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X-RAY 67

PROGRAM SYSTEM FOR X-RAY CRYSTALLOGRAPHY

FOR THE
UNIVAC 1108
CDC 3600/6600
IBM 360/50,65,75
IBM 7094

COMPUTER SCIENCE CENTER
UNIVERSITY OF MARYLAND

UNIVERSITY OF MARYLAND
COMPUTER SCIENCE CENTER
COLLEGE PARK, MARYLAND

IN COLLABORATION WITH -

NATIONAL BUREAU OF STANDARDS,
DEPARTMENT OF COMMERCE,

GEOLOGICAL SURVEY,
DEPARTMENT OF INTERIOR
AND
INSTITUTE OF MATERIALS RESEARCH

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I SHALL TRY TO CORRECT ERRORS WHERE SHOWN
TO BE ERRORS, AND SHALL ADOPT NEW VIEWS
AS FAST AS THEY APPEAR TO BE TRUE VIEWS

ABRAHAM LINCOLN.....

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PREFACE

THE X-RAY SYSTEM OF 1967 IS A REWRITE OF X-RAY-63. IT CONSISTS OF A SET OF FORTRAN PROGRAMS ALL INTERRELATED AND SHARING MUTUAL DATA FILES AND DATA CARD FORMATS. THE PROGRAMS ARE STRUCTURED IN TWO MAIN DIVISIONS. THE NUCLEUS SET (WHICH IS IDENTIFIED BY THE PREFIX NUC) AND THE WORKING DIFFRACTION CALCULATION SET (WHICH IS IDENTIFIED BY THE PREFIX XY). THE NUCLEUS OF THE SYSTEM HAS, IN ACTUALITY, NOTHING TO DO WITH DIFFRACTION CALCULATIONS, PER SE, BUT IS RATHER AN ESSENTIALLY FORTRAN SUB-SYSTEM MONITOR WHICH ALLOWS ANY OTHER FORTRAN PROGRAM TO BE INTEGRATED INTO ITS LIBRARY. THE CODING FOR ALL THE X-RAY SYSTEM HAS BEEN DONE IN A ''NEUTRAL'' FORTRAN IV AND FORTRAN 6, ''PIDGEN'' DIALECT. NUC901 (NUSF) IS ABLE TO TRANSLATE THE SYMBOLIC DECKS TO TAKE CARE OF ANY INDIVIDUAL PECULIARITIES OF THE IBM 7094, UNIVAC 1107,1108, CDC 3600, CDC 6400,6600, AND THE LARGER IBM 360 SERIES. IN ADDITION TO THE CARE EXERCISED IN ASSURING THE UNIVERSALITY OF THE FORTRAN USED, ALL OF THE LOCAL COMPUTER LABORATORY FILE NUMBERS, PAGE LENGTH, FILE COMMANDS, ETC. ARE CODED INTO CAREFULLY MARKED SUBROUTINES OF THE NUCLEUS. THEREFORE CHANGES IN THE DIFFRACTION PROGRAMS ARE, AS FAR AS IS KNOWN FROM EXPERIENCE ON A FEW OF THE ABOVE NAMED MACHINES, ELIMINATED.

DISCLAIMER

ALTHOUGH EACH PROGRAM OF THE NUCLEUS AND X-RAY CRYSTALLOGRAPHIC SYSTEM HAS BEEN TESTED BY ITS CONTRIBUTORS AND FURTHER TESTED ON A NUMBER OF DIFFERENT COMPUTERS, NO WARRANTRY, EXPRESSED OR IMPLIED, IS MADE BY THE CONTRIBUTORS OR THE SYSTEM'S PROGRAMMERS AS TO THE ACCURACY AND FUNCTIONING OF THE PROGRAMS, THEIR SUBPROGRAMS AND THE RELATED PROGRAM MATERIAL AND WRITE-UP. NO RESPONSIBILITY IS ASSUMED BY THE CONTRIBUTORS OR ANY MEMBER OF THE X-RAY SYSTEM GROUP OR SUPPORTERS OF THESE PERSONS IN CONNECTION WITH THE USE OR ATTEMPTED USE OR APPLICATION OF THESE PROGRAMS.

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OBJECTIVES OF THE CODERS OF THE X-RAY SYSTEM

IT MAY BE OF SOME USE TO GIVE THE OBJECTIVES IN ORDER TO HELP USERS UNDERSTAND THE LIMITATIONS AND APPLICATIONS OF THE X-RAY SYSTEM OF FORTRAN PROGRAMS.

I. THE PROGRAMS MUST BE AS MACHINE INDEPENDENT AS PRACTICAL.

II. ALL DATA FORMATS AND METHODS OF INPUT AND OUTPUT MUST BE AS SIMILAR AS POSSIBLE.

III. TREATMENT OF THE DATA MUST BE GENERAL WITH RESPECT TO SYMMETRY, SETTING, AMOUNT OF DATA, NUMBER OF PARAMETERS AND EASE OF USE.

IV. ALL OF THE CODING FOR CRYSTALLOGRAPHY AND MONITORING MUST BE CAREFULLY COMMENTED AND ORGANIZED IN ORDER TO BE PREPARED FOR ANY MAJOR CHANGES IN COMPILERS AND COMPUTERS.

V. ALL PROGRAMS MUST BE CAREFULLY DESCRIBED SO THAT CRYSTALLOGRAPHERS MAY MAKE FULL USE OF THEM WITHOUT RECOURSE TO REPROGRAMMING OR PROGRAM MODIFICATION EXCEPT FOR VERY SPECIAL PROBLEMS.

VI. THE BULK STORAGE DATA SETS MUST BE CAREFULLY DEFINED IN AN OPEN ENDED MANNER SO THAT CHANGES AND ADDITIONS ARE POSSIBLE.

VII. THE CODING REQUIREMENTS FOR ADDING NEW LINKS, EITHER A PRIORI OR FROM EXISTING PROGRAMS WHICH BECOME AVAILABLE, MUST BE STRAIGHT FORWARD AND SIMPLE.

VIII. ALL CRYSTALLOGRAPHIC AND MONITOR PROGRAMS SHOULD GIVE USEFUL INFORMATION TO HELP THE CRYSTALLOGRAPHER ANALYSE AND CORRECT ERRORS IN HIS PROCEDURE OR DATA.

IT SHOULD BE EMPHASIZED THAT THIS SET OF OBJECTIVES IS NOT FULLY REALIZED AT THE TIME OF WRITING.

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THE METHOD OF DISTRIBUTION

THE MATERIAL TO BE SENT TO A USER IS...

1. WRITE-UP
2. SYMBOLIC DECK OF A 'STAND-ALONE' PROGRAM (UPDATE) FOR UPDATING THE SYMBOLIC PROGRAM TAPE. INSTRUCTIONS ARE GIVEN AS COMMENTS IN THE CODE.
3. TAPE OF THE SYMBOLIC PROGRAMS
4. MONCOS TEST DECK

ONE USES THE UPDATE DECK TO PROCESS THE SYMBOLIC TAPE IN PREPARATION FOR COMPILATION IN HIS OWN SHOP. THIS PROGRAM PERMITS WRITING END-OF-FILE BEFORE ALL ROUTINES OR ANY SPECIFIED ROUTINE. IT PERMITS REMOVAL, REPLACEMENT OR ADDITION OF CARDS. IT ALSO WILL PUNCH, PRINT OR COPY THE TAPE WHILE CARRYING OUT THE UPDATING. IT PERMITS PRINTING OR PUNCHING ANY SELECTED SUBSET OF ROUTINES. THE FORMAT OF THE SYMBOLIC TAPE(S) SUPPLIED IS SINGLE RECORD CARD IMAGES AT THE DENSITY AND TRACKS SPECIFICATION OF THE USER. (E.G. 800 BPI 9 TRACK, 556 BPI 7 TRACK, ETC.) EACH SUBROUTINE STARTS WITH A 'SUBROUTINE' CARD AND ENDS WITH AN 'END' CARD. ALL DECKS ARE SEQUENTIALLY NUMBERED IN COLS 77-80 AND LABELED IN COLS 73-76.

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THE OVERALL STRUCTURE OF THE SYSTEM

IN GENERAL THIS MANUAL IS INTENDED AS A WORKING CRYSTALLOGRAPHERS' GUIDE. ONCE THE SYSTEM IS RUNNING IN A GIVEN LABORATORY THE DETAILS OF THE CODING OF THE PROGRAMS WILL BE OF LITTLE IMPORTANCE TO THE SOLUTION OF ANY CRYSTAL STRUCTURE. IN THE INTEREST OF SMOOTHER USAGE, HOWEVER, A BRIEF INTRODUCTION TO THE STRUCTURE OF THE WHOLE SYSTEM IS IN ORDER. IT MAY WELL BE THAT ONE MAY WISH TO ALTER OR ADD TO THE SYSTEM AND THIS WILL BE FACILITATED BY THESE GENERAL REMARKS. THE PROGRAMS THEMSELVES ARE EXTENSIVELY COMMENTED AND THESE COMMENTS SHOULD BE READ CAREFULLY, ESPECIALLY THE GLOSSARIES OF SYMBOLS AND THE LONG DESCRIPTIONS GIVEN IN THE NUCLEUS PROGRAMS. WITH EACH MAJOR 'LINK' A COMMENT CONCERNING ARRAY SIZE REQUIREMENTS IS GIVEN IN ORDER TO FACILITATE CHANGES NECESSARY OR DESIRABLE DUE TO IMMEDIATE ACCESS STORAGE SIZE IN EACH COMPUTER.

**** NUCLEUS- A SET OF SUBROUTINES WHICH ARE USED THROUGHOUT THE

X-RAY SYSTEM

ENTRY POINT	DECKNAME	DESCRIPTION
NUC000	NUCO	MAIN AND SIGN ON ROUTINE THIS IS THE MAIN PROGRAM OF THE X-RAY SYSTEM. THE SYSTEM COMMON IS INITIALIZED BY A CALL TO NUC006 AND THEN THE CONTROL TURNED OVER TO THE PROGRAM CALLING ROUTINE.
NUC001	NUCA	PROGRAM CALLING ROUTINE THIS IS THE PRINCIPAL SUBROUTINE OF THE X-RAY SYSTEM. ITS COMMENTS LIST ALL OF THE OTHER SUBROUTINES OF THE SYSTEM AND IT DIRECTS THE LOADING OF ALL THE MAJOR LINKS. IT IS THE PRINCIPAL RETURN OF ALL LINKS. THIS SUBROUTINE PERMITS THE USER TO DIRECT THE SEQUENCE OF PROGRAM LINKS UTILIZED BY MEANS OF A DATA INPUT STREAM. IT IS INTERESTING TO NOTE THAT CONTROL IS MAINTAINED AS LONG AS THERE ARE NO INVALID FIELDS PUNCHED IN THE INPUT STREAM.
NUC002	NUIF	CARD READING AND SORTING ROUTINE THIS SUBROUTINE SERVES TO SCREEN ALL INPUT DATA, CONTROL, AND FUNCTION CARDS. IT LOADS EVERY CARD INTO A BUFFER AND THEN CHECKS TO FIND THE IDENTIFICATION IN COLUMNS ONE TO SIX. THE PROGRAM CARRIES OUT NAMED FUNCTIONS SUCH AS PRINTING REMARKS AND ESTABLISHING PAGE TITLES, OR ELSE SETS AN INDICATOR FOR CALLING PROGRAM OF WHICH TYPE OF CARD WAS ENCOUNTERED. IN THE EVENT THAT THE CARD IS UNIDENTIFIABLE A STANDARD ERROR MESSAGE IS PRINTED THAT CAN AID THE USER. THE SUBROUTINE ALSO OPERATES WITH THE ERROR MESSAGE SILENCED TO CHECK FOR A MATCH OF INFORMATION ON A WORD BY WORD BASIS. THIS SUBPROGRAM MUST BE USED BY EVERY OTHER SUBPROGRAM WHICH READS DATA CARDS. ****NOTE WELL**** IT DEPENDS ABSOLUTELY ON THE AVAILABILITY OF A REREAD, BUFFER READING OR DECODING FEATURE.
NUC005	NULI	LINE COUNT AND PAGINATION ROUTINE THE FUNCTION OF THIS SUBROUTINE IS TO PROVIDE A MEANS TO ALL SUBPROGRAMS OF THE SYSTEM TO DECREMENT THE LINE COUNT FOR PAGINATION. IT ALSO SERVES TO SIGNAL TO ANY PROGRAM WHEN A NEW PAGE IS WRITTEN SO THAT THAT PROGRAM CAN WRITE ANY NECESSARY SUBHEADING.
NUC006	NUSY	SYSTEM INITIALIZATION ROUTINE (ESTABLISHES SHOP COMPATIBILITY) THIS SUBROUTINE IS CALLED FROM TWO PLACES NUCO AND NUCA STATEMENT NUMBER TWENTY-EIGHT.

IT SERVES TO ESTABLISH CORRECT VALUES FOR THE QUANTITIES STORED IN THE LABELED COMMON AREA 'SYS' TO WHICH ALL THE SUBROUTINES WHICH READ OR WRITE FILES REFER. IT IS IMPORTANT TO SCAN THE DEFINITIONS GIVEN BELOW AND TO REALIZE THAT THE QUANTITIES SET BY THIS ROUTINE ARE THE ONES WHICH ARE MACHINE AND COMPUTER LABORATORY SPECIFIC. IN GENERAL NO EXECUTION OF THE SYSTEM WILL BE POSSIBLE UNLESS APPROPIATE MODIFICATION OF THE QUANTITIES IN THE SYSTEM COMMON ARE SET PROPERLY.

NUC007	NURE	FILE REPOSITION AND UNLOAD OR INTERLOCK ROUTINE THIS SUBROUTINE CONSTITUTES THE FILE HANDLING FUNCTION REWIND, END FILE AND UNLOAD (INTERLOCK, UNLOAD). NO SUBROUTINE OF THE SYSTEM EXCEPT THIS SUBROUTINE MAY CONTAIN THESE INSTRUCTIONS. ****NOTE WELL**** THIS IS AN ABSOLUTE PROHIBITION.
NUC008	NUTI	TIMING ROUTINE INTERVAL TIME PRINTING ROUTINE OF THE SYSTEM. REQUIRES A SHOP SPECIFIC TIME ROUTINE (SEE BELOW)
NUC009	NUON	FILE INITIALIZATION ROUTINE THIS SUBROUTINE SERVES TO DESCRIBE THE BINARY FILE OF CRYSTALLOGRAPHIC DATA IN ITS COMMENTS AND TO READ AND PRINT OR READ, PRINT, AND UPDATE THE VERY FIRST (HISTORY) RECORD. IT IS UTILIZED BY EVERY SUBPROGRAM WHICH MANIPULATES THE BINARY CRYSTALLOGRAPHIC DATA FILE.
NUC010	NUTC	FILE RECORD COPYING ROUTINE THIS IS THE FILE COPYING ROUTINE OF THE SYSTEM.
NUC011	NUTR	FILE READING ROUTINE THIS IS THE FILE READING ROUTINE OF THE SYSTEM
NUC012	NUTW	FILE WRITING ROUTINE THIS IS THE FILE WRITING ROUTINE OF THE SYSTEM
NUC013	NURF	FILE RECORD READING ROUTINE THIS IS THE FILE UNPACKING ROUTINE OF THE SYSTEM

THE FOLLOWING 'NUCLEUS' PROGRAMS ARE ACTUALLY OVERLAYS AND NOT KEPT IN IMMEDIATE ACCESS STORAGE AT ALL TIMES.

NUC801	NUTD	FILE DUMPING ROUTINE THIS IS A MAIN LINK WHOSE FUNCTION IS TO DUMP OR COPY THE BINARY DATA FILE
NUC801	NUWU	WRITE UP GENERATING ROUTINE (FROM CARDS)
NUC901	NUSF	SYSTEM SIFTING ROUTINE
NUC902	SFRD	FILE READING ROUTINE OF NUSF
NUC904	SFSC	ACTUAL SIFTING ROUTINE
NUC950	NUUP	SYMBOLIC TAPE UPDATING ROUTINE
NUC999	NUCZ	GENERAL DIAGNOSTIC RECORDS

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THE NAMING AND FILING OF PROGRAM DECKS AND SUBROUTINE ENTRY POINTS USED BY THE SYSTEM

THE FOLLOWING FILING AND NAMING SYSTEM HAS BEEN DEVISED FOR THE X-RAY SYSTEM. ALL MAJOR PROGRAM DECKS OF THE WORKING NUCLEUS ARE NAMED NUXX WHERE XX IS TWO LETTERS OR NUMBERS WHICH CATALOG THE PROGRAM. THE ENTRY POINTS OF THESE ROUTINES ARE GIVEN AS NUCNNN WHERE NNN IS A THREE DIGIT NUMBER. ALL OF THE MAIN OVERLAYS (LINKS) OF THE DIFFRACTION CALCULATIONS ARE XYXX WHERE THE LAST TWO CHARACTERS ARE THE CATALOG DESIGNATION OF THE PROGRAM. THE ENTRY POINT OF ALL THESE SUBPROGRAMS IS XRYNNN WHERE NNN IS A NUMBER ASSIGNED AT THE TIME THE PROGRAMS ARE ENTERED INTO THE LIBRARY. EVERY SUBROUTINE OF EACH MAJOR LINK IS NAMED WITH THE LEADING TWO CHARACTERS XX OF THE PARENT LINK FOLLOWED BY TWO MORE CHARACTERS TO CATALOG IT. THESE SUBPROGRAMS ARE ALSO ENTERED BY XRYNNN WITH THE VALUE OF THE NUMBERS NNN BEING VERY CLOSE TO THOSE OF THE PARENT LINK.

FOR EXAMPLE THE ATOM PARAMETER LOADING ROUTINES HAVE ENTRY POINTS XRY002, XRY003, AND XRY005. THE PROGRAM DECKS ARE CALLED XYPL, PLGN, AND PLLO. NUC001 (NUCA) CALLS XRY002 (XYPL) ONCE AND IT IN TURN CALLS XRY005 (PLLO) AND XRY003 (PLGN) A NUMBER OF TIMES. IN ADDITION XRY002 CALLS ANY OTHER NECESSARY NUCLEUS SUBROUTINES AND THE FORTRAN LIBRARY ROUTINES.

