNS 79-80 ARE IGNORED.)

RULE 2 - MANDATORY. THE SEQUENCE OF DECKS ON THE TAPE SHALL BE IN INCREASING ORDER OF THEIR ID, TAKEN IN 709 COLLATING SEQUENCE. THE CONTROL OF THE UPDATING PROCESS IS BASED ON THESE =*LABEL= RECORDS.

RULE 3 - OPTIONAL, BUT LEADS TO ELIMINATION OF SPURIOUS INFORMATION FROM THE LISTINGS. AFTER THE LAST SYMBOLIC DECK IN THE JOB (OR AFTER ANY SYMBOLIC DECK WHICH IS FOLLOWED BY OTHER THAN ANOTHER SYMBOLIC DECK

WITH ITS =*LABEL= CARD), INCLUDE A CARD CONTAINING =*ENDIN= IN COLS 1-6. THIS CAUSES ALL LINES ON THE LISTING TO BE SKIPPED, BEGINNING WITH THE =*ENDIN= RECORD, DOWN TO THE NEXT =*LABEL= RECORD OR THE END-OF-FILE.

B. OPERATION OF THE PROGRAM.

THE MASTER LISTING TAPE TO BE UPDATED IS MOUNTED ON UNIT (A5), THE UPDATE LISTING TAPE IS MOUNTED ON UNIT (A6), AND AN UPDATED LISTING TAPE WILL BE WRITTEN ON (B6). CONTROL INFORMATION WILL BE READ FROM UNIT (A2). IN THE FIRST STEP, THE THREE INPUT TAPES (A2), (A5), AND (A6) ARE RUN IN AS FOLLOWS. ALL RECORDS AN (A5) AND (A6) ARE SKIPPED DOWN TO, BUT NOT INCLUDING, THE FIRST =*LABEL= CARD WHICH HAS NON-BLANK ID. (THIS MEANS THAT MONITOR SIGN-ON REMARKS, ETC., ARE SKIPPED. AS LONG AS THEY CONTAIN NO =*LABEL= RECORDS WITH NON-BLANK ID, THERE MAY BE OUTPUT FROM PREVIOUS JOBS ON THE SOURCE TAPES (A5) AND (A6). THIS FEATURE IS CONVENIENT WHEN ONE OF THE TAPES IS PREPARED BY A SYMBOLIC UPDATE JOB FOLLOWED BY AN ASSEMBLY AND COMPILATION JOB.) ALL RECORDS ON (A2) ARE TRANSCRIBED ONTO THE OUTPUT, (B6), UNTIL ONE IS ENCOUNTERED WITH A =*= IN COLUMN 1. THUS PROVISION IS MADE FOR LABELING THE OUTPUT TAPE. NO FURTHER CARDS FROM TAPE (A2) WILL BE TRANSCRIBED (SEE EXCEPTION UNDER =*BREAK=, BELOW). THE FOLLOWING TYPES OF CARDS WILL BE RECOGNIZED ON (A2), ON THE BASIS OF THE PUNCHING IN COLUMNS 1-6-

*REELS ORDINARILY, PROCESSING IS CONCLUDED WHEN ALL THREE INPUT TAPES HAVE REACHED THE END-OF-FILE. IF A =*REELS= CARD APPEARS, THE PROGRAM WILL EXPECT THE MASTER LISTING TO CONTAIN THE NUMBER OF REELS SPECIFIED BY AN INTEGER PUNCHED IN COLUMN 9. AS THE END OF EACH REEL IS REACHED, THE PROGRAM WILL ASK FOR THE NEXT TO BE DIALED ONTO (A5).

*QUIT AS SOON AS THE ID ON THIS CARD BECOMES LESS THAN THE ID ON THE NEXT REMAINING =*LABEL= CARD ON THE MASTER AND UPDATE LISTING, THE UPDATING PROCESS IS TERMINATED, THE OUTPUT TAPE ENDFILED, AND ALL TAPES REWOUND.

*BREAK AS SOON AS THE ID ON THIS CARD BECOMES LESS THAN THE ID ON THE NEXT REMAINING =*LABEL= CARD ON THE MASTER AND UPDATE LISTING, THE OUTPUT TAPE IS ENDFILED AND REWOUND AND A NEW (B6) IS REQUESTED. FOLLOWING A =*BREAK= CARD, ANY CARDS ON (A2) WILL BE COPIED ONTO THE BEGINNING OF THE NEW OUTPUT TAPE, UNTIL A CARD WITH A =*= IN COLUMN 1 IS READ.

* ANY OTHER CARD WITH A =*= IN COLUMN 1 AND NON-BLANK ID WILL CAUSE A LISTING WHOSE =*LABEL= CARD HAS MATCHING ID TO BE OMITTED, WHETHER IT IS ON THE UPDATE OR MASTER TAPE.

WHEN A =*LABEL= CARD ON THE UPDATE LISTING COMES INTO SEQUENCE ON THE MASTER LISTING, THE =*LABEL= CARD AND THE FOLLOWING LISTING ARE COPIED ONTO THE OUTPUT TAPE. IF A =*LABEL= CARD ON THE UPDATE LISTING MATCHES IN ID ONE ON THE MASTER LISTING, THE =*LABEL= CARD AND ITS ASSOCIATED LISTING ON THE MASTER TAPE ARE REPLACED BY THOSE FROM THE UPDATE TAPE. ALL OTHER LISTINGS FROM THE MASTER TAPE ARE COPIED ONTO THE OUTPUT.

THE PROGRAM IS RUN AS A MONITOR SPECIAL JOB, THE CARD ORDER BEING MONITOR CONTROL CARDS, BINARY DECK OF =LISTUP= (THERE ARE NO SUBROUTINES NECESSARY), =*DATA=, AND CONTROL CARDS TO BE READ FROM (A2). THE ONLY OUTPUT OTHER THAN THE MERGED LISTING ON (B6) IS ON THE ON-LINE PRINTER, THERE IS NO OUTPUT ON (A3) BY THE PROGRAM. THE ON-LINE LISTING SHOULD BE CHECKED FOR SEQUENCE OR OTHER ERROR REMARKS.

STATUS (AS OF 11 JULY 1961). THE PROGRAM HAS BEEN USED SEVERAL TIMES FOR STRAIGHTFORWARD MERGING OF LISTINGS, AND THE FEATURE FOR OMITTING LISTINGS UNDER =*=-CARD CONTROL HAS BEEN TESTED IN A CHECKOUT RUN. PROBABLY NOT ALL POSSIBLE SEQUENCING COMBINATIONS HAVE OCCURRED, AND THE =*REELS=, =*QUIT=, AND =*BREAK= FEATURES HAVE NOT BEEN TRIED. THE PROGRAM IS SUPPOSED TO BEHAVE PROPERLY WHEN AN END-OF-FILE CONDITION IS ENCOUNTERED WRITING (B6), BUT THIS FEATURE HAS NOT BEEN TESTED.