PLEASE NOTE THE DISTINCTION BETWEEN DECK NAMES AND SUBROUTINE ENTRY POINTS. THEY MUST NOT BE THE SAME.

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THE STRUCTURE OF THE SYSTEM WHILE IN HIGH SPEED (CORE) STORAGE

NUCLEUS AND SYSTEM STORAGE ARRAYS	ALWAYS IN STORAGE DURING EXECUTION

DIFFRACTION PROGRAMS AND STORAGE ARRAYS MAIN LINK	CALLED INTO STORAGE BY NUCLEUS
SUB-LINKS OF DIFFRACTION PROGRAMS	CALLED INTO STORAGE BY NUCLEUS
SUBROUTINES OF SUB-LINKS	

THE NUCLEUS PROGRAMS READ ALL CARDS AND OTHER FILES. IN THE PROCESS OF READING CARDS NUCA (NUC001) FETCHES INTO THE STORAGE THE PROGRAMS REQUESTED BY THE CRYSTALLOGRAPHER IN HIS CARD DATA DECK. THE DIAGRAM INDICATES THAT THE NUCLEUS ALWAYS REMAINS IN THE MACHINE WHILE EACH OF THE CRYSTALLOGRAPHIC SUBPROGRAMS IS CALLED INTO STORAGE UPON NEED. AN =OVERLAY= MEANS THAT EACH SEPARATE CRYSTALLOGRAPHIC PROGRAM, ITS SUBROUTINES, AND ITS STORAGE ARRAYS OF DATA OCCUPIES THE SAME GENERAL AREA OF HIGH SPEED STORAGE DURING ACTUAL USE. ALL THIS IS NECESSARY BECAUSE OF THE LIMITATION IN IMMEDIATE ACCESS STORAGE EVEN ON THE LARGEST MEMORY COMPUTERS.

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THE SPECIFICATIONS OF THE FORTRAN PROGRAMS

TO BE A SUBROUTINE OF THESE NUCLEUS PROGRAMS A FORTRAN PROGRAM MUST MEET THE FOLLOWING SPECIFICATIONS, THE DETAILS OF WHICH ARE GIVEN IN THE DESIGNATED PROGRAMS.

I. ALL INPUT FROM CARDS MUST BE MADE BY REFERENCE TO NUIF (NUC002) FOLLOWED BY THE APPROPRIATE REREADING OF THE INPUT CARD BUFFER.

II. ALL READS AND WRITES OF MASS STORAGE DEVICES AND OUTPUT TO PRINTERS MUST BE DONE THROUGH GENERAL UNIT DESIGNATIONS AS OUTLINED IN NUSY (NUC006).

III. EVERY TIME A LINE IS WRITTEN ON THE NORMAL PRINT FILE (NTOUT) THE LINES FUNCTION MUST BE USED. NULI (NUC005).

IV. MAIN OVERLAY SEGMENTS MUST BE ENTERED PROPERLY INTO NUCA (NUC001) AND RECOGNITION OF CALLING CARDS ESTABLISHED THERE.

V. ALL CARD FORMATS SHOULD CONFORM TO THE SYSTEM STANDARD CARD FORMATS.

VI. CRYSTALLOGRAPHIC QUANTITIES SHOULD BE DRAWN FROM THE BINARY DATA FILE RATHER THAN CARDS WHENEVER POSSIBLE.

VII. ANY QUANTITY IN THE FILE THAT IS CHANGED OR MODIFIED BY A PROGRAM LINK SHOULD BE ENTERED INTO THE FILE AND ALL, REPEAT ALL, THE REST COPIED AND PRESERVED.

VIII. EVERY PROGRAM MUST RECOGNIZE AN 'END' CARD.

THE PRECEDING SYNOPSIS OF THE ORGANIZATION OF THE X-RAY SYSTEM IS INTENDED AS AN INTRODUCTION TO THE EXTENSIVE COMMENTS INCLUDED IN THE FORTRAN CODING ITSELF. THE IMPORTANT POINTS FROM THE STANDPOINT OF THE CRYSTALLOGRAPHER ARE THE USE OF THE DATA CARDS AND FILE. A DISCUSSION OF THE DETAILS OF THIS USAGE FOLLOWS.

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THE STORAGE AND RETRIEVAL OF CRYSTALLOGRAPHIC DATA

AS FAR AS THE INDIVIDUAL CRYSTALLOGRAPHER'S DATA FOR A GIVEN CRYSTAL ARE CONCERNED THE SYSTEM TREATS THESE IN AN EXCEEDINGLY STYLIZED MANNER. IT IS, THEREFORE, ESSENTIAL THAT THE CRYSTALLOGRAPHER HAVE A CLEAR PICTURE IN HIS MIND OF THE STRUCTURE AND METHOD BY WHICH HIS DATA ARE BEING STORED. THIS WILL HELP HIM MAKE FULL USE OF THE PROGRAMS AND MACHINES NOW AVAILABLE. THE SECOND PART OF THIS MANUAL IS THE REPOSITORY OF INFORMATION ON CARD FORMATS AND THEIR ORDER. ALL OF THE DATA CONCERNING A GIVEN CRYSTAL ARE USUALLY ENTERED FROM CARDS. AS FURTHER READING WILL SHOW THESE CARDS HAVE A FIXED FORMAT AND FUNCTION. THE FUNCTION OF EACH CARD IS FIXED BY THE PUNCHING IN THE FIRST SIX COLUMNS. THUS, FOR EXAMPLE, ALL THE PROGRAMS OF THE SYSTEM READ DATA FROM A STANDARD FORMAT CELL CARD WHICH CONTAINS THE UNIT CELL CONSTANTS.

OF MORE MYSTERY (AND POWER AND CONVENIENCE) IS THE BINARY DATA FILE. THIS FILE MAY BE ANY MASS STORAGE DEVICE (DRUM, TAPE, DISC, BULK CORE) DEPENDING UPON CUSTOM, AVAILABILITY AND EASE OF ACCESS. ALL THE PERTINENT DATA REQUIRED FOR A CRYSTAL STRUCTURE ANALYSIS ARE STORED IN THIS FILE. IT IS, HOWEVER, SLIGHTLY BAFFLING AT FIRST TO THE USER BECAUSE HE HAS SO LITTLE VISIBLE EVIDENCE OF ITS EXISTENCE, ESPECIALLY WHEN THE FILE IS CONTRASTED TO THE BULKY CARDS. ONE WAY OF THINKING OF IT IS AS A MICROFILM COPY OF THE CARDS STACKED IN AN ORDERLY ARRAY AND EASILY RETRIEVABLE BY THE DIFFRACTION COMPUTING PROGRAMS OF THE X-RAY SYSTEM. THE MAIN OBJECTIVE OF THIS BINARY DATA FILE, FROM THE WORKING CRYSTALLOGRAPHER'S STANDPOINT, IS THAT AS SOLUTION PROGRESSES

HE NEED HANDLE FEWER AND FEWER CARDS. THE PROGRAMS AUTOMATICALLY RELY ON THE DATA FILE OF HIS COMPOUND FOR INFORMATION PREVIOUSLY SUPPLIED.

EACH PROGRAM DESCRIPTION, IN ADDITION TO DESCRIBING THE CARDS REQUIRED, SHOWS WHICH DATA FILES ARE UTILIZED AND INDICATES WHICH CARDS ARE OPTIONAL - MEANING THAT IF THE CARDS ARE OMITTED, INFORMATION IS TO BE DRAWN FROM THE FILE. THE EXACT WORD BY WORD STRUCTURE OF THE FILE IS GIVEN IN 1.DATRDN. A NUCLEUS PROGRAM (NUTD) WILL, UPON DEMAND, PRINT THE WHOLE FILE. IN GENERAL THIS WILL NOT BE A DESIRABLE THING TO DO BECAUSE EVERY DIFFRACTION PROGRAM WILL PRINT THE PERTINENT CRYSTALLOGRAPHIC QUANTITIES IN A MUCH MORE READABLE FORM THAN THIS GENERAL DUMP ROUTINE USES. EACH TIME ONE CARRIES OUT A CRYSTALLOGRAPHIC CALCULATION THE BINARY FILE IS UPDATED INTO A NEW MASS STORAGE DEVICE (I.E. TAPE,DRUM,DISC). BY SAVING AND KEEPING TRACK OF THESE FILES THUS GENERATED ONE MAY REDUCE GREATLY THE NUMBER OF CARDS NECESSARY TO CARRY OUT HIS CALCULATIONS. FURTHERMORE, EACH TIME THE FILE IS =UPDATED= THE NUCLEUS PROGRAMS AUTOMATICALLY ADD THE NAMES OF THE PROGRAMS WHICH HAVE REGENERATED THE FILE.

THE FORM GIVEN ON THE NEXT PAGE IS RECOMMENDED TO YOUR ATTENTION AS A MODEL FOR A PERSONAL RECORD TO KEEP AS COMPUTING RUNS ARE MADE DURING THE SOLUTION OF A CRYSTAL STRUCTURE.

RUN RECORD

INITIAL----------
SERIAL NO.----------

COMPOUND ID---------- RUN SEQ. NO.----------

DATE---------- EXECUTION TIME----------

CHARGE NO.---------- TYPE OF JOB----------

FILE ASSIGNMENTS (WITH LAB REGISTRATION NUMBERS)

LINK	NTIN	NTOUT	NFILEA	NFILEB	NFILEC				

A PRIORI REMARKS

A POSTERIORI REMARKS

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CARDS REQUIRED BUT NOT SHOWN IN THE X-RAY SYSTEM WRITE-UP

TO MAKE USE OF THE X-RAY SYSTEM THE FORTRAN DECKS ARE COMPILED AND THE OBJECT PROGRAMS ARE READIED FOR USE. WITH EVERY GIVEN COMPUTER INSTALLATION THERE WILL BE CERTAIN CONVENTIONS AND PROCEDURES FOR OPERATING THE PROGRAMS. THESE CONVENTIONS FALL INTO TWO CATEGORIES. ONE IS THE MODIFICATIONS NECESSARY TO MAKE THE PROGRAM DECKS MEET THE LOCAL REQUIREMENTS TO COMPILE. THIS OPERATION IS HELPED BY =NUSF= A SUBPROGRAM OF THE SYSTEM. BUT ONE MUST READ THE WARNINGS IN THE COMMENTS OF THE NUCLEUS SUBPROGRAMS FOR MACHINE SPECIFIC OPERATIONS. THE SECOND CATEGORY IS USE OF CONTROL AND ACCOUNTING CARDS REQUIRED BY YOUR LOCAL MONITOR. NO SPECIFIC INFORMATION IS GIVEN IN THIS WRITE UP ABOUT THESE CARDS. THERE ARE SOME EXAMPLES IN THE APPENDIX WHICH SHOW THESE CARDS FOR MACHINES UPON WHICH THE PROGRAMS HAVE BEEN RUN. USUALLY WITH LARGE SCALE MACHINES IT IS BEST TO COMPILE AND THEN LOAD THE PROGRAMS AS ABSOLUTE PROGRAMS STORED ON SOME MASS STORAGE DEVICE (TAPE, DISC, DRUM, OR BULK CORE). ONCE THIS HAS BEEN ACCOMPLISHED THE LABORATORY RUN CARDS WILL HAVE TO BE PLACED ON THE FRONT OF AN X-RAY RUN DECK WHICH WILL CAUSE THE ''CALLING UP'' OF THE X-RAY SYSTEM SO STORED. IT IS NOT POSSIBLE HERE TO TREAT, EVEN IF IT WERE KNOWN, ALL THE LOCAL LORE CONCERNING THE METHODS BY WHICH THIS WILL BE ACCOMPLISHED. IN THE APPENDICES ARE GIVEN EXAMPLES OF RUNS FOR THE COMPUTERS AND THEIR INSTALLATIONS WHERE CHECK-OUT HAS BEEN DONE. IT IS LEFT AS AN EXERCISE TO THE READER TO ADAPT THESE EXAMPLES TO HIS OWN USE AND FACILITIES.

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CARD PUNCHING CONVENTIONS

THE OVERALL PLAN OF THE X-RAY SYSTEM IS SUCH THAT THE USER MUST UNDERSTAND FOUR MAJOR TOPICS.

I. FORTRAN CARD FORMAT CONVENTIONS.

II. X-RAY SYSTEM CARD FORMAT CONVENTIONS AND FUNCTIONS.

III. THE STRUCTURE OF THE X-RAY SYSTEM BINARY DATA FILE.

IV. THE MANIPULATION OF DATA FILES IN ORDER TO MAKE PROPER USE OF MASS STORAGE DEVICES AND TO MITIGATE CARD PUNCHING AND HANDLING.

IN ADDITION IF ONE WISHES TO MODIFY OR ALTER PROGRAMS IT WILL BE NECESSARY TO BECOME FAMILIAR WITH THE STRUCTURE OF THE NUCLEUS PROGRAMS AND THE COMMON STORAGE ARRAYS ASSOCIATED WITH THESE PROGRAMS. THE INFORMATION FOR THOSE INTERESTED IN MODIFYING THE PROGRAMS MUST BE OBTAINED BY READING THE COMMENTS SUPPLIED WITHIN THE FORTRAN DECKS.

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I. FORTRAN CONVENTIONS

THE FOLLOWING DISCUSSION IS NOT INTENDED TO BE EXHAUSTIVE, BUT RATHER TO EMPHASIZE THE RULES OF FORTRAN FORMAT STATEMENTS WHICH ARE USUALLY TROUBLESOME TO THE CRYSTALLOGRAPHER USING THE X-RAY SYSTEM WITH NO PREVIOUS FORTRAN PROGRAMMING EXPERIENCE. SOME OF THE FOLLOWING MATERIAL WILL REPRESENT AN OVERSIMPLICATION BUT WILL, HOPEFULLY, BE SUFFICIENT TO INSURE FEWER TERMINATIONS DUE TO 'BAD' CARDS IN THE CRYSTALLOGRAPHIC DATA DECKS.

A FORMAT STATEMENT IS A ONE DIMENSIONAL ARRAY OF CHARACTERS BEGINING WITH (AND ENDING WITH). WITHIN THESE () ARE A SET OF CHARACTERS WHICH DESCRIBE, CARD COLUMN BY COLUMN, THE DECODING OF THE CARD ON AN ITEM BY ITEM BASIS. EACH ITEM IS AN ENTITY OF CRYSTALLOGRAPHIC DATA. IN GENERAL THE X-RAY SYSTEM USES 3 KINDS OF DATA - ALPHANUMERIC CHARACTERS, NUMERIC INTEGERS, AND NUMERIC FLOATING POINT. IN A FORMAT STATEMENT THESE ARE REPRESENTED BY A, I AND F RESPECTIVELY. THE NUMBER OF COLUMNS DESIGNATED FOR EACH ITEM IS PLACED DIRECTLY AFTER THE FORMAT LETTER IN THE CASE OF A, I, AND F. THUS IF AN ITEM CONSISTS OF FOUR COLUMNS OF ALPHABETIC OR INTEGER INFORMATION IT IS CODED A4 OR I4. IF THE ITEM CONSISTS OF 6 COLUMNS OF FLOATING POINT INFORMATION THEN THE NUMBER OF ''DECIMAL POINTS'' AT THE RIGHT OF THE 6 COLUMN FIELD MUST ALSO BE SHOWN. THUS F6.4 MEANS SIX COLUMNS OF FLOATING POINT DATA THE LAST FOUR OF WHICH ARE TO THE RIGHT OF THE DECIMAL POINT. THE NUMBER 543217 PUNCHED IN SUCH A SIX COLUMN FIELD IS ENTERED INTO STORAGE AS THE BINARY EQUIVALENT OF 54.3217 OR ACTUALLY AS .543217 X 10 EXP 2 (HENCE THE NAME =FLOATING POINT=). (NOTE THAT IF ONE MUST PUNCH THE DECIMAL POINT ONLY FIVE FIGURES MAY BE PUNCHED.) THE FORTRAN CONVENTION ON FLOATING POINT IS SUCH THAT IF A DECIMAL POINT IS PUNCHED ANYWHERE IN THE FIELD IT OVERIDES THE DECIMAL POINT SPECIFIED IN THE FORMAT. THUS IN THE SAME F6.4 FIELD ONE MAY PLACE 54321. WHICH WILL ENTER THE STORAGE AS .54321 X 10 EXP 5.

THE RESTRICTIONS ON EACH OF THESE TYPES OF DATA SPECIFICATION ARE AS FOLLOWS....

1. IN I AND F FIELDS NO PUNCHES SAVE NUMERIC (0,1,2,3,4,5,6,7,8,9,+ AND -) ARE ALLOWED OR THE RUN WILL BE TERMINATED. THE F FIELD HAS ONE

EXCEPTION AND THAT IS THE DECIMAL POINT.

2. IN THE I FIELD THE NUMBERS PUNCHED MUST BE RIGHT JUSTIFIED - THAT IS AS FAR TO THE RIGHT AS POSSIBLE IN THE FIELD SPECIFIED FOR THE ITEM. FAILURE TO OBSERVE THIS FORTRAN FORMAT CONVENTION IS A VERY COMMON CAUSE FOR FAILURE OF RUNS. THE INTERPRETER ROUTINE FILLS THE FIELD OUT WITH ZEROS TO THE RIGHT SO THAT A DIGIT '1' BECOMES A '10' OR '100' OR '1000' DEPENDING UPON THE COLUMN PUNCHED IN AN I4 FIELD.

3. ALPHABETIC A FIELDS MAY HAVE ANY PUNCHES PRODUCED BY A CONVENTIONAL KEYPUNCH. IT IS RECOMMENDED THAT IN THE CASE OF IDENTIFICATION ITEMS THAT ARE TO BE PUNCHED IN MANY PLACES THAT THESE ITEMS BE LEFT JUSTIFIED IN THEIR FIELDS. THIS CONVENTION CAN SAVE COMPARISON ERRORS. THE FOUR CHARACTER DESIGNATIONS SHOWN HERE IN VARIOUS CONFIGURATIONS, BETWEEN QUOTES, ARE ALL DIFFERENT AS FAR AS MACHINE COMPARISONS ARE CONCERNED. (VIZ. ' AB', 'AB ', 'A B ', 'A B',) AS A MATTER OF FACT, IN THE BINARY STORAGE, A BLANK IS A SPECIFIC BINARY NUMBER JUST AS UNIQUE AS THE NUMBER WHICH REPRESENTS 1, 2, A, OR Z OR ANY OTHER CHARACTER.