APPENDIX XII

GENERATE AND UPDATE XRAY SYSTEM SYMBOLIC CARD TAPE

THESE 1401 PROGRAMS WERE PREPARED BY S. WAX

DESCRIPTION, THIS PROGRAM MAY BE USED TO GENERATE, UPDATE OR COPY A BCD TAPE CONTAINING THE SOURCE PROGRAM DECKS FOR THE XRAY 63 SYSTEM. THE TAPE HAS THE FOLLOWING FORMAT - SOURCE DECKS ARE ON TAPE AS ONE OR MORE 4400 (55 CARD) RECORDS OR AS A SINGLE VARIABLE, LENGTH RECORDS IF THE PROGRAM IS LESS THAN 55 CARDS IN LENGTH. THE BEGINNING OF EACH PROGRAM IS MARKED BY A FORTRAN * LABEL CARD WITH THE PROGRAM NAME IN COLUMNS 73-77. THIS CARD IS WRITTEN AS A SEPARATE RECORD PRECEEDING THE PROGRAM CARD RECORD(S).

OPERATING INSTRUCTIONS,

A) TO GENERATE A NEW MASTER TAPE FROM CARDS.

1) MOUNT A SCRATCH TAPE ON UNIT 2.
2) TURN ON THE I/O CHECK STOP SWITCH AND SENSE SWITCHES A AND B.
3) LOAD THE PROGRAM FOLLED BY THE CARDS TO BE WRITTEN ON TAPE.
4) PROGRAM WRITES AN END FILE AFTER THE LAST CARD HAS BEEN WRITTEN ON TAPE.

B) TO COPY THE MASTER TAPE.

1) TURN ON THE I/O CHECK STOP SWITCH AND SENSE SWITCHES A AND C.
2) MOUNT THE MASTER TAPE ON UNIT ONE AND A SCRATCH TAPE ON UNIT 2.
3) LOAD THE PROGRAM.

C) TO UPDATE THE MASTER TAPE.

1) UPDATING IS ACCOMPLISHED USING *ALTER CARDS. THE FORMAT OF THESE CARDS AS FOLLOWS.

CARD COLUMN	CONTENTS
1-11	* ALTER (= BLANK)
12-19	FIRST LABEL
20	, (IF SECOND LABEL IS REQUIRED)
21-28	SECOND LABEL (IF REQUIRED)

THE ALTER CARDS MAY BE USED TO ADD, DELETE OR SUBSTITUES DECKS FROM THE MASTER TAPE. THE LABELS MUST BE EXACTLY AS THE DECKS ARE LABELED ON THE MASTER TAPE, IE FROM TWO TO FIVE ALPHA-NUMERIC CHARACTERS FOLLOWED BY ZEROS FOR A TOTAL OF EIGHT CHARACTERS. ALSO, THE LABELS ON ANY SET OF ALTER CARDS MUST BE IN THE SAME ORDER AS THOSE DECKS APPEAR ON THE MASTER TAPE.

2) ADDITIONS TO THE MASTER TAPE

PUNCH AN ALTER CARD WITH A SINGLE LABEL. THIS LABEL SHOULD BE THE DECK NAME BEFORE WHICH THE DECKS FOLLOWING THE ALTER CARD ARE TO BE ADDED. ALL PROGRAMS FOLLOWING THE ALTER CARD WILL BE ADDED TO THE TAPE UNTIL THE NEXT CARD OR LAST CARD IS READ.

3) DELETIONS FROM THE MASTER TAPE.

A) PUNCH AN ALTER CARD WITH TWO LABELS ON IT. THE FIRST OF THESE IS THE NAME OF THE FIRST PROGRAM TO BE DELETED. THE SECOND IS THE NAME OF THE LAST PROGRAM TO BE DELETED.

B) IF ONLY ONE PROGRAM IS TO BE DELETED, THE FIRST AND SECOND LABELS SHOULD BE IDENTICAL.

4) SUBSTITUTIONS ONTO THE MASTER TAPE.

A) PUNCH AN ALTER CARD AS DESCRIBED UNDER DELETIONS.

B) PLACE THIS CARD IN FRONT OF THE DECK OR DECKS TO BE ADDED. THE SYSTEM WILL DELETE THE PROGRAMS INCLUDED BY THE LABELS ON THE ALTER CARD AND SUBSTITUTE THE DECKS FOLLOWING THE ALTER CARD UNTIL THE NEXT ALTER CARD OR LAST CARD IS READ.

5) TO UNDATE.

A) MOUNT THE MASTER TAPE ON UNIT 1 AND A SCRATCH TAPE ON UNIT 2.

B) ARRANGE THE ALTER CARDS AND THEIR FOLLOWING DECKS, IF ANY, IN THE SAME ORDER AS THE PROGRAMS PUNCHED ON THE ALTER CARDS APPEAR ON TAPE.

C) TURN ON THE I/O CHECK TO STOP SWITCH AND SENSE SWITCH A.

D) PLACE THE NEW DECKS AND ALTER CARDS BEHIND THE PROGRAM AND LOAD.

1401 RETRIEVAL OF XRAY 63 SOURCE DECKS

DISCRIPTION, THIS PROGRAM IS DESIGNED FOR USE WITH A TAPE CONTAINING THE SOURCE DECKS OF THE XRAY 63 SYSTEM. THE TAPE HAS THE FOLLOWING FORMAT. THE CARDS OF A SOURCE DECK ARE ON TAPE AS ONE OR MORE 4400 (55 CARD) RECORDS OR AS A SINGLE VERIABLE LENGTH RECORD IF THE PROGRAM IS LESS THAN 55 CARDS IN LENGTH. THE BEGINNING OF EACH AS AN 80 CHARACTER RECORD PRECEEDING THE SOURCE CARD RECORD (S), AS PRESENTLY WRITTEN, THIS PROGRAM MAY BE USED TO PERFORM THE FOLLOWING OPERATIONS, THE SENSE SWITCH SETTINGS ARE GIVEN FOLLOWING THE OPERATION DESCRIPTION. (SENSE SWITCHES TO BE TURNED ON -...)

1) PRINT THE TAPE -A,C

2) PUNCH THE TAPE -A,D

3) ~~PRINT AND~~ PUNCH -A,C,D

4) EXPAND THE TAPE INTO 80 CHARACTER RECORDS ON ANOTHER TAPE -A

5) PRINT ONLY THE *LABEL AND CARDS ON THE TAPE -A,B,E

6) PRINT THE *LABEL AND PUNCH A COMPLETE SET OF RETREIVAL CARDS -A,B,D,E

7) RETRIEVE A PROGRAM FROM THE TAPE AND OUTPUT IT IN ANY OF THE FORMS 1) TO 4) - A,B, ANY SENSE SWITCH SETTING FROM 1),2),3), OR 4)

8) RETRIEVE A PROGRAM, OUTPUT IT IN ANY OF THE ABOVE FORMS AND HALT AT THE END OF THE CURRENT PROGRAM (E.G. TO CHANGE THE SSW SETTINGS FOR THE NEXT PROGRAM TO BE RETRIEVED) - A,B,F, ANY SENSE SWITCH SETTING FROM 1),2),3), OR 4).

9) PRINT APPENDIX I - FIRST CARDS OF EACH ROUTINE - A,B,C,E,G

10) PRINT AND PUNCH APPENDIX I OF USERS MANUAL - A,B,E,G

OPERATING INSTRUCTIONS.

1) TURN ON THE I/O CHECK STOP SWITCH

2) SET THE SENSE SWITCHES FOR THE DESIRED OPERATION.

3) MOUNT THE MASTER TAPE ON UNIT 1.

4) IF EXPANSION OF A PROGRAM INTO 80 CHARACTER RECORDS IS DESIRED, MOUNT A SCRATCH TAPE ON UNIT 2.