THE COMPLETE FORMAT STATEMENT IS THUS FORMED BY A SERIES OF ITEM SPECIFICATIONS SEPARATED BY COMMAS. THERE IS ONE OTHER FEATURE COMMONLY USED IN THE X-RAY PROGRAMS AND THAT IS THE X OR COLUMN SKIPPING FUNCTION. IN THIS CASE THE NUMBER OF COLUMNS TO BE SKIPPED IS WRITTEN BEFORE THE X. THE COMMA AFTER THE X IS NOT NECESSARY. A NUMBER IN FRONT OF AN A, I, OR F DESIGNATES THE NUMBER OF IDENTICAL FIELDS SPECIFIED.

IN ADDITION ONE MUST TAKE CARE NOT TO CONFUSE NUMERIC ZERO AND THE LETTER 'O' (0,O). ON THE PRINTING KEYPUNCHES THEY APPEAR TO BE THE SAME BUT THE HOLE CONFIGURATION IN THE CARD IS UNIQUE FOR EACH. ON MOST PRINTERS THE DIFFERENCE IS SUBTLE BUT USUALLY ONE CAN LEARN TO SEE IT. N.B. I AND 1 MUST BE CAREFULLY WATCHED. THERE NOW EXISTS MORE THAN ONE KIND OF KEYPUNCH AND AT LEAST TWO SETS OF WIDELY USED SYMBOLS (BUSINESS AND SCIENTIFIC). THIS MAY ALSO LEAD TO PROBLEMS BUT USUALLY ONLY IF DATA ARE PUNCHED IN DIFFERENT COMPUTER LABORATORIES. REMEMBER THAT THE HOLE CONFIGURATION IS THE IMPORTANT CONSIDERATION, NOT WHAT SYMBOL IS PRINTED ON THE PRINTER OR CARD.

CONSIDER THE FOLLOWING TYPICAL EXAMPLE, A CARD CONSISTING OF EIGHT ITEMS. THE FIRST FOUR ARE ALPHABETICAL , THE NEXT THREE FLOATING POINT, AND THE LAST AN INTEGER. THE FORMAT WOULD BE

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(A2,A4,1XA4,A2,2X3F10.5,I5)
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THUS THE DATA TO BE SUPPLIED WOULD BE WRITTEN IN THE SECOND PART OF THIS MANUAL -

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COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5   GRUMP                 * NOTE THE IDENTIFICATION IS READ AS TWO ITEMS.
                              THIS IS NECESSARY TO MEET THE RESTRICTIONS OF
                              COMPUTERS THAT NOW HANDLE ONLY FOUR CHARACTERS
                              PER WORD.
6-7   BLANK
8-13  COMPOUND IDENTIFICATION CODE
14-15 BLANK
```

16-25 FIRST VARIABLE
26-35 SECOND VARIABLE
36-45 THIRD VARIABLE
46-50 SERIAL NUMBER OF THESE VARIABLES
51-72 BLANK

AND WOULD BE PUNCHED SUCH THAT READING FROM COL 1 -
GRUMP NACL 3.2 7.9 0.2 1

NOTE THAT WHAT IS GIVEN ABOVE IS A BARE BONES INTRODUCTION TO FORMATING. IT IS, HOPEFULLY, ALL THAT IS NECESSARY FOR THE CRYSTALLOGRAPHER PREPARING DATA CARDS FOR THE X-RAY SYSTEM.

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II. X-RAY SYSTEM CARD FORMAT CONVENTIONS AND FUNCTIONS

THE X-RAY SYSTEM UTILIZES FOUR TYPES OF INPUT DATA CARDS. EVERY CARD, REGARDLESS OF TYPE, IS IDENTIFIED BY THE FIRST SIX COLUMNS (READ A2,A4).

THE FOUR TYPES OF CARDS ARE AS FOLLOWS....

1. SYSTEM FUNCTION CARDS READ BY THE SYSTEM -
   'FILES', 'TITLE', 'RESTART'*, 'FINISH', 'SAVE', 'REMARK'
   (* ONLY THE FIRST SIX COLUMNS ARE CHECKED, THE T IS OPTIONAL)

2. PROGRAM CALLING CARDS READ BY BOTH THE SYSTEM AND THE CALLED PROGRAM -
   E.G. 'DATRDN', 'FC', 'DIAGLS', 'LOADAT', ETC.

3. CARDS ACTUALLY CONTAINING CRYSTALLOGRAPHIC OR OTHER DATA AND READ ONLY WITHIN THE APPROPRIATE PROGRAM -
   E.G. 'ATOM', 'CELL', 'HKL', 'SCALE', 'BETA', ETC.

4. THE 'END' CARD WHICH MARKS THE END OF DATA SETS AND USUALLY DIRECTS THE BEGINNING OF ACTUAL CALCULATION. IT ALWAYS APPEARS JUST BEFORE THE SUBSEQUENT SYSTEM FUNCTION CARDS AND/OR PROGRAM CALLING CARDS IN ANY GIVEN RUN.

EACH CARD HAS IN ADDITION TO ITS IDENTIFICATION COLUMNS A FIXED FORMAT SET IN THE PROGRAMS. EACH CARD IS READ AT LEAST TWICE, ONCE TO IDENTIFY ITS FUNCTION AND ONCE TO DECODE IT ACCORDING TO ITS FORMAT AND THE LIST OF ITEMS WHICH IT SHOULD CONTAIN. THIS DOUBLE READING MAKES POSSIBLE FAIRLY FLEXIBLE CARD ORDERS AND GIVES THE USER CONTROL OF THE CALCULATIONS BY MEANS OF THE STRUCTURE OF HIS DATA DECK. FURTHERMORE AS LONG AS NO 'INVALID' PUNCHING IS CONTAINED IN THE CARD IT MAKES POSSIBLE CHECKING AND DIAGNOSTIC PRINT OUT WHEN IMPOSSIBLE CARD ORDER SEQUENCES ARE ENCOUNTERED. THIS DIAGNOSTIC WHICH, UNFORTUNATELY, WILL BECOME FAMILIAR TO MOST X-RAY-SYSTEM USERS, STATES -

CARD JUST READ.... (IMAGE OF CARD IN QUESTION)
CARD I.D. EXPECTED.... THEN FOLLOWS A LIST OF GROUPS OF SIX CHARACTERS PER ALLOWED CARD SHOWING WHAT CARDS WERE EXPECTED AT THE POINT AT WHICH THE ''CONDEMNED'' CARD WAS ENCOUNTERED. MANY TIMES THIS ERROR IS CAUSED BY SIMPLY NOT PUNCHING WHAT IS SHOWN IN THE WRITE-UP (E.G. DATRON FOR DATRDN).

'INVALID' PUNCHING IS THE PLACING OF CHARACTERS IN 'I' FIELDS WHICH DO NOT BELONG THERE UNDER THE RULES OF THE FORTRAN DECODING ROUTINE. FOR EXAMPLE, A DECIMAL POINT IN AN 'I' FIELD OR A LETTER IN AN 'F' FIELD.

ONE MUST UNDERSTAND THE USE OF THE SYSTEM FUNCTION CARDS WHICH ARE LISTED UNDER 2.GENERL AND THEIR USE AND FORMATS DESCRIBED THERE. THE 'FILES' CARD REQUIRES MOST DILIGENT ATTENTION ON THE PART OF THE USER.

THE DETAILS OF THE QUANTITIES AND INFORMATION AND THE EXACT FIELDS IN WHICH THEY ARE TO BE PUNCHED ALONG WITH THE ORDER IN WHICH THE CARDS MUST BE STACKED IS THE SUBJECT OF THE SECOND PART OF THIS MANUAL. PLEASE TRY TO FOLLOW AS CAREFULLY AS POSSIBLE THE DIRECTIONS GIVEN THERE. READ THE CARD ORDER SUMMARY AND THE FILE USAGE INFORMATION. ALMOST EVERY RUN WILL REQUIRE THE USE OF A 'FILES' CARD.

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III. THE X-RAY SYSTEM DATA FILES

TO TRY TO MAKE CLEARER THE PURPOSE OF THE BINARY FILE A BRIEF DESCRIPTION OF ITS FORMATION AND UPDATING IS GIVEN HERE. IN 1. DATRDN ARE LISTED THE DETAILS OF THE STRUCTURE OF THE X-RAY DATA FILE ON A WORD BY WORD BASIS. SCANNING OF, AND LATER REFERENCE TO, THIS SECTION MAY BE FOUND HELPFUL.

ON ANY COMPUTER EACH MASS STORAGE DEVICE WHETHER IT IS A DRUM, DISC, TAPE OR BULK CORE MUST BE REFERENCED IN SOME WAY BY THE USER. IN FORTRAN PROGRAMS IT HAS BECOME TRADITIONAL TO MAKE THESE REFERENCES BY A ''LOGICAL UNIT NUMBER'' WHICH IS AN INTEGER WHICH POINTS TO A GIVEN PHYSICAL DEVICE. THIS SYSTEM IS GOVERNED VERY MUCH BY LOCAL MACHINE ROOM CUSTOM. THUS ONE CAN NEVER BE SURE EXCEPT BY A REFERENCE TO THE LOCAL COMPUTER LABORATORY WRITE-UP WHICH ''LOGICAL NUMBER'' DESIGNATES WHICH PHYSICAL DEVICE, (TAPE UNIT, DISC, PART OF A DRUM, ETC.). THE HISTORY OF THESE LOGICAL NUMBERS TRACES BACK TO THE IBM 704 ON WHICH THERE WERE 10 TAPE UNITS WHICH WERE REFERRED TO AS 1 TO 10 RESPECTIVELY (AN INGENIOUS ARRANGEMENT). WHEN THE 709 WAS INTRODUCED IT HAD ''CHANNELS'' THAT IS TWO OR MORE SEPARATE DEVICES EACH OF WHICH CONTROLLED UP TO 10 UNITS. THESE BECAME PHYSICAL UNITS A0 TO A9, B0 TO B9 AND SO ON FOR AS MANY AS 8 CHANNELS. BUT BY THIS TIME UNIT NUMBER 5 WAS THE INPUT TAPE UNIT OF THE 704 AND UNIT NUMBER 6 THE STANDARD ''PRINT'' TAPE UNIT IN MANY SHOPS. SO ON THE 709 A2 BECAME ''LOGICAL UNIT'' 5 AND A3 ''LOGICAL UNIT'' 6. WITH THE INTRODUCTION OF IBSYS ON THE 7094 LOGICAL UNIT 6 BECAME PHYSICAL UNIT B1 AT

MANY PLACES. THUS ONE SEES THAT THE USE OF THE LOGICAL NUMBERS HAS SIMPLY DERIVED FROM THE 704. FOR EXAMPLE, ON THE UNIVAC 1108 IT IS NOW COMMON PRACTICE FOR THE INPUT CARDS TO BE FOUND ON LOGICAL UNIT 5 WHICH IS THE AREA ON A DRUM WHERE THE CARD IMAGES ARE TRANSFERED FROM THE MECHANICAL READER TO THE MAGNETIC DRUM. 6 IS THE ''LOGICAL UNIT'' DESIGNATION FOR A DIFFERENT DRUM AREA WHERE THE IMAGES OF THE LINES ARE PLACED READY TO TRANSFER TO THE LINE PRINTER. ''LOGICAL UNITS'' 7 TO 32 ARE PHYSICAL TAPE UNITS A TO Z. (BUT EVEN THIS IS COMPLICATED BY THE FACT THAT THE OPERATOR CONTROLS FROM THE CONSOLE WHICH TAPE DRIVE IS REALLY WHICH PHYSICAL UNIT.) LOGICAL UNITS 35-46 ARE PARTS OF THE FH-432 DRUMS WHICH MAY BE USED TO SIMULATE SCRATCH TAPES (TAKE NOTE 1108 USERS). THESE LOGICAL NUMBERS ARE SET TO CONFORM TO LOCAL CUSTOM IN THE X-RAY SYSTEM IN TWO DISTINCT WAYS. ONE IS IN THE NUCLEUS PROGRAM NUSY (NUC006) WHICH SETS UP THE SYSTEM COMMON BEFORE EXECUTION OF THE SYSTEM BEGINS. THE SECOND AND MOST IMPORTANT WAY FROM THE STANDPOINT OF THE CRYSTALLOGRAPHER IS BY MEANS OF A FILES CARD (TAPES CARD OF THE X-RAY-63 SYSTEM). WITH A FILES CARD ONE IS ABLE TO CHANGE THE LOGICAL UNIT DESIGNATION OF THE X-RAY SYSTEM FILES. THESE FILES ARE NAMED NCDBUF, NTIN, NTOUT, NFILEA, NFILEB, NFILEC, ..., NFILEJ. NCDBUF IS SET ONLY IN =NUSY= AS THE LOGICAL UNIT WHICH DESIGNATES THE BUFFER WHICH HOLDS THE IMAGE OF THE LAST CARD READ FROM THE INPUT DATA STREAM (NTIN). THE REST OF THE UNITS NTIN TO NFILEJ MAY BE SET DURING A RUN BY USE OF A FILES CARD, WHOSE FORMAT IS GIVEN IN SECTION 2.GENERL EVERY TIME A RESTART CARD IS ENCOUNTERED ALL THE LOGICAL UNIT DESIGNATIONS ARE SET BACK TO THE VALUES INITIALIZED BY =NUSY=. IN THE X-RAY SYSTEM THE FILES HAVE THE FOLLOWING USES. NOTE THAT EACH CARD ORDER SUMMARY PAGE (2.XXXXXX- A) STATES WHICH FILES ARE USED BY EACH PROGRAM.

***** BE SURE TO READ SECTION 2.GENERL-A 1. *****

X-RAY FILE	PURPOSE
NTIN	INPUT OF DATA FROM CARDS
NTOUT	OUTPUT OF PRINTED MATTER TO USER
NFILEA	INPUT BINARY FILE OF CRYSTALLOGRAPHIC DATA
NFILEB	OUTPUT OF UPDATED BINARY FILE OF CRYSTALLOGRAPHIC DATA
NFILEC	OUTPUT OF PUNCHED CARDS
NFILED	SPECIAL PRINT OUTPUT
NFILEE	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS
NFILEF	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS
NFILEG	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS
NFILEH	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS
NFILEI	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS
NFILEJ	SCRATCH UNITS FOR VARIOUS INTERMEDIATE JOBS

IF A NUMBER OF CRYSTALLOGRAPHIC CALCULATIONS ARE TO BE CARRIED OUT IN SEQUENCE THE USER MUST INSERT CORRECT 'FILES' CARDS IN THE DATA DECK. REMEMBER THAT NFILEA AND NFILEB ARE INTERCHANGED AUTOMATICALLY AFTER EACH

PROGRAM LINK IS EXECUTED. THUS THESE TWO FILES MAY REQUIRE RESETTING ONLY OCCASIONALLY, BUT ONE MUST 'VISUALIZE' BEFORE THE RUN HOW THE COURSE OF THE CRYSTALLOGRAPHIC BINARY DATA STORAGE WILL RUN.

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THE X-RAY SYSTEM DECK STRUCTURE

THE COURSE OF THE CRYSTALLOGRAPHIC CALCULATIONS, WHICH MAY INVOLVE ANY NUMBER OF THE LINKS IN THE SYSTEM, IS CONTROLLED BY THE SEQUENCE OF CARDS IN THE INPUT DATA. A SEQUENCE OF INTERDEPENDENT CALCULATIONS MAY BE PERFORMED BY STACKING AN APPROPRIATE SET OF DATA DECKS (FOR EXAMPLE, DATA REDUCTION, FOLLOWED BY FC, FOLLOWED BY A DIFFERENCE FOURIER, FOLLOWED BY AN FO FOURIER, FOLLOWED BY A BOND LENGTH AND ANGLE CALCULATION.) EACH SET OF DATA DECKS WILL START WITH A 'RESTART' CARD IF IT DOES NOT DEPEND UPON THE SUCCESSFUL COMPLETION OF ANY CALCULATION AHEAD OF IT. THUS EACH INDEPENDENT SET OF CALCULATIONS IS PRECEEDED BY A 'RESTART' CARD. AT THE END OF THE DECK ONE PLACES A 'FINISH' CARD WHICH CAUSES EXECUTION TO TERMINATE AND CONTROL TO BE RETURNED TO THE COMPUTER LABORATORY EXECUTIVE ROUTINE OR MONITOR.

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

A 'RESTART' CARD CAUSES IMMEDIATE INITIALIZATION OF FILE ASSIGNMENTS, RESETTING OF PAGE NUMBER TO ZERO, AND THE CLEARING OF THE TITLE ARRAY TO BLANKS. A 'TITLE' CARD AND 'FILES' CARD USUALLY FOLLOWS THE 'RESTART' CARD. AFTER THIS COMES THE CALLING CARD FOR THE FIRST CRYSTALLOGRAPHIC PROGRAM NEEDED FOR THE PROBLEM AT HAND. 'REMARK' CARDS, IF ONE WISHES, MAY BE INSERTED NEXT, AND FINALLY THE DATA CARDS DEMANDED BY THE PROGRAM BEING CALLED. IF THE BINARY DATA FILE IS BEING USED AS THE SOURCE OF CRYSTALLOGRAPHIC DATA AND INSTRUCTIONS THEN AN 'END' CARD MAY FOLLOW THE PROGRAM CALLING CARD WITH NO OTHER DATA CARDS BEING PRESENT. AT ANY RATE, ONCE THE REQUIRED DATA IS ASSEMBLED IN ORDER, AN 'END' CARD IS ALWAYS PLACED BEFORE ANY OTHER CALL OR FUNCTION CARD. USUALLY ONE WILL PLACE A 'TITLE' CARD BEFORE EACH SUCCESSIVE CALL FOR ANOTHER CRYSTALLOGRAPHIC COMPUTATION. EACH PROGRAM READS AND PROCESSES DATA CARDS UNTIL THE 'END' CARD IS REACHED, WHEREUPON THE PROGRAM FINISHES THE CALCULATION, WRITES SUMMARY DATA, FINISHES UPDATING THE OUTPUT BINARY DATA FILE (IF ANY) AND RETURNS CONTROL TO THE SYSTEM PROGRAM NUCA (NUC001). THIS CONTROLLING PROGRAM INTERCHANGES NFILEA AND NFILEB (LOGICALLY) AND THEN SEEKS THE NEXT JOB SPECIFIED. THERE MAY BE SOME SYSTEM FUNCTION CARDS AS THEY ARE NEEDED AND THEN ANOTHER CALLING CARD CAN INITIATE A NEW CALCULATION WITH THE SAME OR ANY OTHER SYSTEM PROGRAM THE CRYSTALLOGRAPHER MAY REQUIRE.

IF FOR ANY REASON THERE IS A FAILURE BECAUSE OF THE PROGRESS OF THE CALCULATION (E.G. SINGULAR MATRIX, ETC.) THE PROGRAMS TRY TO SALVAGE THE OUTPUT BINARY FILE, IF ANY, AND GIVE A DIAGNOSTIC OF THE CAUSE OF FAILURE. THEY ALSO GIVE A PHRASE, THAT DEALS WITH ENDING, IN A NUMBER OF DIFFERENT LANGUAGES.

THESE MESSAGES SERVE THE PURPOSE OF IDENTIFYING THE DYING PROGRAM FOR THE PROGRAMMERS AND HAVE NO DEEP SIGNIFICANCE. WHEN NUCA IS SIGNALED THAT A SERIOUS CALCULATION ERROR HAS BEEN DETECTED, ALL THE SUBSEQUENT DATA, FUNCTION, AND CALLING CARDS ARE SKIPPED UNTIL EITHER A 'RESTART' OR 'FINISH' CARD IS ENCOUNTERED. SINCE VERY OFTEN THE FAILURE OF ONE CALCULATION PRECLUDES THE NEED FOR A SUBSEQUENT ONE IT IS BEST TO USE 'RESTART' CARDS DISCREETLY. (E.G. IF THE STRUCTURE FACTOR CALCULATION FAILS THERE IS NO PURPOSE IN CARRYING OUT THE FOLLOWING FOURIER.)

IN SUMMARY, BECAUSE OF THIS PROCEDURE THE CALCULATIONS WHICH RUN INDEPENDENTLY SHOULD BE HEADED BY A 'RESTART' CARD. A DEPENDENT SEQUENCE OF CALCULATIONS ARE NOT TO BE SEPARATED BY 'RESTART' CARDS SO THAT FAILURE OF ONE LINK WILL CAUSE DELETION OF THE REMAINING REQUESTS. THE END OF ALL CALCULATIONS IS INDICATED BY A 'FINISH' CARD.

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THE TREATMENT OF SYMMETRY

THE CRYSTALLOGRAPHIC PROGRAMS OF THE X-RAY SYSTEM ARE DESIGNED TO OPERATE FOR ANY SPACE GROUP IN ANY SETTING. THE DESIGN OF THE PROGRAMS IS SUCH THAT THE DATA REDUCTION LINK READS THE SYMMETRY SPECIFIED BY THE CRYSTALLOGRAPHER AND RECASTS IT INTO SUITABLE FORMS FOR USE BY THE VARIOUS PROGRAM LINKS OF THE SYSTEM. SEVERAL ARBITARY RULES MUST BE OBSERVED BY THE CRYSTALLOGRAPHER IN ORDER TO PRODUCE COMPUTATIONALLY CORRECT RESULTS WITH RESPECT TO SYMMETRY.

I. A UNIQUE ASYMMETRIC SET OF REFLECTIONS MUST BE SUPPLIED. IF ONE HAS SPACE GROUP P4, FOR EXAMPLE, THEN ANY REFLECTION FROM THE SETS HKL, HK-L, -H-KL, -H-K-L, -KHL, K-HL, K-H-L, OR -KH-L MUST BE SUPPLIED, BUT FROM NO MORE THAN ONE OF THESE SETS. A SIMILAR CONSIDERATION APPLIES TO THE NON EQUIVALENT SETS RELATED TO -HKL.

II. WHETHER THE CELL IS CENTRIC OR ACENTRIC AND WHAT BRAVAIS LATTICE IT POSSESSES IS SPECIFIED SEPARATELY.

III. ALL THE REST OF THE SYMMETRY IS SPECIFIED BY MEANS OF A STATEMENT OF THE SYMMETRY OPERATIONS IN TERMS OF GENERAL EQUIVALENT POSITIONS.

THIS MEANS THAT FOR EXAMPLE C 2/C WHICH HAS THE FULL SET OF EQUIVALENT POSITIONS.

X, Y, Z
X + 1/2, Y + 1/2, Z
X, -Y, Z + 1/2
X + 1/2, -Y + 1/2, Z + 1/2
-X, Y, -Z + 1/2
-X + 1/2, Y + 1/2, -Z + 1/2

-X, -Y, -Z
-X + 1/2, -Y + 1/2, -Z

IN THE X-RAY SYSTEM THIS EXAMPLE MUST BE ENCODED BY THE FOLLOWING INPUT.