5) IF RETRIEVAL OF PROGRAMS IS DESIRED PUNCH THE NAMES OF EACH PROGRAM IN COLUMNS 1-8 OF A CARD. THE NAME MUST PUNCHED ONE NAME TO A CARD AND MUST BE EXACTLY AS THE DECK IS LABELED ON TAPE, IE TWO THROUGH FIVE ALPHANUMERIC CHARACTERS. FOLLOWED BY ZEROS FOR A TOTAL OF EIGHT CHARACTERS. PLACE THESE CARDS BEHIND THE PROGRAM DECK MAKING SURE THAT THE CARDS ARE IN THE SAME ORDER AS THE DECKS APPEAR ON TAPE.

6) PRESS THE START RESET AND CHECK RESET KEYS ON THE 1401 AND THE CHECK RESET KEY ON THE 1402.

7) PLACE THE PROGRAM DECK AND DATA, IF ANY, IN THE READER AND PRESS THE LOAD KEY.

```
          JOB   GENERATE AND UPDATE XRAY SYMBOLIC TAPE                UPDT001
          CTL   441                                                   UPDT002
*
* TO GENERATE A SYMBOLIC TAPE FOR USE ON A 1401 WITH 4000 POS.
* OF STORAGE, CHANGE THE FOLLOWING...
* CHANGE THE B ADDRESSES OF THE COMPARE INSTRUCTIONS
* AT LOCATIONS INCRCT+3 AND NEXTE-3 FROM 32* TO 480
* CHANGE THE OUTBUF DA SPECIFICATION FROM 1X4400,G TO 1X560,G
*
X1        EQU   89                                                    UPDT003
X2        EQU   94                                                    UPDT004
X3        EQU   99                                                    UPDT005
READ      EQU   DEKSEQ                                                UPDT006
INTAP     EQU   (U1                                                   UPDT007
INTAPE    EQU   (U1                                                   UPDT008
OUTTAP    EQU   (U2                                                   UPDT009
OTTPER    EQU   WRTPER                                                UPDT010
INTPER    EQU   RDTPER                                                UPDT011
INBUF     EQU   OUTBUF                                                UPDT012
LBLBUF    DA    1X80,G                                                UPDT013
CPALSW    DCW   '0'                                                   UPDT014
ENDSW     DCW   '0'                                                   UPDT015
LBCDSW    DCW   '0'                                                   UPDT016
GRPMK     DCW   '  '                                                  UPDT017
ALCDSW    DCW   '0'                                                   UPDT018
RTRYCT    DCW   '01'                                                  UPDT019
PRLBNM    DCW   =9                                                    UPDT020
CRLBNM    DCW   =9                                                    UPDT021
NAMCNT    DCW   =1                                                    UPDT022
SPACE     DS    10                                                    UPDT023
*                                                                     UPDT024
* SENSE SWITCH A ALWAYS ON                                            UPDT025
* SENSE SWITCH B ON TO GENERATE NEW MASTER TAPE FROM CARDS            UPDT026
* SENSE SWITCH C ON TO COPY MASTER TAPE                               UPDT027
* SENSE SWITCHES B AND C OFF TO UPDATE                                UPDT028
*                                                                     UPDT029
* SET GROUP MARK-WORD MARK  AT END OF READ AREA AND NAME-COUNT AREAUPDT030
BEGIN     LCA   GRPMK,81                                              UPDT031
          LCA   GRPMK,NAMCNT+9                                        UPDT032
          SW    1,87                                                  UPDT033
          SW    92,97                                                 UPDT034
          SW    77,76                                                 UPDT035
          SW    75,74                                                 UPDT036
          SW    73,INBUF+72          BEGINNING OF LBL FIELD           UPDT037
          RWD   INTAP                                                 UPDT038
          MCW   '000',X3             INITIALIZE XR3                   UPDT039
          BSS   STCPSW,C             COPY TAPE IF SSW C ON            UPDT040
          B     CKSSWB                                                UPDT041
STCPSW    MCW   '1',CPALSW           SET COPY SW                      UPDT042
          B     RDTAPA                                                UPDT043
CKSSWB    BSS   CKFSTL,B             CHK FRST CD FOR *LABEL IF SSWB ONUPDT044
          RWD   OUTTAP               B OFF C OFF SO UPDATE            UPDT045
          RT    INTAPE,INBUF         READ FIRST RECORD                UPDT046
          SBR   SETWMB+3                                              UPDT047
SETWMB    SW    0                                                     UPDT048
          SW                                                          UPDT049
          BER   RSTPER                                                UPDT050
          MCW   '01',RTRYCT                                           UPDT051
          B                          READ FIRST CARD                  UPDT052
* SSW B OFF SO CHECK THAT FIRST CARD IN READER IS *ALTER CARD         UPDT053
          C     11,'*     ALTER'                                      UPDT054
          BU    BDFSTA               NO ALTER                         UPDT055
          C     19,'000'                                              UPDT056
          BE    CKARGA               CONTINUE IF ALTER CARD           UPDT057
BDFSTA    CS    332                  WORD 'ALTER' BUT NO ZEROS        UPDT058
          CS                           IN COLS. 17-19                 UPDT059
          CC    1                                                     UPDT060
          MCW   'FIRST CARD NOT A *ALTER CARD. CHECK CARDS',244       UPDT061
          W                                                           UPDT062
          CS    299                                                   UPDT063
          MCW   'PRESS START TO RESTART',223                          UPDT064
          W                                                           UPDT065
          CC    1                                                     UPDT066
          H     BEGIN                                                 UPDT067
* IF SSW B ON, CHECK THAT FIRST CARD IN READER IS *LABEL CARD         UPDT068
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CKFSTL    R                          READ FIRST CARD
          C     11,  '*      LABEL'
          BE    NEXTB
          C     12,'*       LABEL'
          BE    NEXTB
          CS    332                  FIRST CARD NOT A *LABEL
          CS
          CC    1
          MCW   'FIRST CARD NOT A *LABEL CARD. CHECK CARDS',244
          W
          CS    299
          MCW   'PRESS START TO RESTART',223
          W
          CC    1
          H     BEGIN
*
* FOLLOWING ROUTINE  SEQUENCE NUMBERS AND LABELS THE CARDS OF A
* PROGRAM DECK AND WRITES THE PROGRAM ON TAPE AS ONE OR MORE
* 4400 CHARACTER (55 CARD) RECORDS OR AS A VARIABLE LENGTH RECORD
* IF THE PROGRAM IS LESS THAN 55 CARDS IN LENGTH
* THE *LABEL CARD MARKING THE BEGINNING OF THE PROGRAM IS WRITTEN
* AS A SINGLE 80 CHARACTER RECORD
*
* ALL CARDS ARE READ WITH THE FOLLOWING READ INSTRUCTION
DEKSEQ    BCE   NOCRDS,ENDSW,1       BR IF READER EMPTY
          R
          BSS   LASTCD,A             SET SW IF LAST CARD
NEXTB     BSS   NEXTG,B              B ON TO WRITE NEW TAPE
          C     11,'*      ALTER'    CHECK FOR *ALTER
          BU    NEXTG
          C     19,'000'
          BE    ALTRCD               WE JUST READ AN ALTER CARD
NEXTG     MCW   '0',ALCDSW           TURN OFF ALTER CRD SW
          C     11,'*      LABEL'    CHECK FOR *LABEL CRD
          BE    LBLCRD
          C     12,'*       LABEL'
          BE    LBLCDA               LBL CARD STARTING IN COL 8
          MCW   '0',LBCDSW           TURN OFF LBL CARD SW
          C     '9999990',NAMCNT+8     CHECK FOR COUNT OVERFLOW
          BE    MXCTER               BR IF OVERFLOW
INCRCT    A     '10',NAMCNT+8        INCREASE COUNT
          MRCM  NAMCNT+1,73          MOVE NAME AND CNT TO DETAIL CARD
          MRCM  1,OUTBUF+X3          MOVE CARD TO OUTPUT BUFFER
          C     X3,'32*              CONTINUE IF ALTER CARD
          BE    WRTBUF               BR IF FULL
          MA    '080',X3             OTHERWISE INCREASE X3
          B     READ                 RD NEXT CARD
WRTBUF    WT    OUTTAP,OUTBUF        WRITE BUFFER
          BER   WRTPER
          MCW   '01',RTRYCT
          BEF   NDOTAP
          BSS   NEXTE,B
* IF BUFFER WAS NOT FULL WHEN WRITTEN, WE NEED TO CLEAR THE WORD
* MARK AT THE END OF THE RECORD SO WE CAN READ RECORDS INTO THE
* BUFFER WHEN THE NEXT ALTER CARD IS ENCOUNTERED.
          C     X3,'32*              READ FIRST CARD
          BE    NEXTE                YES
          CW    OUTBUF+X3            NO-CLEAR WM
NEXTE     MCW   '000',X3             RESET XR3
          BSS   FINTST,B
          B     NEXTF
FINTST    BCE   FINISH,ENDSW,1       END OF CARD TO TAPE
NEXTF     BCE   COPY,CPALSW,1        COPY REMAINDER OF TAPE IF SW ON
          BCE   NXTALT,ALCDSW,1      PROCESS ALTER CARD
          BCE   READ,LBCDSW,0        GET NEXT DETAIL CARD
          B     NEWNAM               PROCESS LABEL CARD
*
* SET LAST CARD SWITCH
LASTCD    MCW   '1',ENDSW            SET END SWITCH
          B     NEXTB
* END OF CARD TO TAPE
FINISH    CS    332
          CS
          CC    1
          MCW   'END OF JOB',220
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            W                                                          UPDT144
            CC    1                                                    UPDT145
            WTM   OUTTAP                WRITE EOF                      UPDT146
            WTM   OUTTAP                                               UPDT147
            H                                                          UPDT148
            MCW   '0',ENDSW                                            UPDT149
            B     BEGIN                                                UPDT150
*                                                                      UPDT151
* CARD READER EMPTY                                                    UPDT152
NOCRDS      BSS   MARKND,B              WRT BUFFR AND HALT IF SSW B ON UPDT153
            MCW   '1',CPALSW            SSW B OFF - SET COPY SWTCH     UPDT154
            BCE   COPY,ALCDSW,1         IF SSW B OFF AND LAST CARD IS NOTUPDT155
            BCE   COPY,LBCDSW,1         A *LABEL OR *ALTER CARD, WRITE OUUPDT156
            LCA   GRPMK,OUTBUF+X3       BUFFER BEFORE COPYING REMAINDER UPDT157
            B     WRTBUF                OF TAPE                        UPDT158
COPY        MRCM  LBLBUF,OUTBUF         RESTORE PREVIOUS LABEL         UPDT159
            B     WRTAPA                COPY TAPE                      UPDT160
MXCTER      MCW   CRLBNM-1,MESSF-42     COUNT OVERFLOW                 UPDT161
            CS    332                                                  UPDT162
            CS                                                         UPDT163
            MCW   MESSF,285                                            UPDT164
            W                                                          UPDT165
            CC    L                                                    UPDT166
            MCW   '0000000',NAMCNT+8    RESET COUNT                    UPDT167
            B     INCRCT          GO ON                                UPDT168
*                                                                      UPDT169
* LABEL CARD PROCESSING                                                UPDT170
* MOVES NAME FROM LABEL CARD AND SETS WORD MARK                        UPDT171
* IN THE NAMCNT AREA                                                   UPDT172
* NAME IS MOVED ONE CHARACTER AT A TIME                                UPDT173
LBLCDA      MCW   'LABEL ',12       PUT WORD LABEL IN COL 7-12         UPDT174
LBLCRD      MCW   CRLBNM-1,PRLBNM-1     SAVE PREV LABEL NAME           UPDT175
            MRCM  73,CRLBNM-8       GET NEW LABEL NAME                 UPDT176
            BCE   PRVLBL,LBCDSW,1       BRANCH IF PREV CRD A LABEL CARD UPDT177
            MCW   '1',LBCDSW        SET LABEL CARD SWITCH              UPDT178
* NOTE-- +BWRTBF IS THE ADDRESS OF THE LABEL BWRTBF                    UPDT179
BRNCH       B     *+1                   SKIP THE BUFFER WRITING FOR    UPDT180
            MCW   +BWRTBF,BRNCH+3       THE FIRST LABEL CARD FOUND     UPDT181
            B     NEXTA                                                UPDT182
BWRTBF      C     '000',X3                                             UPDT183
            BE    NEWNAM                                               UPDT184
MARKND      LCA   GRPMK,OUTBUF+X3                                      UPDT185
            B     WRTBUF                                               UPDT186
NEWNAM      CW    NAMCNT+X1         CLEAR WORD MARK IN NAMCNT FIELD    UPDT187
*                                                                      UPDT188
* COL 73 OF THE LABEL CARD MUST NOT BE BLANK                           UPDT189
* ANY LABEL NAME WITH MORE THAN 5 LETTERS                              UPDT190
* WILL BE TRUNCATED TO FIVE LETTERS                                    UPDT191
* THE FIRST ZERO OR BLANK FOUND IN COL 74-78 MARKS THE LABEL END       UPDT192
*                                                                      UPDT193
NEXTA       MCW   '00000000',NAMCNT+8                                  UPDT194
            BCE   BLKLBL,73,        BRANCH IF COL 73 IS BLANK          UPDT195
            MCW   73,NAMCNT+1                                          UPDT196
            MCW   '002',X1          INITIALIZE X1                      UPDT197
NAMCHK      BCE   ENDFLD,72+X1,0        CHECK FOR END OF NAME          UPDT198
            BCE   ENDFLD,72+X1,                                        UPDT199
            C     X1,'006'          WAS COL 78 NON ZERO                UPDT200
            BE    LNGNAM            BRANCH IF YES                      UPDT201
            MCW   72+X1,NAMCNT+X1       MOVE NEXT CHAR OF NAME TO NAMCNT UPDT202
            A     '001',X1          INCREASE X1                        UPDT203
            B     NAMCHK            CHECK NEXT CHAR OF NAME            UPDT204
*                                                                      UPDT205
* SET WORD MARK IN NAMCNT FIELD ONE POSITION AFTER LAST                UPDT206
* CHARACTER OF NAME                                                    UPDT207
*                                                                      UPDT208
ENDFLD      SW    NAMCNT+X1                                            UPDT209
            MRCM  NAMCNT+1,73           ZERO REMAINDER OF NAME FIELD UPDT210
            WT    OUTTAP,1          WRITE LBL CARD ON TAPE             UPDT211
            BER   WRTPER        TAPE ERROR                             UPDT212
            MCW   '01',RTRYCT                                          UPDT213
            BEF   NDCTAP        END OF TAPE                            UPDT214
            MCW   '000',X3                                             UPDT215
            B     READ        READ NEXT CARD                           UPDT216
*                                                                      UPDT217
* PROCESS ALTER CARD                                                   UPDT218
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* WRITE OUT BUFFER IF PREVIOUS CARD NOT A *LABEL OR *ALTER
*
ALTRCD    BCE   PRVLBA,LBCDSW,1     NO PROG CRDS AFTER LAST LBL CRD