```
LATICE      C  C
SYMTRY       X, Y, Z
SYMTRY       X, -Y, Z + 1/2
```

NOTE THAT THE SECOND 'SYMTRY' CARD COULD JUST AS WELL HAVE BEEN -X, Y, -Z + 1/2 (BECAUSE IT IS IMPLIED BY THE CENTER). THE IDENTITY (X, Y, Z) IS ALWAYS EXPECTED AND MUST BE GIVEN. IN THE SYSTEM THE SYMMETRY DATA SUPPLIED IS TRANSFORMED INTO TWO FORMS. ONE IS A SET OF ROTATION MATRICES AND TRANSLATION VECTORS USED BY ALL PROGRAMS WHICH MUST GENERATE EQUIVALENT POSITIONS IN DIRECT SPACE OR EQUIVALENT REFLECTIONS IN RECIPROCAL SPACE. THE OTHER IS A SET OF INTEGER DIRECTORS ASSOCIATED WITH EACH REFLECTION IN THE BINARY DATA FILE. THESE INTEGERS MAKE POSSIBLE THE GENERATION OF ALL THE EQUIVALENT RECIPROCAL SPACE POINTS AND STRUCTURE FACTORS (PHASES INCLUDED). THUS ONE MAY SAY THAT ALL THE VARIOUS PROGRAMS ARE CODED AS IF THE STRUCTURES WERE TRICLINIC AND THE SYMMETRY IS IMPOSED BY MACHINE DIRECTING CODES ESTABLISHED BY THE DATA REDUCTION LINK. THIS, THEN, IS THE 'RAISON D'ETRE' FOR THE EXISTENCE OF THE BINARY DATA FILE AS FORMED BY DATA REDUCTION (DATRDN). THE CRYSTALLOGRAPHER WORKS ONLY WITH AN ASYMMETRIC SET OF ATOMS AND REFLECTIONS.

=BLOKLS= BLOCK DIAGONAL LEAST SQUARES PARAMETER REFINEMENT

THIS MODIFICATION OF THE =ORFLS= LINK WAS MADE BY J.M. STEWART, C.W. DICKINSON AND F.A. KUNDELL. IT MAKES POSSIBLE THE TREATMENT OF MANY ATOMS AND THE VARYING OF MANY PARAMETERS SIMULTANEOUSLY. DERIVATIVE BLOCKS ARE FORMED FOR EACH ATOM EQUAL, ON A SIDE, TO THE NUMBER OF PARAMETERS OF THAT ATOM TO BE VARIED. EACH BLOCK IS THEN TREATED, IN TURN, EXACTLY AS IN THE FULL MATRIX CASE. SEE THE =ORFLS= AND =DIAGLS= WRITE-UPS FOR DETAILS. THIS METHOD MITIGATES CORRELATION EFFECTS OF TYPE ONE AS DESCRIBED IN THE =DIAGLS= WRITE-UP.

BOND LENGTH AND ANGLE AND CONTACT DISTANCE PROGRAM

THE =BONDLA= PROGRAM OF THE X-RAY SYSTEM IS A REWRITTEN VERSION OF THE =BONDLA= OF X-RAY-63. IT HAS BEEN WRITTEN BY F.A. KUNDELL IN COLLABORATION WITH J.M. STEWART AND R.V. CHASTAIN.

THE OBJECTIVES OF THE CODE ARE TO PRODUCE TWO CATEGORIES OF DISTANCES AND ONE OF ANGLES, TO FIND ALL DISTANCES INCLUDING THOSE OF ATOMS RELATED BY SYMMETRY, AND TO ESTIMATE THE ERRORS IN THE CALCULATED QUANTITIES BASED UPON THE DIAGONAL ELEMENTS FROM THE LEAST-SQUARES REFINEMENT.

THE TWO KINDS OF DISTANCES ARE DEFINED--- ''BOND'' DISTANCES AND ''CONTACT'' DISTANCES IN TERMS OF THREE LENGTHS. THESE THREE LENGTHS ARE MINIMUM DISTANCE TO DEFINE A ''BOND'', MAXIMUM DISTANCE TO DEFINE A ''BOND'' (WHICH IS THE MINIMUM DISTANCE TO DEFINE A ''CONTACT'') AND MAXIMUM DISTANCE TO DEFINE A ''CONTACT''. TAKING EACH ATOM OF THE ASYMMETRIC SET IN TURN, ALL OF THE INTERIOR ANGLES OF THE 'BONDED' ATOMS OF THE ASYMMETRIC SET ARE CALCULATED. THE ASYMMETRIC SET IS THAT SET OF ATOMS WHICH DEFINE THE STRUCTURE AND ARE REQUIRED BY THE STRUCTURE FACTOR TYPE PROGRAMS (E.G. FC, ORFLS)

THE PROGRAM IS RESTRICTIVE WITH RESPECT TO THE MAXIMUM DISTANCES WHICH MAY BE CALCULATED. IF NO SPECIFICATION IS SUPPLIED, THE THREE VALUES WILL BE SET TO 0.03, 1.80, AND 2.50 ANGSTROMS RESPECTIVELY. IN NO CASE SHOULD THE DIFFERENCE IN MAXIMUM AND MINIMUM BOND DISTANCE BE SET TOO LARGE SINCE THIS WILL RESULT IN A HUGE NUMBER OF POSSIBLE ''BOND'' ANGLES BEING PRODUCED. THE MINIMUM BEING SET EQUAL TO A NUMBER GREATER THAN ZERO ASSURES THE PROPER DETECTION OF ATOMS IN SPECIAL POSITIONS. ALL OF THESE RESTRICTIONS MAY BE OVERRIDDEN BY THE USER AS HE SEES FIT.

THE CALCULATION PROCEEDS BY A SERIES OF SYMMETRY OPERATIONS ON THE ASYMMETRIC SET OF ATOMS. ALL CONTACT DISTANCE CALCULATIONS ARE FROM ATOMS OF THE ASYMMETRIC SET TO SYMMETRICALLY RELATED SETS (INCLUDING THE IDENTITY). DURING THE COURSE OF THIS CALCULATION ANY GENERATED ATOM WHICH HAS A ''BOND'' DISTANCE TO A MEMBER OF THE ASYMMETRIC SET IS SAVED (EXCLUDING THOSE GENERATED BY THE IDENTITY). DISTANCES ARE PRINTED OUT SYMMETRY OPERATION BY SYMMETRY OPERATION. EACH ATOM OF THE ASYMMETRIC UNIT IS ACTED UPON FOR EACH OF THE FOLLOWING OPERATIONS IN TURN.

I BASIC SYMMETRY OPERATIONS OF THE SPACE GROUP

II CENTER OF SYMMETRY (IF IT EXISTS)

III BRAVAIS LATTICE TRANSLATIONS

IV 27 SURROUNDING UNIT CELL TRANSLATIONS

THUS FOR A SPACE GROUP SUCH AS C 2/C 216 GENERATIONS WILL BE CARRIED OUT. THE PRINT OUT, HOWEVER, WILL ONLY BE FOR THOSE OPERATIONS FOR WHICH CONTACT

DISTANCES ARE ACTUALLY FOUND. FOR SPEED AN ASYMMETRIC UNIT CENTROID IS ESTIMATED AND USED TO ELIMINATE THOSE SYMMETRY OPERATIONS WHICH HAVE NO CHANCE OF PRODUCING CONTACT DISTANCES TO THE ASYMMETRIC UNIT SUPPLIED. IT IS IMPORTANT TO NOTE THAT IF THE ASYMMETRIC SET OF ATOMS SUPPLIED IS NOT NEAR THE ORIGIN (I.E. MOSTLY IN THE MODULO ONE UNIT CELL) THE BEST RESULTS MAY NOT BE OBTAINED. THERE IS A WARNING MESSAGE.

WHENEVER A BOND DISTANCE IS DETERMINED TO EXIST, THE COORDINATES OF THE GENERATED ATOM ARE SAVED AND AN INDEX OF THE SYMMETRY OPERATION WHICH PRODUCED IT IS APPENDED TO THE ASYMMETRIC UNIT ATOM NAME. (THIS IS PRINTED AS ZERO FOR ATOMS OF THE ASYMMETRIC UNIT ITSELF.)

FINALLY AN ATOM BY ATOM PRINT OUT IS GENERATED GIVING ALL OF THE BOND DISTANCES, AND INCLUDED ANGLES TO THE OTHER ATOMS IN THE STRUCTURE TO WHICH THEY ARE BONDED.

THE COORDINATES AND THE STANDARD DEVIATION OF THE COORDINATES OF THE EXTENDED BONDED SET ARE WRITTEN IN THE BINARY DATA FILE IN LOGICAL RECORD 18.

IN ADDITION TO THE ''AUTOMATIC'' FEATURES OF THE PROGRAM ONE MAY USE CARDS TO REQUEST THE DISTANCE BETWEEN ANY TWO NAMED ATOMS OF THE ASYMMETRIC SET, THE ANGLE BETWEEN ANY THREE, OR THE ANGLE BETWEEN THE TWO LINES FORMED BY ANY FOUR ATOMS, WHICH, IN PAIRS, DEFINE THE LINES.

THE BASIC ORIENTATION OF THE PROGRAM IS TO FINDING ''NEAREST NEIGHBORS''. HOWEVER, BY JUDICIOUS USE OF THE MAXIMUM AND MINIMUM BOND DISTANCE SPECIFICATIONS, ONE MAY INVESTIGATE ANY REGION OF NEXT OR NEXT TO NEXT NEAREST NEIGHBORS.

THE PROGRAM WILL RUN FROM THE BINARY DATA FILE OR FROM THE CARD INPUT STREAM AS DESIRED.

DATA PRE-PROCESSING FOR CARD CONTROLLED, TWO THETA SCANNED, XRD-6 DIFFRACTOMETER

THIS LINK WAS WRITTEN BY J.M.STEWART. THE PURPOSE OF THIS PROGRAM IS TO SCAN THE CARDS OUTPUT FROM THE DIFFRACTOMETER, TO READ THEM ALL, REGARDLESS OF PUNCHING ERRORS AND TO GIVE, IN GRAPHICAL FORM, A REPRESENTATION OF THE HISTORY OF THE STANDARD REFLECTIONS. A SET OF HKL CARDS TO USE WITH DATA REDUCTION (DATRDN) MAY BE PUNCHED.

THE CALLING CARD SERVES TO SET SEVERAL PARAMETERS OF THE DATA SCAN. THESE ARE THE FOLLOWING...

1 CARD PUNCHING
2 OBSERVABILITY IN TERMS OF COUNTING STATISTICS
3 BACKGROUND TIME (SEC)
4 INTENSITY SCALING
5 BACKGROUND INBALANCE WARNING LEVEL

THESE QUANTITIES ARE DESCRIBED FURTHER BELOW AND IN DETAIL IN THE FORMAT SECTION.

AFTER THE CALLING CARD A MODEL OUTPUT CARD IS SUPPLIED IN WHICH ALL THE COLUMNS THAT ARE FIXED FOR CORRECT OUTPUT ARE PUNCHED AND ALL THE COLUMNS THAT HAVE VARIABLE NUMERIC VALUES ARE PUNCHED AS 9. THIS CARD SERVES AS A MODEL TO THE PROGRAM TO ENABLE IT TO DETECT SKIPPED COLUMNS AND EXTRANEOUS PUNCHES.

AN EXAMPLE OF A TYPICAL CONTROL CARD 10 COLUMN WORD BY 10 COLUMN WORD FOLLOWS-

W999999999	THE H,K,L WORD ONLY THE W IS FIXED
1600699999	SET PHI AT SLEW SPEED
Y600609999	SET CHI AT SLEW SPEED (QUARTER CIRCLE)
S200699999	SET TWO THETA AT SLEW SPEED COUNT FOR PRESENT TIME
V209999999	FIRST BACKGROUND DECACOUNTS
S400699999	SCAN AND COUNT TWO THETA
V409999999	SCAN DECACOUNTS
V309999999	SECOND BACKGROUND DECACOUNTS

THE PROGRAM THEN SCANS, COLUMN BY COLUMN, THE FOLLOWING DIFFRACTOMETER OUTPUT CARDS. WHEN 80 SUCCESSIVE COLUMNS ARE FOUND WHERE THE FIXED COLUMNS OF THE CONTROL CARD ARE MATCHED AND THE 9 COLUMNS CONTAIN ONLY VALID NUMBERS THE CARD IS TREATED AS AN EXPERIMENTAL OBSERVATION.

THE NUMERIC COLUMNS ARE TRANSFORMED TO BINARY. THE REFLECTION WORD CONSISTS OF THREE SUBFIELDS OF 3 COLUMNS EACH, ONE FOR H, ONE FOR K AND ONE FOR L. COLUMNS 2,5, AND 8 ARE FOR SIGNS, 0 FOR POSITIVE 1 FOR NEGATIVE. IN ADDITION COL 2 IS USED TO INDICATE A STANDARD REFLECTION,4 FOR POSITIVE H AND 5 FOR NEGATIVE H. CONTROL OF THE STATISTICS IS BASED ON THESE COLUMNS. BECAUSE OF THE RESTRICTION OF THE DATEX LOGIC, NUMBERS MUST BE USED TO REPRE-

SENT SIGNS.

THE MAXIMUM NUMBER OF DIFFERENT REFLECTIONS THAT MAY BE TREATED AS STANDARDS IS TEN. 5000 MEASUREMENTS MAY BE MADE AMONG THE SPECIFIED STANDARDS. THESE MAY THEN BE MIXED IN THE DECK IN ANY WAY. THE PROGRAM PLOTS THEM STANDARD BY STANDARD IN ORDER OF ENCOUNTER.

THE INTENSITY IS CALCULATED ON THE FOLLOWING BASIS...

FIRST A QUANTITY K IS CALCULATED-

```
K = (60)*(DELTA TWO THETA)
    ----------------------------------------------------
    (2)*(TIME FOR ONE BACKGROUND IN SEC)*(SCAN RATE IN DPM)
```

THEN THE OVERALL BACKGROUND IS FOUND-

```
BKG = K*(BACKGROUND1 + BACKGROUND2)
```

NOTE THAT SINCE THE PARTIAL DERIVATIVE OF BKG WITH RESPECT TO THE TWO BACKGROUNDS IS K, THE VARIANCE BACKGROUND IS GIVEN BY...