          BCE   RESTLB,ALCDSW,1     AN ALTER OR LABEL CARD
          MCW   '1',ALCDSW
          C     X3,'000'             DONT WRITE BUFFER IF IT WAS
          BE    RESTLB              JUST WRITTEN
          LCA   GRPMK,OUTBUF+X3     OTHERWISE MARK END OF RECORD
          B     WRTBUF              AND WRITE OUT BUFFER
PRVLBA    MCW   '1',PRLBSW=1        SET PRV LBL SW
          B     PRVLBL              BRNCH TO PRVLBL ERROR ROUTINE
PRVLBB    MCW   '0',PRLBSW          RESET SWITCH
          MCW   '0',LBCDSW          RESET LABEL CRD SW
          B     NXTALT              PROCESS ALTER CARD
*
* BEGINNING OF TAPE SEARCH TO COMPARE LABELS ON ALTER CARD WITH
* LABELS ON THE MASTER TAPE AND ADD AND/OR DELETE DECKS FROM THE
* MASTER TAPE
*
NXTALT    MCW   '1',ALCDSW
RESTLB    MRCM  LBLBUF,OUTBUF       RESTORE PREV LBLCRD TO OUTBUF
CKARGA    C     19,OUTBUF+79        COMPR LBL WITH FRST LBL ON ALTR
          BE    CKTWAR              IF EQL CHK FOR SECND LBL ON ALTR
*
* TAPE COPY
*
WRTAPA    WT    OUTTAP,OUTBUF       WRITE RECRD ON NEW TAPE
          BER   WRTPER
          MCW   '01',RTRYCT
          BEF   NDOTAP              END OF OUTPUT TAPE
*
* BEFORE READING NEXT RECORD, WE NEED TO CLEAR THE WORD MARK AT THE
* END OF THE RECORD JUST WRITTEN FROM THE OUTBUF AREA
* THE ADDRESS OF THE CLRWMA INSTRUCTION IS FILLED IN BY THE
* SBR CLRWM+3 INSTRUCTION FOLLOWING THE RDTAPA INSTRUCTION
* THE DUMMY ADDRESS 'ANYWHR' IS NECESSARY ONLY THE FIRST TIME THE
* CLRWMA INSTRUCTION IS EXECUTED SINCE A CW WITH ADDRESS ZERO
* WOULD CAUSE A PROGRAM STOP
*
          CW    OUTBUF+80           CLEAR WM IF PREV REC A LBL CRD
CLRWMA    CW    ANYWHR=2
          CW                        CLEAR WM AT END OF PREV RECRD
          LCA   GRPMK,END-1    NECSRY ONLY IF RECRD LNGER THAN BUFR
RDTAPA    RT    INTAP,INBUF         READ NEXT RECORD
          SBR   SETWMA+3            STORE ADDR OF END OF REC IN ADDR
          SBR   CLRWMA+3            OF SW AND CW INSTRUCTIONS
          BEF   NDINTP
          BER   INTPER
          MCW   '01',RTRYCT
SETWMA    SW    0
          SW                        SET WM AT END OF RECRD
          BCE   WRTAPA,CPALSW,1     KEEP COPYING IF COPY SW ON
          C     OUTBUF+10,'*     LABEL'     CHECK FOR *LABEL CARD
          BE    CKARGA              LBL CRD-CHK IF MATCHES ALTER CRD
          B     WRTAPA              NO LBL- COPY RECORD
*
* CHECK FOR SECOND LABEL ON ALTER CARD
* THERE MUST BE A COMMA IN COL. 20 AND ZEROS IN COL. 26-28
*
CKTWAR    BCE   NEXTD,20,,          BR IF COMMA IN COL.20
          B     SAVLBL              NO COMMA-SO NO SECOND LBL
NEXTD     C     28,'000'            CHK FOR ZEROS IN COLS. 26-28
          BE    CKARGB              BR IF TWO LBLS ON ALTER CARD
*
* WE NOW HAVE A MATCH OF THE CURRENT LBL CRD WITH THE SINGLE LBL
* ON THE ALTER CARD
* SAVE THE *LABEL CARD AND READ THE NEXT CARD IN THE READER
*
SAVLBL    MRCM  OUTBUF,LBLBUF       SAVE LBL CARD
          B     DEKSEQ              READ NEXT CARD
*
* WE HAVE TWO LABELS ON THE ALTER CARD-DELETE DECKS THROUGH
* THE SECOND LABEL
*
CKARGB    C     28,OUTBUF+79        COMPARE LBL WITH 2ND LBL ON ALT
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          BE    SKP1OK                                                  UPDT294
          MCW   '0',SKPSW=1                                             UPDT295
          B     SKPDEK                                                  UPDT296
SKP1OK    MCW   '1',SKPSW                                               UPDT297
*                                                                       UPDT298
* SKIP DECKS UNTIL WE FIND A MATCH OF A LBL CARD WITH THE SECOND        UPDT299
* LABEL ON THE ALTER CARD                                               UPDT300
* THEN SKIP TO THE NEXT LABEL CARD ON THE TAPE                          UPDT301
*                                                                       UPDT302
SKPDEK    RT    INTAPE,INBUF                                            UPDT303
          BEF   NOMTCH                                                  UPDT304
          BER   RSTPER                                                  UPDT305
          MCW   '01',RTRYCT                                             UPDT306
          C     OUTBUF+10,'*     LABEL'    CHECK FOR *LABEL CARD        UPDT307
          BE    CKSKSW              CHECK SKIPSW IF *LABEL CARD         UPDT308
          B     SKPDEK              OTHERWISE KEEP SKIPPING             UPDT309
CKSKSW    SW    OUTBUF+80                                               UPDT310
          BCE   SAVLBL,SKPSW,1      SAVE NEW LBL AND READ NEXT CARD     UPDT311
          B     CKARGB              CHK FOR MTCH WITH 2ND LBL ON ALT    UPDT312
*                                                                       UPDT313
* ROUTINES FOR ERRORS IN LABEL NAME                                     UPDT314
*                                                                       UPDT315
PRVLBL    MCW   PRLBNM-1,MESSA-37   PREV CARD A LABEL CARD              UPDT316
          CS    332                                                     UPDT317
          CS                  PRINT MESSAGE AND CONTINUE                UPDT318
          MCW   MESSA,270                                               UPDT319
          W                                                             UPDT320
          CC    L             BUT DO NOT WRITE OUT                      UPDT321
          BCE   PRVLBB,PRLBSW,1     BACK TO ALTER CD IF SW IS ON        UPDT322
          MCW   '1',LBCCSW    THE BUFFER                                UPDT323
          B     NEWNAM                                                  UPDT324
BLKLBL    MCW   PRLBNM-1,MESSB-9    BLANK NAME IN LABEL CARD            UPDT325
          CS    332                                                     UPDT326
          CS                  PRINT MESSAGE                             UPDT327
          MCW   MESSB,258                                               UPDT328
          W                                                             UPDT329
          CC    L                                                       UPDT330
          MCW   '    ',NAMCNT+3   SET NAME TO THREE BLANKS              UPDT331
          MCW   '004',X1                                                UPDT332
          B     ENDFLD        GO ON                                     UPDT333
LNGNAM    MCW   CRLBNM-1,MESSC-35   NAME TOO LONG                       UPDT334
          CS    332                                                     UPDT335
          CS                  PRINT MESSAGE                             UPDT336
          MCW   MESSC,263     TRUNCATE NAME TO FIVE CHAR                UPDT337
          W                                                             UPDT338
          CC    L                                                       UPDT339
          B     ENDFLD        GO ON                                     UPDT340
*                                                                       UPDT341
* TAPE ERROR WHILE WRITING                                              UPDT342
*                                                                       UPDT343
WRTPER    SBR   WTERRT+3      STORE RETURN ADDRESS                      UPDT344
          BSP   OUTTAP        BACKSPACE AND TRY TO WRITE FIVE TIMES     UPDT345
          C     RTRYCT,'05'                                             UPDT346
          BE    BDCTTP                                                  UPDT347
          A     '1',RTRYCT                                              UPDT348
          MA    '180',WTERRT+3      GET BACK TO WRT TAPE INSTRUCTN      UPDT349
WTERRT    B     0                                                       UPDT350