```
SIGMA(BKG) = KSQRT((SIGMA(B1))**2 + (SIGMA(B2))**2)
```

BUT FROM COUNTING STATISTICS-

```
(SIGMA(B1))**2 = B1
```

THUS SIGMA(BKG) = K*SQRT(B1 + B2) = SQRT(K**2(B1 + B2)) OR SIGMA(BKG) = 0.31623 *SQRT(K*BKG). THE FACTOR 0.31623 IS DERIVED FROM THE FACT THAT ALL BACKGROUNDS ARE IN DECACOUNTS.

IT MAY, BY SIMILAR REASONING, BE SHOWN THAT...

```
SIGMA(I) = 0.31623*(SQRT(I + K*BKG))  WHERE I = (SCAN DEKACOUNTS) - BKG
```

THE PROGRAM ALSO TREATS 1/LP AND LISTS OR PUNCHES F VALUES.

THE BACKGROUNDS ARE CHECKED AND ANY REFLECTIONS FOR WHICH THE TWO BACKGROUNDS ARE DIFFERENT BY MORE THAN A SPECIFIED FACTOR ARE FLAGGED. ONE SHOULD INVESTIGATE ALL FLAGGED REFLECTIONS CAREFULLY. THE CRITERION IS AS FOLLOWS.... THE STANDARD DEVIATION OF BACKGROUND 1 IS DETERMINED AND THE PARAMETER SPECIFIED IN THE CALLING CARD MULTIPLIES IT. THE RESULTANT FACTOR IS SUBTRACTED FROM THE ABSOLUTE DIFFERENCE IN THE TWO BACKGROUNDS AND REFLECTIONS FOR WHICH THE RESULT IS POSITIVE ARE FLAGGED. THIS TEST IS SUPERCEDED BY THE 'LESS-THAN' TEST WHICH FOLLOWS.

WHEN AN INTENSITY IS DISCOVERED TO BE LESS THAN A SPECIFIED NUMBER OF BACKGROUND STANDARD DEVIATIONS ABOVE THE BACKGROUND IT IS FLAGGED AS A ''LESS-THAN''. CAUTION IS DICTATED ON THE SETTING OF THIS PARAMETER NOT TO BE TOO OPTIMISTIC WITH RESPECT TO THE DATA TO BE CALLED ''OBSERVED''. THIS WARNING IS VERY IMPORTANT TO OBSERVE FOR DATA TAKEN AT HIGH TWO THETA.

ONCE ALL THE DATA HAVE BEEN READ THE STATISTICS FOR THE STANDARD

REFLECTIONS ARE PLOTTED AND A SET OF SUMMARY COUNTS GIVEN.

THE INTENTION IS THAT ONE PROCESSES, WITHOUT PUNCHING OUTPUT CARDS, ON A DAY BY DAY BASIS THE OUTPUT FROM THE DIFFRACTOMETER. THIS PROCEDURE MAY THEN GIVE THE CRYSTALLOGRAPHER A GOOD INDICATION OF PROBLEMS IN HIS DATA AS THEY ARISE DURING THE COLLECTION AND BEFORE THE CRYSTAL IS REMOVED FROM THE DIFFRACTOMETER.

DATA SCALING PROGRAM - DATFIX

THIS PROGRAM WAS WRITTEN BY J.R. HOLDEN. IT SERVES TO ESTIMATE THE OVERALL TEMPERATURE AND SCALE FACTOR AND TO CALCULATE QUASI-NORMALIZED STRUCTURE FACTORS (E(H,K,L)). THE DATA SCALING PROGRAM TAKES THE RELATIVE STRUCTURE FACTORS FROM THE BINARY DATA FILE PRODUCED BY THE DATA REDUCTION PROGRAM AND PRODUCES AN UPDATED BINARY DATA FILE CONTAINING A SET OF QUASI-NORMALIZED STRUCTURE FACTORS DEFINED AS FOLLOWS-