BDCTTP    SKP   OUTTAP        BAD TAPE, SKIP AND BLANK TAPE             UPDT351
          MCW   '01',RTRYCT                                             UPDT352
          B     WTERRT-7      GO ON                                     UPDT353
*                                                                       UPDT354
* OUTPUT TAPE FULL                                                      UPDT355
NDCTAP    SBR   EOTRTN+3      STORE RETURN ADDRESS                      UPDT356
          CS    332                                                     UPDT357
          CS                                                            UPDT358
          MCW   MESSE,260                                               UPDT359
          CC    L                                                       UPDT360
          W                                                             UPDT361
          WTM   OUTTAP                                                  UPDT362
          RWU   OUTTAP        REWIND OUTPUT TAPE                        UPDT363
          H                                                             UPDT364
EOTRTN    B     0             GO ON                                     UPDT365
          DCW   'THE LABEL CARD          IS NOT FOLLOWED BY ANY PRO'    UPDT366
MESSA     DC    'GRAM CARDS'                                            UPDT367
MESSB     DCW   'THE LABEL CARD FOLLOWING LABEL          IS BLANK'      UPDT368
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          DCW   'THE LABEL          HAS BEEN TRUNCATED TO FIVE LETT'UPDT369
MESSC     DC    'ERS'                                                UPDT370
MESSE     DCW   'OUTPUT TAPE FULL.  MOUNT A NEW TAPE AND PUSH START'UPDT371
          DCW   'THE CARD COUNT FOR LABEL          HAS OVERFLOWED A'UPDT372
MESSF     DC    'ND HAS BEEN RESET TO ZERO'                          UPDT373
MESSG     DCW   'END OF JOB'                                         UPDT374
* TAPE ERROR WHILE READING LABELS AND SKIPPING UNTIL A MATCH IS     UPDT375
* FOUND                                                             UPDT376
RSTPER    SBR   RSERRT+3                                             UPDT377
          C     RTRYCT,'25'                                          UPDT378
          BH    NEXTJ                                                UPDT379
          B     BADTP                                                UPDT380
          B     RSERRT                                               UPDT381
NEXTJ     BSP   INTAP                                                UPDT382
          A     '1',RTRYCT                                           UPDT383
          RT    INTAPE,INBUF                                         UPDT384
          BER   RSTPER+4                                             UPDT385
RSERRT    B     0                                                    UPDT386
* TAPE ERROR WHILE READING AND COPYING TAPE                          UPDT387
RDTPER    C     RTRYCT,'25'                                          UPDT388
          BE    BKSPAC                                               UPDT389
          A     '1',RTRYCT                                           UPDT390
          BSP   INTAPE                                               UPDT391
          B     RDTAPA                                               UPDT392
* BACKSPACE THREE TIMES AND REREAD                                   UPDT393
* TRY THIS THREE TIMES AND THEN GIVE UP                              UPDT394
BKSPAC    C     BKSPCT=1,'3'                                         UPDT395
          BE    BDINTP                                               UPDT396
          A     '1',BKSPCT                                           UPDT397
          MCW   '01',RTRYCT                                          UPDT398
          BSP   INTAPE                                               UPDT399
          BSP   INTAPE                                               UPDT400
          BSP   INTAPE                                               UPDT401
          RT    INTAPE,INBUF                                         UPDT402
          RT    INTAPE,INBUF                                         UPDT403
          B     RDTAPA                                               UPDT404
BDINTP    MCW   '1',BKSPCT                                           UPDT405
          B     BADTP                                                UPDT406
          B     SETWMA                                               UPDT407
BADTP     SBR   BDTPRT+3            STORE RETURN ADDR                UPDT408
          MCW   '01',RTRYCT                                          UPDT409
          CS    332                                                  UPDT410
          CS                                                         UPDT411
          MCW   OUTBUF+79,280                                        UPDT412
          MCW                                                        UPDT413
          CC    1                                                    UPDT414
          W                                                          UPDT415
          CS    299                                                  UPDT416
          MCW   'RECORD BEGINNING WITH ABOVE CARD',267               UPDT417
          MCW   'TAPE ERROR WHILE READING '                          UPDT418
          W                                                          UPDT419
          CS    299                                                  UPDT420
          MCW   'CANNOT READ AFTER 75 ATTEMPTS',230                  UPDT421
          W                                                          UPDT422
          CS    299                                                  UPDT423
          MCW   'PUSH START TO IGNORE ERROR AND CONTINUE', 240       UPDT424
          W                                                          UPDT425
          CC    1                                                    UPDT426
          W                                                          UPDT427
BDTPRT    B     0                                                    UPDT428
*                                                                    UPDT429
* END OF FILE ON INPUT TAPE                                          UPDT430
NDINTP    BCE   FINCPY,CPALSW,1     EOF OK IF COPY SWITCH IS ON      UPDT431
          CS    332                 EOF NOT LEGAL WHILE SEARCHING    UPDT432
          CS                        FOR MATCHING LABEL               UPDT433
          CC    1                                                    UPDT434
          MCW   28,228                                               UPDT435
          W                                                          UPDT436
          CS    299                                                  UPDT437
          MCW   'ON ABOVE ALTER CARD',258                            UPDT438
          MCW   'CANNOT FIND DECK MATCHING FIRST LABEL '             UPDT439
          W                                                          UPDT440
          CS    299                                                  UPDT441
          MCW   'CORRECT CARD AND PRESS START TO CONTINUE',241       UPDT442
          W                                                          UPDT443
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          CS    299                                                   UPDT444
          MCW   'UPDATE HAS BEEN DONE UP TO ABOVE ALTER CARD',244     UPDT445
          W                                                           UPDT446
          CS    299                                                   UPDT447
          MCW   'USE THE TAPE ON UNIT 2 AS THE NEW INPUT TAPE '       UPDT448
          MCW   'ON UNIT 1',255                                       UPDT449
          W                                                           UPDT450
          CS    299                                                   UPDT451
          MCW   'AND RESTART WITH THE ABOVE ALTER CARD',235           UPDT452
          W                                                           UPDT453
          CS    299                                                   UPDT454
          CC    1                                                     UPDT455
          WTM   OUTTAP                                                UPDT456
          WTM   OUTTAP                                                UPDT457
          H     BEGIN                                                 UPDT458
FINCPY    WTM   OUTTAP                                                UPDT459
          WTM   OUTTAP                                                UPDT460
          CS    332                                                   UPDT461
          CS                                                          UPDT462
          CC    1                                                     UPDT463
          MCW   'UPDATE COMPLETED.  NEW MASTER TAPE ON UNIT 2.',246   UPDT464
          W                                                           UPDT465
          CS    299                                                   UPDT466
          MCW   'PUSH START TO REW IND AND UNLOAD TAPES',238          UPDT467
          W                                                           UPDT468
          CC    1                                                     UPDT469
          H                                                           UPDT470
          RWU   INTAPE                                                UPDT471
          RWU   OUTTAP                                                UPDT472
          H     *-3                 STOP STOP STOP                    UPDT473
* END OF FILE WHILE SEARCHING FOR SECOND LABEL MATCH                  UPDT474
NOMTCH    CS    332                                                   UPDT475
          CS                                                          UPDT476
          CC    1                                                     UPDT477
          MCW   28,228                                                UPDT478
          W                                                           UPDT479
          CS    299                                                   UPDT480
          MCW   'ON ABOVE ALTER CARD',259                             UPDT481
          MCW   'CANNOT FIND DECK MATCHING SECOND LABEL '             UPDT482
          W                                                           UPDT483
          CS    299                                                   UPDT484
          MCW   'CORRECT CARD AND RESTART ENTIRE RUN',236             UPDT485
          W                                                           UPDT486
          CC    1                                                     UPDT487
          H     *-3                 STOP STOP STOP                    UPDT488
          LTORG*                                                      UPDT489
OUTBUF    DA    1X4400,G                                              UPDT490
END       NOP                                                         UPDT491
          END   BEGIN
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          JOB          XRAY PROGRAM RETRIEVAL                          RTRV001
          CTL   441                                                    RTRV002
*                                                                      RTRV003
* SENSE SWITCH SETTINGS                                                RTRV004
* PRINT TAPE-A,C                                                       RTRV005
* PUNCH TAPE-A,D                                                       RTRV006
* PRINT AND PUNCH-A,C,D                                                RTRV007
* EXPAND INTO 80 CHAR RECORDS-A                                        RTRV008
* PRINT LABEL CARDS-A,B,E                                              RTRV009
* PRINT AND PUNCH LABEL CARDS-A,B,D,E                                  RTRV010
* RETRIEVE A PROGRAM-A,B,ANY COMBINATION OF C,D OR NEITHER             RTRV011
* RETRIEVE AND HALT BEFORE OUTPUT -A,B,F,ANY COMBINATION OF C,D        RTRV012
*                                                                      RTRV013
X1        EQU   89                                                     RTRV014
X2        EQU   94                                                     RTRV015
CBUFFR    DSA   -BUFFR-80                                              RTRV016
EXPBUF    DA    1X80,G                                                 RTRV017
C80       DSA   -80                                                    RTRV018
C5        DSA   -5                                                     RTRV019
BEGIN     SW    1,87                                                   RTRV020
          SW    92,101                                                 RTRV021
          SW    201                                                    RTRV022
          CS    332                                                    RTRV023
          CS                                                           RTRV024
          MCW   '1',SRCHSW=1          TURN ON SEARCH SW                RTRV025
          MCW   '0',MTCHSW=1          TURN OFF MATCH SW                RTRV026
          B     SSWCHK                CHECK SSW                        RTRV027
          RT    (U1,BUFFR                                              RTRV028
          SBR   X1                  STORE END OF REC ADDR              RTRV029
          BEF   ENDFIL                                                 RTRV030
          BER   TAPERR                                                 RTRV031
          MCW   '01',RTRYCT         RESET RD RTRY CT                   RTRV032
          BSS   RDCARD,B            B ON TO RETRIEVE                   RTRV033
          B     OUTPUT              NO SEARCH JUST PRINT OR PUNCH      RTRV034
RDCARD    BSS   LBLCRD,E            BRNCH TO PRINT LBL CARDS           RTRV035
          BCE   NOCRDS,LSTCDS,1     BRANCH IF NO MORE CARDS            RTRV036
          R                                                            RTRV037
          BSS   HALTA,F             STOP AT END OF PROG IF SSW F ON    RTRV038
          B     *+2                                                    RTRV039
HALTA     H                                                            RTRV040
          BSS   SLSTCS,A            SET LST CD SW                      RTRV041
          B     LBLCRD                                                 RTRV042
SLSTCS    MCW   '1',LSTCDS=1                                           RTRV043
LBLCRD    C     BUFFR+10,'*     LABEL'      CHECK FOR *LABEL CARD      RTRV044
          BSS   PRTLBL,E            PRINT LBL CRD IF SSW E ON          RTRV045
          BU    TMCHSW              NO LBL CRD- TEST MATCH SW          RTRV046
          C     BUFFR+79,B          YES LABEL - DOES IT MATCH          RTRV047
          BU    TSCHSW              NO MATCH- TEST SEARCH SW           RTRV048
          MCW   '0',SRCHSW          LBL MATCHES -TURN OFF SRCH SW      RTRV049
          MCW   '1',MTCHSW          TURN ON MATCHSW                    RTRV050
          CCB   SSWCHK,1            CHECK  SSW FOR TYPE OF OUTPUT      RTRV051
          B     OUTPUT              OUTPUT THE RECORD                  RTRV052
TMCHSW    BCE   OUTPUT,MTCHSW,1     NOT YET FINISHED THIS PRGRM DECK   RTRV053
RDTAPB    RT    (U1,BUFFR           FINISHED THIS DECK -RD NXT RECRD   RTRV054
          SBR   X1                                                     RTRV055