```
E(H,K,L) = K(I)*F(H,K,L)*EXP(B*(SIN(THETA)/LAMBDA)**X)/(EPSILON(H,K,L)*
           SUMMATION(F(J)**2)*N(J)))**0.5
```

F(H,K,L) - RELATIVE STRUCTURE FACTOR OF THE H,K,L REFLECTION

THETA - BRAGG ANGLE FOR REFLECTION

LAMBDA - WAVELENGTH

F(J) - FORM FACTOR FOR THE J TH TYPE OF ATOM

N(J) - NUMBER OF ATOMS OF TYPE J IN THE UNIT CELL

EPSILON - WEIGHT FACTOR DEPENDING UPON SPACE GROUP REFLECTION CLASS EXTINCTIONS.

B AND X - CORRECTION FACTORS FOR THERMAL MOTION

K(I) - SCALE FACTOR FOR REFLECTION GROUP I

THE E VALUES CONTAINING THE EPSILON FACTOR ARE THOSE USED IN THE KARLE-HAUPTMAN METHODS FOR STATISTICAL PHASE DETERMINATION. E VALUES NOT CONTAINING THE EPSILON FACTOR ARE USED AS FOURIER COEFFICIENTS IN THE CALCULATION OF THE SHARPENED PATTERSON FUNCTION. THIS PROGRAM PLACES VALUES OF E NOT CONTAINING THE EPSILON FACTOR IN THE REFLECTION RECORDS WITH THE VALUE OF EPSILON STORED AS A SEPARATE WORD. THE VALUE OF E BOTH WITH AND WITHOUT THE EPSILON FACTOR IS THEN AVAILABLE TO SUBSEQUENT PROGRAMS USING THE REFLECTION FILE.

THE VALUES REQUIRED FOR THE CALCULATION OF E ARE OBTAINED AS FOLLOWS- F, SIN(THETA/LAMBDA), AND F(J) ARE READ FROM THE REFLECTION FILE. THE VALUES OF N(J) ARE READ FROM CONTROL CARDS (THE CELCON CARDS) FOR THE PROGRAM. VALUES OF K(I) ARE ESTIMATED BY THE PROGRAM SO THAT THE AVERAGE VALUE OF E SQUARED IS EQUAL TO 1.00 FOR THE REFLECTIONS WITHIN EACH SCALE FACTOR GROUP. AN OVERALL SCALE FACTOR IS ALSO ESTIMATED. VALUES OF INDIVIDUAL GROUP SCALE FACTORS ARE USED ONLY IF THEY FALL WITHIN THE RATIO LIMITS SPECIFIED IN A K(I)/K CONTROL CARD. (THESE RATIO LIMITS REFER TO THE RATIO OF THE GROUP SCALE FACTOR TO THE OVERALL SCALE FACTOR.) IF NO K(I)/K CARD IS READ, THE OVERALL SCALE FACTOR IS

USED, AND THOSE DETERMINED FOR INDIVIDUAL GROUPS ARE LISTED IN THE OUTPUT AS ''SUGGESTED SCALE FACTORS''. THE GROUP LEVEL SCALE FACTORS DETERMINED BY THIS PROGRAM ARE PROBABLY NOT VERY RELIABLE, THEREFORE, THE OVERALL SCALE FACTOR SHOULD BE USED IF THE DATA HAS BEEN PLACED ON A COMMON SCALE BY SOME OTHER MEANS.

THE ESTIMATED VALUES FOR B AND X ARE THOSE FOR WHICH THE E VALUES SHOW NO TREND WITH INCREASING VALUE OF SIN(THETA/LAMBDA). THE PROGRAM APPROXIMATES THIS CONDITION BY CHOOSING VALUES WHICH MINIMIZE THE SUM OF THE SQUARES OF (E**2-1) FOR INDIVIDUAL REFLECTIONS. THE SUM IS TAKEN OVER ALL REFLECTIONS IN AN ENTIRE HEMISPHERE, THAT IS, ALL REFLECTIONS WHICH WOULD BE MEASURED IF THE STRUCTURE WERE TRICLINIC. ''LESS THANS'' ARE ENTERED AT HALF THEIR MAXIMUM POSSIBLE VALUE, AND SPACE GROUP EXTINCTIONS ARE ENTERED AS ZERO. THE FINAL B AND X VALUES ARE OBTAINED BY A METHOD OF SUCCESSIVE APPROXIMATION. A TABLE OF SUMMATION (E**2-1)**2 FOR COMBINATIONS OF VALUES OF B AND X WITHIN LIMITS SET AS INPUT DATA OR SPECIFIED BY BRANGE AND XRANGE CARDS IS CALCULATED. THIS TABLE IS THEN SEARCHED FOR THE MINIMUM ENTRY. THESE VALUES OF B AND X ARE THEN PRINTED AND THE AREA OF THE MINIMUM SEARCHED FOR THE LOWEST VALUE OF (E**2-1)**2 AND THE CORRESPONDING B AND X PRINTED AND USED IN THE CALCULATION OF THE E(H,K,L) VALUES. IF ONE RESTRICTS THE FINAL VALUES OF B OR X SUCH THAT THE MINIMUM CORRESPONDS TO VALUES AT THE EDGE OF THE TABLE IT MAY BE ADVISABLE TO REPEAT THE CALCULATION. THE VALUE OF THE ESTIMATED OVERALL TEMPERATURE FACTOR WHICH IS PLACED IN THE BINARY DATA FILE IS THE ONE CORRESPONDING TO THE MINIMUM VALUE OF SUMMATION (E**2-1)**2 WITH X=2.0. ONE MAY FORCE THE E(H,K,L) VALUES TO PREDETERMINED VALUES OF B AND X BY SPECIFYING A 1X1 ARRAY.

DATA REDUCTION PROGRAM

THE INITIAL CODING FOR THE DATA REDUCTION PROGRAM WAS WRITTEN BY JAMES M. 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 NEW X-RAY SYSTEM VERSION WAS DONE BY J.M. STEWART AND R.V. CHASTAIN. THE PROGRAMMING OF THE 1/LP CORRECTIONS WAS DONE BY A. MIGHELL, A. SANTORO, AND M. ZOCCHI.

THIS PROGRAM IS DESIGNED TO ORGANIZE THE RAW DATA NEEDED IN THE DETERMINATION OF A CRYSTAL STRUCTURE INTO A COHERENT COLLECTION STORED IN A BINARY FILE SO THAT THE STRUCTURE FACTOR, AND REFINEMENT PROGRAMS WILL CALCULATE AUTOMATICALLY. THE FORTRAN STATEMENTS OF THE PROGRAM 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) BOND ABSORPTION CORRECTIONS (OPTIONAL).

(11) REFLECTION DATA. H, K, AND L. I, F, OR F**2.

THE CELL DIMENSIONS ARE READ AND CHECKED FOR REASONABLENESS- NO ZERO OR NEGATIVE AXIAL LENGTHS. EITHER DIRECT CELL OR RECIPROCAL CELL LENGTHS MAY BE GIVEN. ANGLES EITHER AS ALL COSINES OR ALL DEGREES MAY BE SUPPLIED. THE RECIPROCAL CELL CONSTANTS, THE METRIC TENSOR, AND INVERSE METRIC TENSOR ARE CALCULATED (1, PAGE 360).

THE SCATTERING FACTOR INFORMATION IS READ IN AND STORED IN TABLES. 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 FOUR CHARACTERS (E.G.- N FOR NITROGEN, CU2+ FOR COPPER(II), ETC.). THE DESIGNATION IS STORED IN A =DICTIONARY= ON THE BINARY FILE FOR USE OF THE FOLLOWING PROGRAMS. X-RAY FORM FACTORS MAY BE USED DIRECTLY FROM 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 OCCASIONAL 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 THERE MUST BE 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).

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, SEE THE STATEMENT ON SYMMETRY IN 1.GENERL

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 =DRGC= (GENERATION CHECKING SUBROUTINE) WHICH SORTS AND EXAMINES THE OPERATIONS TO CHECK FOR CRYSTALLOGRAPHIC VALIDITY.

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 INTO THE BINARY DATA FILE.

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 (E.G. POWDER, SPECTROMETER, WEISSENBERG, PRECESSION, ETC.), 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.

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.

'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 IN THE FILE. THESE WEIGHTS CAN THEN BE CALCULATED AT SOME FUTURE TIME BY PROGRAM =WEIGHT=. THE LEAST SQUARES PROGRAMS ALLOW THE SETTING OF WEIGHTS = 1.0 AS WELL AS TO USE THOSE IN THE BINARY DATA FILE.

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-

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WEIGHT = Q1/MAX1F(SIGMA,Q2*FREL+Q3,Q4*FRELM+Q5)
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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 A 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 0.0.

THE SCHEME APPLIES WEIGHTING FUNCTION- WEIGHT=Q1/(J) IN WHICH (J) IS THE MAXIMUM OF THESE THREE FUNCTIONS- (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

NOTE- Q1 IS INITIALIZED TO 2.0 ALL THE REST TO ZERO

ABSORPTION CARDS SUPPLY INFORMATION SPECIFIC TO THE TYPE OF ABSORPTION CORRECTION BEING APPLIED. THE INFORMATION ON SPHERES AND CYLINDERS OF BOND (11) IS GIVEN IN VOLUME II OF THE INTERNATIONAL TABLES (3). THE DATA IS READ INTO THE CORE FROM CARDS AND INTERPOLATED FROM THE VALUE OF (SIN THETA)/LAMBDA BY AITKEN'S METHOD (6). DIFFERENT ABSORPTION CORRECTIONS ARE REQUIRED FOR EACH LEVEL, THROUGH THE ANGULAR DEPENDENCE IS COMPUTER DETERMINED.

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 READ BY THE SUBROUTINE =RDRR=.

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.

ON THE OUTPUT BINARY FILE , A CODE OF =1= IS USED FOR OBSERVED REFLECTIONS, =2= FOR 'LESS-THANS', =3= FOR REFLECTIONS EXHIBITING SECONDARY EXTINCTION (WHICH ARE NOT MARKED AT DATA-REDUCTION TIME, BUT MAY BE IDENTIFIED LATER AT FC TIME), =4= IS A REFLECTION TO BE IGNORED, AND =5= IS A SYSTEMATICALLY ABSENT REFLECTION.

THE VALUE OF (SIN THETA)/LAMBDA IS COMPARED WITH THE MAXIMUM ANTICIPATED VALUE PUNCHED IN THE 'CONDIT' 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 DATA GATTERING METHOD 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). THERE ARE A FEW ADDITIONAL DATA, MOST OF WHICH APPEARED IN THE LITERATURE SUBSEQUENT TO THE PUBLICATION OF THE =INTERNATIONAL TABLES=.
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. IT IS MANDATORY THAT THE REFLECTION CARDS THEMSELVES FOLLOW IMMEDIATELY BEHIND THE 'REFIN' CARD AND THAT THE EXACT NUMBER SUPPLIED OR THE LAST INDEX IN THE STACK BE GIVEN IN THE 'REFIN' CARD.

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 =RDGN= USING THE SYMMETRY OPERATIONS PREPARED BY SUBROUTINE =DRGC=. SEE FOURIER PROGRAM WRITE-UP (SECTION 1.FOURR) FOR DETAILS CONCERNING THESE CODES. FINALLY, THE CALCULATED INFORMATION IS WRITTEN OUT ON TWO FILES, A NORMAL PRINT FILE AND THE BINARY DATA FILE WHICH SERVES AS INPUT TO THE OTHER PROGRAMS OF THE SYSTEM.

THE BINARY DATA FILE CONTAINS THE INFORMATION WHICH CONSTITUTES THE DATA WHICH ARE KNOWN ABOUT A CRYSTAL UNDER STUDY. THE REDUCTION OF DATA PROGRAM PLACES IN THE FILE 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 BINARY FILE IS THEREFORE FIXED BY THE MOST GENERAL CALCULATION OR COMBINATION OF CALCULATIONS PROGRAMMED FOR THE SOLUTION OF STRUCTURES.

IN ADDITION TO ITS BINARY FILE, DATA REDUCTION PRINTS A SUMMARY OF THE DATA PROCESSED. 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.

(NOTE - FOR DESCRIPTION OF THE X-RAY SYSTEM BINARY DATA FILE SEE 3.APENDX-2)

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=DIAGLS= DIAGONAL LEAST SQUARES PARAMETER REFINEMENT

THIS MODIFICATION OF THE ORFLS LINK BY J.M. STEWART, F.A. KUNDELL AND E.C. LINGAFELTER MAKES POSSIBLE THE TREATMENT OF MANY ATOMS AND THE VARYING MANY PARAMETERS SIMULTANEOUSLY. THE SHIFTS ARE DETERMINED USING ONLY THE SUM OVER ALL THE REFLECTIONS OF THE SQUARE OF THE PARTIAL DERIVATIVE OF A GIVEN PARAMETER DIVIDED INTO THE SUM OVER ALL THE REFLECTIONS OF THE PRODUCT OF DELTA F TIMES THE DERIVATIVE. THIS MEANS THAT IT IS STRICTLY APPLICABLE ONLY TO SPACE GROUPS AND/OR UNIT CELLS IN WHICH THERE ARE NO LARGE OFF DIAGONAL SUMS. THESE KINDS OF SUMS MAY OCCUR FOR TWO MAIN REASONS, 1) NON-ORTHOGONALITY OR SYMMETRY INTERACTIONS OF THE ATOMS WITHIN THE UNIT CELL OR, 2) SOME ADDITIONAL SYMMETRY CONDITION BETWEEN PARAMETERS OF UNIQUE ATOMS IN THE ASSYMMETRIC SET, THESE UNIQUE ATOMS ACTUALLY BEING PLACED IN =GENERAL= POSITIONS FROM THE STANDPOINT OF THE SPACE GROUP SYMMETRY. LARGE OFF DIAGONAL SUMS FROM THE FIRST CAUSE WILL, IN GENERAL, SIMPLY CAUSE CONVERGENCE TO BE DELAYED. WHERE A FULL MATRIX OR BLOCK DIAGONAL LEAST SQUARES, FOR EXAMPLE, ON A MONOCLINIC CELL WILL BRING RESULTS IN TWO REFINEMENT CYCLES, THE DIAGONAL TREATMENT WILL REQUIRE FOUR OR FIVE TO GET THE SAME RESIDUAL AND FINAL PARAMETERS. AS A RULE OF THUMB ONE MAY EXPECT IN THIS EXAMPLE THAT X,Z POSITION PARAMETER CORRELATION COEFFICIENT OF THE FULL MATRIX WILL APPROXIMATE THE COSINE OF THE INTERAXIAL ANGLE. CORRELATIONS OF TYPE 1 MAY BE CIRCUMVENTED, IF DESIRED, BY RECOURSE TO =BLOKLS= OR =ORFLS= . CORRELATIONS OF TYPE 2 WILL CAUSE MORE SUBTLE KINDS OF PROBLEMS TO DEVELOP AND THESE MUST THEN BE HANDLED WITH SUITABLE FINESSE. IN ORDER TO AID IN CONTROLLING, PROVISION IS MADE TO EITHER DAMP ALL PARAMETER SHIFTS BY A GIVEN FACTOR OR ELSE TO LIMIT THE MAGNITUDE OF ANY GIVEN SHIFT OR BOTH. THERE IS A BUILT-IN SHIFT LIMITING FACTOR ON ALL VARIABLES, 1 UNIT IN B, 0.1 ANGSTROMS IN POSITION. REFERENCE TO THE WRITE UP OF =ORFLS= WILL SERVE TO SHOW THE DETAILS OF THE USE OF THE PROGRAM. THIS PROGRAM REQUIRES PATCHES JUST LIKE THE =ORFLS= LINK.

AUTOMATIC DIFFRACTOMETER OUTPUT PROCESSOR

THE PROGRAM 'DIFOPP' WAS PREPARED BY F. A. MAUER FOR PROCESSING THE OUTPUT OF GENERAL ELECTRIC - DATEX DIFFRACTOMETERS HAVING EITHER PUNCHED-CARD OR PUNCHED-PAPER-TAPE OUTPUT.

DATA IN THE FORM OBTAINED USING THE FOLLOWING TECHNIQUES (WITH EITHER A SINGLE FILTER OR A BALANCED FILTER PAIR) CAN BE PROCESSED...

A. STATIONARY CRYSTAL, STATIONARY COUNTER (PEAK HEIGHT)
   1. BACKGROUND MEASURED AT TWO THETA MINUS BACKSET AND AT TWO THETA PLUS BACKSET.
   2. BACKGROUND MEASURED AT TWO THETA MINUS BACKSET ONLY.
   3. BACKGROUND MEASURED AT TWO THETA PLUS BACKSET ONLY.
   4. BACKGROUND NOT MEASURED.

B. MOVING CRYSTAL, MOVING COUNTER (TWO THETA SCAN)

THE PROGRAM IS WRITTEN TO TOLERATE VARIATIONS IN WORD ORDER AND NUMBER OF WORDS PER REFLECTION SO THAT ERRORS THAT OCCUR DURING MANUAL OPERATION MAY BE CORRECTED BY RE-WRITING ONLY THE AFFECTED WORDS.

CARDS ARE READ IN 80A1 FORMAT BY SUBROUTINE XRY329 WHENEVER THE INPUT BUFFER IS EMPTY, AND ONE CHARACTER IS RETURNED EACH TIME THE SUBROUTINE IS CALLED. SUBROUTINE XRY323 EXTRACTS INDIVIDUAL WORDS FROM THE INPUT CHARACTER STREAM.

PUNCHED PAPER TAPE MUST BE CONVERTED TO MAGNETIC TAPE BY A DEVICE SUCH AS THE DIGI-DATA PAPER TAPE TO MAGNETIC TAPE CONVERTER. BECAUSE THE PAPER TAPE CODE MAY BE AN EIGHT-BIT CODE, WHILE THE MAGNETIC TAPE CODE IS LIMITED TO SIX BITS, EACH PAPER TAPE FRAME IS SPLIT. THE FOUR LOW ORDER BITS ARE RECORDED AS THE FIRST OF TWO 6-BIT FRAMES, AND THE FOUR HIGH ORDER BITS AS THE SECOND. FOR EXAMPLE, THE DIGIT 5, FOR WHICH THE ASCII CODE IS 00110101 (CHANEL 8---1) IS RECORDED AS

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000101  IN MAG TAPE FRAME 1
000011  IN MAG TAPE FRAME 2
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THE MAGNETIC TAPE IS BLOCKED WITH 510 PAPER TAPE (1020 MAG TAPE) FRAMES PER BLOCK. SUBROUTINE XRY327 (UNIVAC 1108 SPECIFIC) READS IN ONE OF THESE BLOCKS WHENEVER THE INPUT BUFFER IS EMPTY AND RETURNS THE OCTAL REPRESENTATION OF ONE PAPER TAPE FRAME (RIGHT JUSTIFIED) EACH TIME THE SUBROUTINE IS CALLED. SUBROUTINE XRY326 EXTRACTS ONE TEN-CHARACTER OUTPUT WORD FROM THE INPUT STREAM EACH TIME IT IS CALLED. SUBROUTINE XRY328 (UNIVAC 1108 ASSEMBLY LANGUAGE) CAUSES ERROR INDICATORS RESULTING FROM RECORDS THAT ARE NOT A MULTIPLE OF SIX FRAMES TO BE IGNORED.

THE DIFFRACTOMETER OUTPUT MUST CONSIST OF TEN-CHARACTER WORDS, THE FIRST CHARACTER BEING ONE OF THE LEGAL BEGIN WORD CODES RECOGNIZED BY SUBROUTINE XRY323 (CARDS) OR XRY326 (TAPE).

WORD IDENTIFICATION	CARDS	TAPE
HKL	W	F
CHI	Y	X
PHI	/	Q
OMEGA	U	T
TWO-THETA	S	R
SCALER	V	U

THE CARDS OR TAPE ARE TREATED AS A STREAM OF CHARACTERS WITH NO ASSUMPTION ABOUT WHERE A WORD MUST START. EACH TIME A NEW WORD IS REQUIRED, THE INPUT STREAM IS SEARCHED UNTIL A BEGIN-WORD CODE IS FOUND. THE NEXT NINE CHARACTERS MUST BE DIGITS, AND THERE MUST BE A NON-DIGIT FOLLOWING THE LAST CHARACTER OF THE WORD. EXTRANEOUS CHARACTERS BETWEEN WORDS ARE IGNORED UNLESS THEY HAPPEN TO FIT THIS PATTERN. EXTRANEOUS LETTERS THAT CORRESPOND TO BEGIN WORD CODES WILL AFFECT THE WORD COUNT THAT APPEARS AS PART OF THE PRINTED OUTPUT FOR EACH REFLECTION.

WHEN A NEW HKL WORD IS READ THE CORRESPONDING SETTINGS FOR CHI, PHI, AND TWO THETA (BACKGROUND, PEAK, BACKGROUND) ARE CALCULATED USING A SIMPLIFIED VERSION OF 'DIFSET'. READING CONTINUES UNTIL A SECOND HKL WORD IS ENCOUNTERED. THIS IS STORED WHILE DATA FROM THE PREVIOUS HKL ARE PROCESSED, AND THE RESULTS ARE WRITTEN ON OUTPUT TAPES. FOR THIS REASON, MESSAGES ABOUT CONDITIONS ENCOUNTERED WHILE READING WILL PRECEED THE CORRESPONDING DATA.

FOR PURPOSES OF DEFINING LIMITATIONS ON THE CORRECTION PROCEDURE, THE WORDS REQUIRED FOR A COMPLETE SET OF DATA MAY BE GROUPED AS FOLLOWS-

1. HKL
2. CHI AND PHI
3. (TWO THETA - SCALER)