          BEF   ENDFIL                                                 RTRV056
          BER   TAPERR                                                 RTRV057
          MCW   '01',RTRYCT                                            RTRV058
          B     LBLCRD              CHECK FOR LBL MATCH                RTRV059
TSCHSW    BCE   MCHSOF,SRCHSW,1     NON MATCHING LBL-KEEP SEARCHING    RTRV060
          MCW   '0',MTCHSW            IF SECHSW ON                     RTRV061
          MCW   '1',SRCHSW          OTHERWISE RESET SWTCHS AND         RTRV062
          BCE   RDCARD,PRNTSW,1     GET NEXT LBL CRD IF PRINTING       RTRV063
          BCE   RDCARD,XPNDSW,1     OR EXPANDING                       RTRV064
          CS    180                 OTHERWISE FEED LAST CRD FRM PNCH   RTRV065
          P                         PUNCH BLANK CARD                   RTRV066
          SSB   RDCARD,4            SELECT INTO NEXT STACKER           RTRV067
MCHSOF    MCW   '0',MTCHSW          STILL LOOKING FOR MATCH            RTRV068
          B     RDTAPB                                                 RTRV069
* ROUTINE TO PRINT, PUNCH, PRINT AND PUNCH, OR EXPAND A TAPE           RTRV070
* RECORD ACCORDING TO INDICATORS SET BY THE SSWCHK ROUTINE             RTRV071
OUTPUT    CS    280                                                    RTRV072
          CS    180                                                    RTRV073
          SW    101,201                                                RTRV074
          MCW   '01',RTRYCT                                            RTRV075
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```
            MCW   '079',X2              RESET XR2
            MA    CBUFFR,X1             GET REC LENGTH
MORE        MA    C80,X1
            C     '001',X1              ARE WE FINISHED WITH THIS RECORD
            BE    ENDREC
            BCE   NOXPND,XPNDSW,0       IF EXPAND SW ON WRITE RECRD
            MCW   BUFFR+X2,EXPBUF+79       AS 80 CHAR REC
WRTAPA      WT    (U2,EXPBUF
            BER   WRTERR
            MCW   '01',RTRYCT
            BEF   ENDFIL
            B     INCRX2
NOXPND      BCE   PRTREC,PRNTSW,1       PRINT RECRD
            BCE   PCHREC,PNCHSW,1       PUNCH
            BCE   PPREC,PPSW,1          PRINT AND PUNCH
            B     SSWCHK
            B     NOXPND
PRTLBL      BE    MOVLBL                BR TO MOVE IF LBL CRD
            B     RDTAPB                OTHERWISE READ NEXT RECORD
MOVLBL      MCW   BUFFR+79,280          MOVE LBL CRD TO PRINT
            BSS   PCHLBL,C              PUNCH LBL IF SSW C ON
            W
            B     NEXTA
PCHLBL      MCW   BUFFR+79,108
            WP
NEXTA       BCV   NUPAGC                CHECK FOR PAGE OVERFLOW
            B     RDTAPB                GET NEXT RECORD
NUPAGC      CCB   RDTAPB,1              NEW PAGE
PPREC       MCW   BUFFR+X2,280
            MCW   BUFFR+X2,180
            WP    INCRX2
PRTREC      MCW   BUFFR+X2,280
            W     INCRX2
PCHREC      MCW   BUFFR+X2,180
            P
INCRX2      MA    '080',X2              INCRSE X2 TO GET NEXT 80 CHAR
            BCV   NUPAGA                CHECK FOR PAGE OVERFLOW
            B     MORE                  MORE RECORD TO OUTPUT
NUPAGA      CCB   MORE,1                NEW PAGE
ENDREC      BSS   RDTAPB,B              RD NXT REC IF RETRIEVING
            BCE   RDTAPC,XPNDSW,1       SKIP DOUBLE SPACING IF EXPNDING
            BCE   RDTAPC,PNCHSW,1          OR PRINTING
            CC    J                     DOUBLE SPACE AT END OF REC
            BCV   NUPAGB                OTHERWISE STAY IN THIS READ LOOP
RDTAPC      RT    (U1,BUFFR
            SBR   X1
            BEF   ENDFIL
            BER   TAPERR
            MCW   '01',RTRYCT
            B     OUTPUT
NUPAGB      CCB   RDTAPC,1
* END OF OUTPUT ROUTINE
* ROUTINE TO CHECK SENSE SWITCHES AND SET INDICATORS
* FOR THE OUTPUT ROUTINE
SSWCHK      SBR   SSWRTN+3
            MCW   '0',PRNTSW=1          RESET INDICATORS
            MCW   '0',PNCHSW=1
            MCW   '0',PPSW=1
            MCW   '0',XPNDSW=1
SSWCK*      BSS   SPRTSW,C              SSW C ON TO PRINT
TSSWD       BSS   TPRTSW,C              CHECK FOR C IF D IS ON
            BCE   SSWRTN,PRNTSW,1       D OFF C ON SO CONTINUE
            MCW   '1',XPNDSW            D AND C OFF SET XPND SW
            B     SSWRTN
SPRTSW      MCW   '1',PRNTSW            SET PRNT SW
            B     TSSWD                 CHECK PUNCH SW
TPRTSW      B     SPCHSW,PRNTSW,0
            MCW   '1',PPSW              D ON C ON SO PRT AND PNCH
            MCW   '0',PRNTSW            TURN OFF PRINT SW
            MCW   '0',PNCHSW            TURN OFF PUNCH SW
            B     SSWRTN
SPCHSW      MCW   '1',PNCHSW            D ON C OFF SO PNCH
SSWRTN      B     0                     GO ON
* END OF SSWCHK ROUTINE
NOCRDS      CS    332
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```
          CS
          MCW   'CARD READER EMPTY',218
          CC    1
          W
          CC    1
          MCW   '0',LSTCDS          RESET LAST CARD SW
          H     BEGIN
ENDFIL    BSS   CHKSWE,B            CHECK FOR RETRIEVAL SW
          B     ENDTPA              SSW B OFF
CHKSWE    BSS   ENDTPA,E            B ON E ON
          B     NOMTCH              B ON E OFF
ENDTPA    CS    332
          CS
          MCW   'END OF TAPE',212
          CC    1
          W
          CC    1
          H     BEGIN
NOMTCH    CS    332                 SWTCH IS ON
          CS                        PRNT MESSAGE
          CC    1
          MCW   80,280
          W
          CC    J
          MCW   'DECK',251
          MCW   'END OF TAPE REACHED WHILE SEARCHING FOR ABOVE '
          W
          CS    332
          CS
          MCW   'CHECK CARD ORDER AND DECK NAME',231
          W
          CC    J
          CS    332
          CS
          MCW   'PUSH START TO REWIND TAPE AND CONTINUE',239
          W
          CC    1
          H
          RWD   (U1
          MCW   '0',LSTCDS          RESET LSTCDSW TO TRY AGAIN  LSTCD
          B     BEGIN
* TAPE ERROR ROUTINES
TAPERR    SBR   TPERRT+3
          C     RTRYCT=2,'25'       TRY TO RD 25 TIMES
          BE    BACKUP
          A     '1',RTRYCT
          BSP   (U1
          RT    (U1,BUFFR
          BER   TAPERR+4
TPERRT    B     0
BACKUP    C     BSPCNT=1,'3'
          BE    BADTAP
          BSP   (U1                 TRY TO CLEAN TAPE
          BSP   (U1
          BSP   (U1
          RT    (U1,BUFFR
          RT    (U1,BUFFR
          A     '1',BSPCNT
          MCW   '01',RTRYCT
          B     TPERRT-11
BADTAP    CS    332
          CS
          MCW   BUFFR+79,279
          CC    1
          W
          CS    299
          MCW   'BEGINNING WITH ABOVE CARD',262
          MCW   'TAPE ERROR DURING READING OF RECORD '
          W
          CC    J
          CS    299
          MCW   'CANNOT READ AFTER 75 ATTEMPTS',230
          W
          MCW   'PUSH START TO IGNORE ERROR AND CONTINUE',240
          W
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```
                CC    1
                MCW   '01',RTRYCT
                MCW   '0',BSPCNT
                H      TPERRT
                RT    (U1,BUFFR
* TAPE WRITE ERROR
WRTERR          C     RTRYCT,'10'
                BE    BOTPWR
                A     '1',RTRYCT
                BSP   (U2
                B     WRTAPA
BOTPWR          CS    332
                CS
                MCW   'BAD TAPE ON UNIT 2. CANNOT WRITE',233
                W
                CS    299
                MCW   'CHANGE TAPES AND RESTART',225
                CC    1
                W
                CC    1
                H     BEGIN
                LTORG*
BUFFR           DA    1X6000,G
                END   BEGIN
```