WORDS WITHIN ANY GROUP MAY BE REPEATED. THE LAST WORD OF EACH TYPE MUST BE CORRECT BEFORE THE FOLLOWING GROUP IS BEGUN. IN GROUP 3, TWO THETA AND SCALER WORDS MUST APPEAR IN PAIRS IN THIS ORDER. THE TWO THETA SETTING IS COMPARED WITH CALCULATED SETTINGS IN ORDER TO CLASSIFY THE SCALER READING THAT FOLLOWS IT AS BACKGROUND (LOW), PEAK, OR BACKGROUND (HIGH). IF THE BALANCED FILTER OPTION IS USED, SCALER READINGS OBTAINED WITH FILTER 2 ARE DISTINGUISHED FROM THOSE OBTAINED WITH FILTER 1 BY CHECKING THE FILTER IDENTIFICATION CODE OF THE SCALER WORD. AS MANY AS SIX DIFFERENT SCALER WORDS MAY BE STORED FOR A SINGLE REFLECTION. THE NAMES GIVEN TO THESE IN THE PROGRAM ARE OF THE FORM SC11, SC21,...SC23 WHERE THE FIRST DIGIT DESIGNATES THE FILTER, AND THE SECOND, THE TWO THETA SETTING (1-BACKGROUND(LOW), 2-PEAK, 3-BACKGROUND(HIGH)). IN THE CASE OF DATA OBTAINED BY THE TWO THETA SCAN TECHNIQUE, THE TWO THETA SETTING THAT GOES WITH THE SCALER WORD CONTAINING THE NUMBER OF COUNTS ACCUMULATED DURING THE SCAN IS THE SAME AS THE SETTING FOR EITHER BACKGROUND(LOW) OR BACKGROUND(HIGH). IT IS DISTINGUISHED FROM THESE BY THE FACT THAT THE SCANNING SPEED CODE CHARACTER IS DIFFERENT FROM SIX, AND THE SCALER WORD IS STORED AS SC12 OR SC22. IF A TWO THETA SETTING THAT MATCHES NONE OF THE CALCULATED SETTINGS OCCURS, THE SCALER WORD IS

DROPPED, ERROR INDICATOR 5 IS SET, AND READING CONTINUES. THE USE OF THIS SCHEME FOR CLASSIFYING SCALER READINGS PERMITS PEAK AND BACKGROUND READINGS TO OCCUR IN ANY ORDER, AND MAKES IT POSSIBLE TO CORRECT ANY TWO THETA-SCALER PAIR AT ANY TIME BEFORE THE NEXT HKL IS RECORDED. IF IT BECOMES NECESSARY TO MAKE A CORRECTION IN A PREVIOUS GROUP, THE GROUPS THAT FOLLOW IT MUST BE REPEATED.

IN ORDER TO ACCOMMODATE DATA TAKEN BY THE TWO-THETA SCAN METHOD WHERE THE AXIS POSITION HAS NOT BEEN RECORDED BEFORE THE SCALER READING FOR THE SECOND BACKGROUND (TO MAKE THE DATA FOR ONE REFLECTION FIT ON ONE CARD) THE PROGRAM HAS BEEN CHANGED TO THAT THE END OF THE TWO-THETA CAN RANGE IS TAKEN AS THE SETTING FOR THE SECOND BACKGROUND.

WHEN A NEW HKL IS READ, DATA FROM THE PREVIOUS HKL ARE CHECKED FOR COMPLETENESS. IF ALL DATA REQUIRED FOR THE TECHNIQUE SPECIFIED HAVE BEEN RECORDED, THE NET COUNTS AND STANDARD DEVIATION OF THE NET COUNTS (BASED ON COUNTING STATISTICS ONLY) ARE COMPUTED. IF THE DATA ARE NOT COMPLETE, ERROR INDICATOR 8 IS SET. IN EITHER CASE, 'XRY324' IS CALLED TO COMPUTE THE INTEGRATED INTENSITY, APPLY CORRECTION FACTOR (AS RECOMMENDED BY ALEXANDER AND SMITH (1962)), COMPUTE F(OBSERVED) AND SIGMA (F-OBSERVED), AND TAG REFLECTIONS THAT ARE TO BE TREATED AS HAVING INTENSITIES LESS THAN THE MINIMUM OBSERVABLE. THE OUTPUT WRITTEN ON NTOUT, FOR PRINTING, INCLUDES ERROR MESSAGES AND INCOMPLETE DATA AS WELL AS COMPLETE AND CORRECT DATA. THAT WRITTEN ON NTAPEB INCLUDES ONLY THE LATTER AND IS IN A FORMAT SUITABLE FOR INPUT TO =DATA REDUCTION=. THE LAST RECORD BEFORE THE END OF FILE MARK ON NTAPEB IS 'TAPES N' WHERE N IS THE LOGICAL NUMBER OF THE CARD READER (NTINM IN NUC006)

IN RUNNING =DATA REDUCTION=, ALL THE INPUT DATA REQUIRED BY THAT PROGRAM ARE SUPPLIED ON CARDS IN THE USUAL WAY. AT THE PLACE IN THE DECK WHERE REFLECTION DATA WOULD BEGIN, A =TAPES= CARD IS USED TO REDEFINE THE USUAL INPUT TAPE =NTIN= TO HAVE THE LOGICAL TAPE NUMBER OF =NTAPEB=. THIS CAUSES =DATA REDUCTION= TO READ THE REFLECTION DATA TAPE PREPARED BY THIS PROGRAM. THE 'TAPES N' RECORD CAUSES THE PROGRAM TO GO BACK TO READING CARDS SO THAT IT WILL FIND ANY REMAINING CARDS IN THE DATA DECK.

ERROR INDICATORS ARE PRINTED IN TEN COLUMNS HEADED 'ERRORS'. THE TYPE OF ERROR IS DETERMINED BY THE NUMBER OF THE COLUMN IN WHICH THE INDICATOR IS WRITTEN. EXCEPT IN COLUMN 6, WHICH IS USED FOR TWO INDICATORS, THE COLUMN NUMBER IS WRITTEN TO INDICATE THAT AN ERROR OCCURRED. THE NUMBERS THAT MAY APPEAR IN COLUMN 6 ARE 0/1/6/7.

1. ERROR IN WORD LENGTH
2. ILLEGAL BEGIN WORD CODE (WORD IS SKIPPED)
*3. CHI SETTING IS INCORRECT (PHI AND TWO THETA WILL NOT BE TESTED)
*4. PHI SETTING IS INCORRECT (TWO THETA WILL NOT BE TESTED)
*5. TWO THETA SETTING INCORRECT (THIS TEST IS MADE WHEN A SCALER WORD IS ENCOUNTERED. IF TEST IS FAILED, BOTH TWO-THETA WORD AND SCALER WORD ARE REJECTED)
*6. 0 NO ERROR
   1 NUMBER OF COUNTS EXCEEDS MAXIMUM FOR LINEARITY OF COUNTER.
   6 SCALER READING BELOW TEN COUNTS
   7 BOTH OF ABOVE

IN CASE OF 1, 6, OR 7 OUTPUT ON NTAPEB IS SUPPRESSED AND SETTINGS ARE WRITTEN ON NTAPEA FOR USE IN REMEASURING THIS REFLECTION.

*7. SCALER READING SAME AS PREVIOUS (THE OPERATOR MAY HAVE SKIPPED THE COUNTING CYCLE)

8. DATA INCOMPLETE
OUTPUT ON NTAPEB IS SUPPRESSED AND SETTINGS ARE WRITTEN ON NTAPEA FOR USE IN RE-MEASURING THE REFLECTION

9. ILLEGAL SIGN BIT IN HKL WORD (THIS, OR ANY OTHER ERROR IN HKL WORD WILL USUALLY CAUSE INDICATORS 3, 4, 5, AND 8 TO OCCUR)

10. HKL READ IS OUTSIDE THE SPHERE OF REFLECTION

* 3, 4, 5, 6, AND 7 INDICATE THAT AN ERROR CONDITION EXISTED AT ONE TIME. UNLESS AN 8 ALSO OCCURS, IT WAS CORRECTED. IF 3 OR 4 OCCURS TESTS FOR 5, 6, AND 7 ARE SKIPPED. IF 3 AND 4 DO NOT OCCUR BUT 5 DOES TESTS FOR 6 AND 7 ARE SKIPPED. WHEN A TEST IS SKIPPED, THE INDICATOR FOR THAT TEST REMAINS SET TO ZERO. ALL TESTS ON SETTINGS ARE MADE BEFORE ROUNDING OFF FOR PRINTING.

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DIFFRACTOMETER SETTING PROGRAM

=DIFSET= WAS ORIGINALLY CODED BY STEVEN T. FREER AND JOSEPH KRAUT. IT WAS MODIFIED AND ADAPTED TO THE SYSTEM BY HERMAN L. AMMON, AND THE SUBROUTINE FOR DETERMINING SYSTEMATIC ABSENCES WAS ADDED BY ROGER V. CHASTAIN. THE FORTRAN IV VERSION, WHICH INCLUDES PROVISIONS FOR MAKING A CONTROL TAPE OR CARD DECK FOR AN AUTOMATIC DIFFRACTOMETER, WAS PREPARED BY FLOYD A. MAUER.

THE PROGRAM WILL GENERATE MILLER INDICES AND COMPUTE SETTINGS FOR A DIFFRACTOMETER EQUIPPED WITH AN EULERIAN CRADLE (GONIOSTAT). FOR EACH HKL, SETTINGS FOR CHI, PHI, START TWO-THETA, PEAK TWO-THETA, AND STOP TWO-THETA, AS WELL AS THE SCANNING TIME, ARE COMPUTED. THE PROGRAM IS GENERAL FOR ALL SPACE GROUPS.

NECESSARY INPUT DATA CONSIST OF CELL PARAMETERS AND THE ORIENTATION OF TWO RECIPROCAL AXES WITH RESPECT TO THE PHI AXIS AND THE PHI=0 PLANE. CELL CONSTANTS MAY BE SUPPLIED ON A =CELL= CARD, OR THEY MAY BE LEFT IN MEMORY BY A =PARAM= RUN THAT PRECEEDS THE =DIFSET= RUN. IN THE LATTER CASE, A =PARAMC= CARD REPLACES THE =CELL= CARD TO INDICATE THAT THE CELL CONSTANTS CAME FROM A PREVIOUS LEAST SQUARES REFINEMENT.

SOME CARE MUST BE EXERCISED IN SPECIFYING THE ORIENTATION OF THE RECIPROCAL LATTICE ON THE GONIOSTAT. TWO RECIPROCAL LATTICE VECTORS DO NOT UNIQUELY FIX THE POSITION OF A THREE DIMENSIONAL LATTICE AND IT IS NECESSARY TO FOLLOW THE CONVENTION THAT A RIGHT HANDED SYSTEM OF AXES IS BEING USED. WHEN SPECIFYING A RECIPROCAL LATTICE VECTOR LYING ON THE PHI AXIS, A VECTOR MUST BE CHOSEN WHICH IS COINCIDENT WITH THE POSITIVE DIRECTION OF THE PHI AXIS (I.E., A VECTOR COMING OUT OF THE GONIOSTAT, NOT GOING INTO IT).

THE SUBROUTINE =XRY271= WRITTEN TO GIVE REFLECTIONS IN AN ORDER SUITABLE FOR AUTOMATIC OPERATION WORKS BEST IF ONE OF THE RECIPROCAL AXES IS PARALLEL TO THE PHI AXIS OF THE DIFFRACTOMETER. SCANNING IS UP AND DOWN ROWS PARALLEL TO PHI. THE PHI SETTING DOES NOT CHANGE WITHIN A ROW, AND CAN BE MADE TO PROGRESS ALWAYS IN ONE DIRECTION TO MINIMIZE THE EFFECT OF BACKLASH. CHI AND TWO THETA CHANGE FOR EACH REFLECTION BUT DATA ARE TAKEN UP ONE ROW AND DOWN THE NEXT SO THAT NO TIME IS LOST IN RESETTING EITHER AXIS AT THE END OF A ROW. SETTINGS MAY BE GENERATED AUTOMATICALLY FOR AS MUCH AS A HEMI-SPHERE OR AS LITTLE AS AN OCTANT OF RECIPROCAL SPACE.

THE TWO-THETA SCAN RANGE MAY BE CALCULATED IN THREE WAYS. TWO OF THE METHODS INVOLVE SUBTRACTING A 'QUANTITY' FROM THE TWO THETA FOR THE ALPHA(1) WAVELENGTH TO OBTAIN 'START TWO THETA' AND ADDING THIS 'QUANTITY' TO THE TWO THETA FOR THE ALPHA(2) WAVELENGTH TO OBTAIN 'STOP TWO THETA'. THE PRESENCE OF A =BAKSET= CARD SIGNALS THAT THIS 'QUANTITY' WILL BE CONSTANT (THE VALUE CONTAINED ON THE CARD) AND NOT A FUNCTION OF TWO

THETA.

FOR COPPER RADIATION, THIS 'QUANTITY' MAY BE OBTAINED FROM AN INTERNALLY STORED TABLE (DETERMINED EMPIRICALLY BY THE J. KRAUT GROUP) AND IS A FUNCTION OF TWO THETA. THE TABLE VALUES ARE AUTOMATICALLY APPLIED IF NEITHER OF THE OTHER TWO OPTIONS IS CALLED (AS DETERMINED BY THE ABSENCE OF =BAKSET= AND =EQNCON= CARDS). THE TABLE VALUES ARE ---

TWO-THETA RANGE (DEGREES)	TWO-THETA INCREMENT APPLIED (DEGREES)
0 - 10	0.75
10 - 20	0.75
20 - 30	0.75
30 - 40	0.75
40 - 50	0.80
50 - 60	0.80
60 - 70	0.80
70 - 80	0.85
80 - 90	0.85
90 - 100	0.85
100 - 110	0.85
110 - 120	0.85
120 - 130	0.95
130 - 140	0.95
140 - 150	1.05
150 - 160	1.20
160 - 170	1.20

THE THIRD OPTION IS SIGNALLED BY THE PRESENCE OF AN =EQNCON= CARD CONTAINING THE CONSTANTS 'A' AND 'B'. THESE QUANTITIES ARE USED IN THE FOLLOWING EQUATION ---

TWO THETA SCAN RANGE = A + B*TAN(THETA)

FACTORS (E.G., CRYSTAL SIZE, CRYSTAL MOSAICITY AND SOURCE SIZE) INFLUENCING THE SCAN RANGE BUT WHICH ARE CONSTANT FOR A GIVEN CRYSTAL MAY BE LUMPED INTO 'A' WHILE SPECTRAL DISPERSION, A FUNCTION OF THETA, MAY BE EXPRESSED BY THE SECOND TERM. THE AVERAGE OF THE TWO THETA'S FOR THE ALPHA(1) AND ALPHA(2) WAVELENGTHS IS DETERMINED AND HALF OF THE ABOVE RANGE USED TO CALCULATED 'START' AND 'STOP'. VALUES RECOMMENDED BY ALEXANDER AND SMITH (1) FOR A AND B ARE 1.80 AND 0.86 FOR COPPER RADIATION, AND 1.80 AND 1.00 FOR MOLYBDENUM. (THESE ARE TYPICAL VALUES FOR A DIFFRACTOMETER OF THE RADIUS OF THE G.E. XRD-6.)

OUTPUT FROM THE PROGRAM MAY BE IN SEVERAL FORMS. PRINTED OUTPUT IS ALWAYS FURNISHED. SETTING CARDS CONTAINING THE SAME INFORMATION ARE OPTIONAL. IF SETTING CARDS ARE MADE, PUNCHING OF CARDS FOR REFLECTIONS THAT ARE SYSTEMATICALLY ABSENT IS OPTIONAL. A CONTROL TAPE OR CARD DECK FOR AN AUTOMATIC DIFFRACTOMETER IS GENERATED IF AN =XRDC= CARD AND AN =XRDFMT= CARD ARE SUPPLIED. (AT NBS A TTYFMT CARD IS ALSO REQUIRED.)

DATA ON THE =XRDC= CARD DETERMINES WHETHER ---

(1) A CARD DECK OR
(2) A MAGNETIC TAPE FOR OFF-LINE PUNCHING

WILL BE MADE. THE TAPE FOR PUNCHING MAY BE OBTAINED WITH TEN CHARACTER COMMAND WORDS ONLY, AS REQUIRED BY DATEX PAPER-TAPE INPUT DIFFRACTOMETERS, OR WITH TELETYPE CONTROL CHARACTERS BETWEEN THE COMMAND WORDS. THE CHARACTERS THAT OCCUR ON THE MAGNETIC TAPE WILL BE THE INTEGERS 0-9 AND ANY OTHERS THAT MAY BE WRITTEN IN THE 5A1 FIELDS OF THE =XRDFMT= CARD. THE RECORDS WILL CONTAIN A VARIABLE NUMBER OF CHARACTERS THAT ARE TO BE PUNCHED AND ARE FILLED WITH BLANKS TO MAKE 120 CHARACTERS IN EACH RECORD. THESE BLANKS MUST NOT BE PUNCHED. IF THE =TTYFMT= CARD IS USED (NBS ONLY) THE FOUR CHARACTERS (B, A, C, +) OCCUR AND ARE TO BE TRANSLATED TO THE ASCII (AMERICAN STANDARD CODE FOR INFORMATION INTERCHANGE) CODE FOR CARRIAGE RETURN, LINE FEED, SPACE, AND ASTERISK, RESPECTIVELY. DIFFERENT CHARACTERS MAY BE SELECTED FOR THESE PURPOSES BY CHANGING THE DATA STATEMENT-

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DATA ICR,LF,ISPACE,ISTAR /1H$,1H',1H=,1H* /
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IN SUBROUTINE XRY276. THE CHARACTER BLANK (IBLNK IN SUBROUTINE XRY276) AND ANY CHARACTERS THAT WILL OCCUR AS BEGIN WORD CODES OR IN COMPOUND IDENTIFICATION CODES MUST BE AVOIDED.

THE CODE THAT IS TO BE PUNCHED IN THE PAPER TAPE MAY DIFFER FOR INDIVIDUAL DIFFRACTOMETERS. ANY DISTINCTIVE CHARACTER MAY BE USED FOR ANY BEGIN WORD CODE IF IT IS TRANSLATED APPROPRIATELY BEFORE PUNCHING. FOR EXAMPLE, THE CHARACTERS THAT ARE USED FOR THE GE-DATEX CARD INPUT DIFFRACTOMETER ARE SUITABLE FOR THE PAPER-TAPE INPUT MACHINE IF THE FOLLOWING CONVERSION TABLE IS USED.

TYPE OF WORD	BEGIN WORD CODE	TAPE CODE 87654.321
HKL	W	01000.110
CHI	Y	01001.000
PHI	/	01000.001
TWO-THETA	S	01000.010
OMEGA	U	01000.100
(DIGITS)	0-9	8-4-2-1 BCD

IF THE TAPE IS TO BE PUNCHED IN ASCII CODE, TWO SETS OF LETTERS GIVE THE REQUIRED BIT CONFIGURATIONS IN CHANNELS 1-4 AND 7, WHICH ARE THE ONLY ONES THE EQUIPMENT READS. THE DIGITS 0-9 ALSO CONFORM WITH RESPECT TO THESE CHANNELS.

TYPE OF WORD	BEGIN WORD CODE	TAPE CODE 87654.321	BEGIN WORD CODE	TAPE CODE 87654.321
HKL	F	11000.110	V	01010.110
CHI	H	01001.000	X	11011.000

PHI	A	01000.001	Q	11010.001
TWO-THETA	B	01000.010	R	11010.010
OMEGA	D	01000.100	T	11010.100

(AT NBS, X,Q,R, AND T ARE USED FOR AXIS POSITION COMMANDS AND F IS USED FOR HKL IDENTIFICATION DATA TRANSFER.)

CONSIDERABLE FLEXIBILITY IN GENERATING THE DIFFRACTOMETER TAPE OR CARDS IS PROVIDED. THE PROGRAM IS DESIGNED AROUND A TEN-CHARACTER COMMAND WORD SUCH AS IS USED BY THE GE-DATEX DIFFRACTOMETER, BUT OTHER FORMATS CAN BE OBTAINED. AS MANY AS TWELVE COMMAND WORDS CAN BE SPECIFIED FOR MEASUREMENTS ON EACH DATA REFLECTION AND (INDEPENDENTLY) ON UP TO NINE STANDARD REFLECTIONS. IF FEWER THAN TWELVE COMMANDS ARE USED FOR A REFLECTION, THE UNUSED ONES ARE IGNORED. THE SAME IS TRUE IF FEWER THAN NINE STANDARD REFLECTIONS ARE SPECIFIED.

THE CURRENT DATA REFLECTION, WHICH CHANGES EACH TIME A NEW HKL IS GENERATED, AND THE NINE STANDARDS ARE NUMBERED SEQUENTIALLY FROM 1 TO 10 FOR IDENTIFICATION. THE DATA REFLECTION IS ALWAYS NUMBER 1. THESE NUMBERS APPEAR ON THE =STDREF=, =XRDFMT=, AND =TTYFMT= CARDS TO INDICATE WHICH REFLECTION THEY APPLY TO. ALL THE CARDS FOR A GIVEN STANDARD MUST BE TOGETHER, FOLLOWED BY THE =HKL= OR SETTING CARD THAT DETERMINES WHICH REFLECTION IS TO BE MEASURED. ALL STANDARD REFLECTIONS MUST BE ORDERED ACCORDING TO IDENTIFICATION NUMBER. PARAMETERS ON THE =STDREF= CARD DETERMINE HOW MANY DATA REFLECTIONS ARE TO BE DONE BEFORE THAT STANDARD IS INSERTED. ALL REFLECTIONS WITHIN THE INDEX AND ANGLE LIMITS (INCLUDING SYSTEMATICALLY ABSENT REFLECTIONS, BUT NOT STANDARD REFLECTIONS ARE COUNTED. DURING EACH OUTPUT CYCLE COMMANDS FOR ONE DATA REFLECTION, AND ANY STANDARD REFLECTIONS WHOSE TURN HAS COME UP, ARE PUT ON THE DIFFRACTOMETER CONTROL TAPE OR IN THE CARD DECK.

EITHER AND =HKL= CARD OR A SETTING CARD MAY BE USED TO PROVIDE THE SETTING ANGLE DATA FOR A STANDARD REFLECTION. AN =HKL= CARD CAUSES SETTINGS TO BE COMPUTED. THE INDEX AND ANGLE LIMITS ARE CHECKED, AND THE PHI ANGLE CORRECTION, IF ANY, IS APPLIED. SETTING CARDS (GENERATED BY THIS PROGRAM IN A PREVIOUS RUN, OR PUNCHED IN THE SAME FORMAT) MAY BE USED TO PROVIDE UP TO FIVE ANGLE SETTINGS. THE INDICES AND THE ANGLES IN THE CHI, PHI, START TWO-THETA, PEAK TWO-THETA, AND STOP TWO-THETA FIELDS ARE USED AS SPECIFIED ON THE =XRDFMT= CARD. THERE ARE NO CHECKS MADE, AND FICTITIOUS INDICES AND ANGLES MAY BE USED FOR SPECIAL PURPOSES SUCH AS CHECKING ARC ALIGNMENT, TWO-THETA DRIFT AND CRYSTAL DETERIORATION. IT IS POSSIBLE TO USE TWO STANDARD REFLECTIONS TOGETHER TO MANIPULATE AS MANY AS TEN ANGLE SETTINGS WITH AS MANY AS 24 COMMANDS.

ONLY THE FIRST =HKL= OR SETTING CARD AFTER A =STDREF= CARD IS TREATED AS A STANDARD REFLECTION. ANY OTHERS ARE TREATED AS DATA REFLECTIONS. THUS IT IS POSSIBLE TO USE =HKL= AND SETTING CARDS AS INPUT TO THIS PROGRAM IN ORDER TO PREPARE A CONTROL TAPE OR CARD DECK IN A SPECIAL ORDER OR FOR A FEW SCATTERED REFLECTIONS. FOR EXAMPLE, IT IS CONVENIENT TO HAVE THE =DIFOPP= PROGRAM THAT PROCESSES THE DIFFRACTOMETER OUTPUT PUNCH SETTING CARDS FOR THOSE REFLECTIONS THAT MUST BE RE-MEASURED. THESE CAN BE USED AS INPUT TO =DIFSET= TO MAKE UP A NEW CONTROL TAPE OR CARD DECK.

WITH THE FLEXIBILITY AFFORDED BY THIS PROGRAM, IT IS QUITE POSSIBLE TO TAKE DATA IN A WAY THAT HAS NOT BEEN PROVIDED FOR IN THE PROGRAM =DIFOPP= THAT PROCESSES THE OUTPUT DATA. IT IS A GOOD IDEA TO CHECK OUT THE PROCESSING OF OUTPUT DATA BEFORE DOING A LARGE JOB.

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BINARY DATA FILE DUMP, COPY OR PUNCH

THIS LINK IS DESIGNED TO AID IN CHECKING OUT PROGRAMS. IT WILL DUMP THE CONTENTS OF THE BINARY DATA FILE, PHYSICAL RECORD BY PHYSICAL RECORD. THE ALPHABETIC MATERIAL IN THE FILE WILL NOT BE PRINTED CORRECTLY BUT ALL INTERGERS AND FLOATING POINT QUANTITIES WILL BE PRINTED PROPERLY. IF ONE DESIRES TO BY PASS =DATRDN= DURING CHECK OUT OF A TEST CASE, THE WHOLE BINARY DATA FILE MAY BE PUNCHED IN CARDS BY DUMCOP - THESE CARDS ARE THEN READ BY THE 'STAND-ALONE' NUCLEUS CHECK OUT PACKAGE.

THIS LINK MAY ALSO BE USED TO SIMPLY COPY THE BINARY DATA FILE. THIS FUNCTION MAY BE FOUND USEFUL WHEN ONE WISHES TO TRANSFER A FILE FROM ONE MASS STORAGE DEVICE TO ANOTHER (E.G. DRUM OR DISC TO TAPE).

PROGRAM FOR THE CALCULATION OF STRUCTURE FACTORS

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 CURRENT FORTRAN VERSION WAS PREPARED IN 1965 BY ROBERT BRAUN AND J.M. STEWART.

THE STRUCTURE FACTOR CALCULATION IS ACCOMPLISHED IN TWO OVERLAYS AND THEIR SUBROUTINES- THE FIRST READS THE ATOM PARAMETERS FROM THE BINARY DATA FILE AND GENERATES THE FULL CELL OF ATOMIC COORDINATES AND THE SECOND CALCULATES THE STRUCTURE FACTORS.

THIS METHOD OF CALCULATING STRUCTURE FACTORS IS USEFUL IN THAT IT MAKES POSSIBLE THE DETECTION OF ATOMS IN SPECIAL POSITIONS, IN ADDITION IT IS A FASTER METHOD FOR STRUCTURE FACTOR SUMMATION BECAUSE OF THE SIMPLER SUMMATION ALGORITHIM. THIS INFORMATION IS THEN PUBLISHED BY THE PROGRAM AND THE ATOM SCATTERING FACTOR SCALED APPROPRIATELY. THESE SCALE FACTORS ARE EXACTLY THE ONES REQUIRED BY STRUCTURE FACTOR PROGRAMS (I.E. LEAST-SQUARES) WHICH GENERATE SYMMETRY BY OPERATING UPON THE MILLER INDICES. IN ADDITION TO THIS FEATURE THE PROGRAM IS FASTER THAN A LEAST SQUARES PROGRAM BECAUSE NO DERIVATIVES ARE CALCULATED. IT THUS SERVES AS THE BEST LINK TO USE WHEN FIXED ATOM STRUCTURE FACTORS ARE PREPARED OR WHEN ONE WISHES TO CALCULATE STRUCTURE FACTORS TO GIVE PHASES, FOR EXAMPLE, FOR A FOURIER OR DIFFERENCE FOURIER CALCULATION.

SINCE THE PROGRAM GENERATES ALL THE ATOMS IN THE UNIT CELL THE RESTRICTIONS ON NUMBERS OF ATOMS IS DEPENDENT ON THE NUMBER OF SYMMETRY OPERATIONS SUPPLIED AT DATA REDUCTION TIME. FOR A TRICLINIC CELL P1 OR P1 BAR THE PROGRAM WILL HANDLE THOUSANDS OF ATOMS IN THE ASYMMETRIC UNIT CELL.

THERE IS A 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), 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 MAY BE STORED ON TAPE AT DATA REDUCTION TIME. IT IS MORE USUAL TO LET THE SYMMETRY GENERATION SUBROUTINE OF THIS FC PROGRAM, ESTABLISH THE INDIVIDUAL ATOM SCALE FACTORS TO BE USED BY THE =FC= PROGRAM.

THE ATOMIC FORM FACTOR SCALING FEATURE (POPULATION PARAMETER)

FACILITATES CALCULATIONS FOR STRUCTURES CONTAINING VARIATE ATOM EQUI-POINTS.

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 IN THE BINARY FILE DURING DATA REDUCTION. THE SCATTERING FACTOR IS GIVEN BY EQUATION 1. FOR THIS CORRECTION, THE MAGNITUDE OF FC WHICH IS TO BE COMPARED WITH THE EXPERIMENTAL VALUE IS GIVEN BY EQUATION 2, THE CORRECT COEFFICIENT FOR ELECTRON-DENSITY MAPS IS GIVEN BY EQUATION 3, AND THE AMPLITUDE FOR DIFFERENCE SYNTHESIS IS GIVEN BY EQUATION 4.

(1) F(J) = F(J) + F'(J) + F''(J) WHERE F(J) IS THE SCATTERING FACTOR FROM THE TABLES SUPPLIED AT DATA REDUCTION, F'(J) IS THE TEMPLETON CORRECTION TO THE REAL PART OF THE SCATTERING FACTOR, F''(J) THE IMAGINARY PART OF THE DISPERSION CORRECTION.

(2) TO BE ADDED

(3) TO BE ADDED

(4) TO BE ADDED

THE LIMIT TO THE NUMBER OF NON-EQUIVALENT ATOMS WHICH MAY BE CALCULATED DEPENDS UPON THE TEMPERATURE FACTOR MODE AND CORE SIZE OF THE MACHINE USED. IT IS NOTEWORTHY, HOWEVER, THAT THIS LIMITATION ON THE NUMBER OF ATOMS IN THE UNIT CELL CAN BE READILY OVERCOME BY ANY MULTIPLE BY THE USE OF A =PARTIAL CONTRIBUTION= CALCULATION IN A MULTI-PASS METHOD. THE STRUCTURE FACTOR PROGRAMS 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.

IN ORDER TO FACILITATE THE USE OF ''FIXED ATOMS'' A BRIEF OUTLINE OF THE METHOD USED WILL BE FOUND USEFUL. THE VERY LIMITED MUMBER OF PARAMETERS THAT FULL MATRIX LEAST SQUARES IS CAPABLE OF HANDLING MAKES THE USE OF FIXED ATOMS DESIREABLE FOR MANY COMPOUNDS. (BLOCK DIAGONAL OR DIAGONAL REFINEMENTS MAY BE CARRIED OUT.) THE STRUCTURE FACTOR PROGRAM CAN BE UTILIZED TO CALCULATE STRUCTURE FACTORS FOR A PORTION OF THE ATOMS IN THE ASSYMMETRIC UNIT OF A GIVEN UNIT CELL. THESE ARE ATOMS WHOSE PARAMETERS ARE NOT TO BE VARIED. THE RESULTING STRUCTURE FACTORS MAY THEN BE USED AS ''FIXED ATOM'' CONTRIBUTIONS TO THE STRUCTURE FACTORS CALCULATED FOR THE WHOLE CELL, OR THAT PORTION DETERMINED SO FAR IN THE STRUCTURE

ANALYSIS. THE STORAGE RESTRICTION ON THE FC PROGRAM IS SUCH THAT IT CAN HANDLE MANY ATOMS IN THE UNIT CELL SO THAT BY JUDICIOUS USE OF THE ATOM LIMITATION OF THE FULL MATRIX LEAST SQUARES PROGRAM A NUMBER OF LARGE BLOCK REFINEMENTS MAY BE CARRIED OUT. THIS PROCEDURE WILL RESULT IN THE REFINEMENT OF THE WHOLE STRUCTURE. SOME ''OVERLAP'' OF PARAMETERS MAY BE DESIREABLE. THE BINARY DATA FILE HAS QUANTITIES STORED, AMONG OTHERS, FOR EACH REFLECTION FOR A, B, AND FIXED CONTRIBUTION TO A AND B (WHERE A AND B REFER TO THE REAL AND IMAGINARY PARTS OF THE STRUCTURE FACTOR). DATA REDUCTION INITIALIZES ALL FOUR TO ZERO. AFTER AN FC CALCULATION A AND B HAVE BEEN GIVEN A VALUE AND THIS IS WRITTEN ON =NFILEB=. THE LOGICAL UNIT =NFILEB= MAY NOW BE SWITCHED TO BE A =NFILEA= AND THIS BINARY DATA FILE BECOMES INPUT INFORMATION FOR THE NEXT CALCULATION OF STRUCTURE FACTORS (FOR LEAST SQUARES OR OTHER STRUCTURE FACTOR TYPE PROGRAMS). AT THIS POINT THE STRUCTURE FACTOR TYPE PROGRAM IS KEYED TO ESTABLISH AND APPLY THE PREVIOUS FC AS A FIXED ATOM CALCULATION. THIS RESULTS IN THE A AND B ON THE NEW =NFILEA= BEING PLACED IN THE FIXED ATOM A AND B ON =NFILEB= AND THE STRUCTURE FACTOR TYPE PROGRAM USING THESE VALUES INSTEAD OF ZEROS TO START THE STRUCTURE FACTOR SUMMATIONS. THE =NFILEB= AT THE END OF THE RUN THEN HAS A SET OF FIXED ATOM CONTRIBUTIONS STORED UPON IT AND MAY BE USED AS AN =NFILEA= IN SUBSEQUENT RUNS AND CODED EITHER TO USE PREVIOUS FC TO ESTABLISH AND APPLY AS FIXED ATOM CONTRIBUTION OR SIMPLY TO APPLY THE FIXED ATOM CONTRIBUTION NOW ESTABLISHED. NOTE THAT IN THE FIRST CASE CASCADING OCCURS AND IN THE SECOND THE SET ALREADY ESTABLISHED IS CONTINUED AS THE FIXED ATOM SET. LARGE TIME SAVINGS MAY RESULT FROM THE USE OF THE FIXED ATOM FACILITY, ESPECIALLY IN THE CASE OF FULL MATIRX LEAST SQUARES REFINEMENT OF A FEW PARAMETERS OF A SMALL PORTION OF A LARGE NUMBER OF ATOMS IN AN ASYMMETRIC UNIT.

WHEN THE CALCULATION FOR A GIVEN REFLECTION IS COMPLETE THE INFORMATION IS PLACED IN =NFILEB=, THE STATISTICS COMPILED AND THE NEXT REFLECTION PROCESSED. FINALLY, REFLECTION COUNTS AND NEW SCALE FACTORS FOR EACH LEVEL ARE CALCULATED AND PRINTED. THE NEW RESCALE FACTORS ARE PLACED IN THE BINARY DATA FILE ALONG WITH THE LEAST SQUARES CHANGE IN OVERALL TEMPERATURE FACTOR. THE RELIABILITY INDEX, R, IS PRINTED FOR EACH LEVEL AND FOR ALL REFLECTION DATA.

THE NEW SCALE FACTOR, K, IS OBTAINED FROM THE OLD SCALE FACTOR, K-PRIME, BY EQUATION 5, THE LEAST SQUARES CORRECTION TO THE OVERALL ISOTROPIC TEMPERATURE FACTOR IS COMPUTED BY MINIMIZING THE SUM OF THE SQUARE OF THE RESIDUAL IN EQUATION 6, AND THE RELIABILITY INDEX IS GIVEN BY EQUATION 7.

IN THE FOLLOWING EQUATIONS THE SUMMATION SYMBOL SIGMA IS WRITTEN AS JUST THAT. ABS IMPLIES ABSOLUTE VALUE.

(5) K = (K')(SIGMA(FC))/SIGMA(FO))

(6) RESIDUAL = DELTA(B)(SINSQUARE THETA/LAMBDA SQUARE) + LN(FO/FC) + LN(RESCALE CONSTANT)

(7) R = SIGMA(ABS(DELTA F))/SIGMA(ABS(FO)) WHERE SUM IS OVER ALL REFLECTIONS.

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FOURIER SYNTHESIS PROGRAM

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, JAMES M. STEWART, AND HIROSHI TAKEDA.

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) OR AUTOMATIC LAYOUT TO INCH/ANGSTROM SCALE IF DESIRED.

(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 FILE 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 MODIFICATION OF THE PHASE OF THE SYMMETRICALLY RELATED REFLECTION. THE ACTUAL FOURIER SUMMATION IS ACCOMPLISHED BY SUMMING ALL SPACE GROUPS AS IF THEY WERE TRICLINIC USING THE METHOD OF FACTORING SHOWN BELOW.

******EQUATIONS TO BE ADDED HERE******

THE BINARY DATA FILE, HOWEVER, CONTAINS ONLY A UNIQUE SET OF REFLECTIONS PLUS THE NECESSARY INDICATORS TO MAKE POSSIBLE THE AUTOMATIC GENERATION OF SYMMETRY-RELATED REFLECTIONS. SUBROUTINES OF THE DATA REDUCTION PROGRAM ARE USED TO ANALYZE THE SPACE-GROUP SYMMETRY OPERATIONS

FOR A SET OF ROTATION MATRICES (R) AND TRANSLATION VECTORS (T) WHICH ARE STORED IN THE BINARY DATA FILE. AT DATA REDUCTION TIME THE GENERATIONS ARE APPLIED TO EACH UNIQUE REFLECTION AND A SET OF CODES ARE FORMED WHICH DEFINE FOR EACH UNIQUE 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. A SUBROUTINE OF THE FOURIER PROGRAM USES THESE CODES 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 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 HEMISPHERE 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 ********** GIVES ALL ALLOWED VALUES FOR PHASE CHANGES 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.

FOR NON-DIAGONAL ROTATIONS THE MAGNITUDE OF H,K,L AS WELL AS THE SIGNS WILL BE ALTERED.

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=.

IN ORDER TO SIMPLIFY THE USE OF THE FOURIER PROGRAM AND MAKE INTERPRETATION EASIER IT IS POSSIBLE TO LEAVE OUT THE =LAYOUT= CARD AND LET THE PROGRAM ESTABLISH GRID DIVISIONS BASED ON A CONSIDERATION OF RESOLUTION DESIRED AND TYPE POSITION CHARACTERISTIC OF THE LINE PRINTER. AN ARTICLE IN SCIENCE, VOL 143 NO. 3611, 1162-1163 (1964) GIVES A METHOD SUGGESTED BY J. D. H. DONNAY AND H. TAKEDA. THE PROGRAM USES AN IMPROVEMENT OF THIS APPROACH. A FOURIER LAID OUT IN THE FOLLOWING MANNER RESULTS IN DEVELOPING THE ELECTRON OR PATTERSON OR DIFFERENCE FOURIER AT THE POINT OF THE TYPE WHEEL. IN THE AUTHORS TERMINOLOGY THE =MACHINE GRID= POINT. IN ORDER TO PRINT OUT UNDEFORMED SECTIONS TRUE TO A SPECIFIED SCALE (IN ANGSTROMS/INCH) THE FOLLOWING VALUES MAY

BE SUPPLIED IN THE =LAYOUT= CARD OR IF THE =LAYOUT= IS OMITTED THEY WILL BE SUPPLIED AUTOMATICALLY. THE COSINE OF THE ANGLE ALPHA, BETA, OR GAMMA (QU) BETWEEN THE AXIS IN THE PRINTED PAGES (SUM DIRECTIONS 2 AND 3), THE NUMBER OF DIVISIONS ACROSS THE PAGE (THIRD SUM DIRECTIONS) MUST BE EQUAL TO (CELL LENGTH(3) * (INCHES/ANGSTROM) * 10.0)/(NUMBER OF TYPE WHEELS PER EACH FOURIER GRID COLUMN). THE NUMBER OF DIVISIONS DOWN THE PAGE (SECOND SUM DIRECTION) MUST BE EQUAL TO (CELL LENGTH(2) * SINF(QU) * (INCHES/ANGSTROM * 6.0)/(NUMBER OF PRINT LINES PER EACH FOURIER GRID LINE). THE NUMBER OF DIVISIONS FROM PAGE TO PAGE MAY REPRESENT ANY SENSIBLE RESOLUTION. (I.E. QUARTER OR THIRD ANGSTROM). REMEMBER THAT IF THERE IS AN ANGLE BETWEEN ANY AXIS AND THE PAGE TO PAGE AXIS THEN ONE MUST OFF-SET EACH LAYER ACCORDINGLY.

THE FOLLOWING COEFFICIENTS ARE PRESENTLY CODED INTO THE FOURIER PROGRAM.

(1) USERS FUNCTION. BY MEANS OF SUBROUTINE XRY061. (PRESENT FORM OF XRY061 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. THE =DATFIX= LINK MUST BE RUN FIRST IN ORDER TO GENERATE E VALUES.

(4) FO FOURIER. SUBSTITUTE FO/2 FOR LESS-THANS AND THEN TEST ALL REFLECTIONS- 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 QUAZI-NORMALIZED 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 FO 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 QUAZI-NORMALIZED STRUCTURE FACTORS (E) GENERATED BY =LATFIX= PROGRAM AS COEFFICIENTS. PHASES PREDETERMINED FROM KARLE AND KARLE SYMBOLIC ADDITION PROCEEDURE. REJECT ALL REFLECTIONS WITH UNDETERMINED PHASE, REJECT WHEN THE MAGNITUDE OF (E) IS LESS THAN (RR), REJECT ALL LESS-THAN REFLECTIONS. ESTIMATED PHASES MUST HAVE BEEN PLACED IN THE BINARY DATA FILE BY USE OF =PHASE=, =MODIFY=, OR SIMILAR PROGRAM.

(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 THE PROGRAM READS, REFLECTION BY REFLECTION, THE UNIQUE SET SUPPLIED ON THE BINARY DATA FILE. 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 IN THE BINARY DATA FILE AT DATA REDUCTION TIME IF NO 'MAXHKL' CARD USED. ON THE FIRST PASS THROUGH THE BINARY DATA FILE THE BCD LIST OF FC MAY BE MADE IF THE USER SO DESIRES. ALL THE REFLECTIONS IN THE FILE ARE LISTED, AND THOSE REFLECTIONS REJECTED ARE MARKED WITH =R=. THE CORRECT COEFFICIENTS ARE FORMED FOR THE CURRENT REFLECTION AND CONTRIBUTED TO THE FIRST SUMMATIONS. (NO SORTING IS REQUIRED EXCEPT TO GAIN MAXIMUM COMPUTING SPEED). ONCE ALL REFLECTIONS IN THE BINARY DATA FILE HAVE BEEN TREATED, THE SECOND AND THIRD SUMS ARE CALCULATED FOR ALL THE FIRST SUM COEFFICIENTS STORED.

THE FOURIER CALCULATION SUBROUTINE WHICH DOES THE ACTUAL FOURIER SUMMATION CONTAINS A PROVISION FOR BREAKING THE SUMMATION UP INTO AN OPTIMUM NUMBER OF PASSES. THIS IS DONE WHEN THE WHOLE CALCULATION CANNOT

BE ACCOMPLISHED IN A SINGLE PASS THROUGH THE BINARY DATA FILE. FOR EXAMPLE THE FOLLOWING LIMITATIONS MAY APPLY (DEPENDING UPON 32000 WORDS OF CORE AVAILABLE FOR PROGRAM AND STORAGE - E.G. 65K 1108).

(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 AND COMMENTS FOR DETAILS.

BECAUSE OF THE PARTICULAR METHOD OF SUMMATION A VERY LARGE NUMBER OF REFLECTIONS CAN BE ACCOMMODATED.

NO INTERMEDIATE FILES 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 THE CALCULATION IS DIVIDED 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 OUTPUT LINE PRINTER FILE. IT IS POSSIBLE TO SUPPRESS PRINTING VALUES BETWEEN SELECTED MAXIMUM AND MINIMUM CUT-OFF POINTS BY THE USE OF A =MAP= CARD. THIS GREATLY FACILITATES INTERPRETATION OF THE PRINTED MAPS.

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ATOMIC PARAMETER LOADING PROGRAM

PROGRAMMING FOR THIS LINK WAS DONE BY J.M. STEWART AND LINDA PLASTAS.

THE FUNCTION OF THIS LINK OF THE X-RAY-SYSTEM IS TO SERVE TO PLACE THE ATOMIC PARAMETERS IN THE PROPER ARRAYS IN THE BINARY DATA FILE. THIS MEANS THAT THIS PROGRAM MUST ALWAYS BE USED AT LEAST ONCE BEFORE ANY PROGRAM WHICH CALCULATES STRUCTURE FACTORS (E.G. FC, ORFLS, FOUREF, ETC.) MAY BE USED. THIS PROGRAM PERMITS EITHER AN A PRIORI LOADING OF ATOMIC COORDINATES OR THE EDITING OF PARAMETERS ALREADY STORED IN THE DATA FILE. THE PROGRAM ACCEPTS PARAMETERS IN THREE GROUPS. THE FIRST GROUP CONSISTS OF QUANTITIES WHICH, BY THEIR NATURE, ARE FEW. THE F RELATIVE SCALE FACTORS, THE FOURIER GRID COORDINATES, THE MAXIMUM VALUES OF THE MILLER INDICES, AN OVERALL ISOTROPIC TEMPERATURE PARAMETER, OR A MOLECULAR SHIFT ARE THESE KINDS OF QUANTITIES. THE SECOND GROUP IS THE ACTUAL INDIVIDUAL ATOMIC PARAMETERS. THESE INCLUDE THE FRACTIONAL OR GRID COORDINATES (X,Y,Z), THE POPULATION PARAMETER (SITE OCCUPANCY), THE INDIVIDUAL ISOTROPIC OR ANISOTROPIC TEMPERATURE FACTOR, THE SCATTERING FACTOR TYPE, AND THE ATOMIC DESIGNATION. THE SECOND CATEGORY OF DATA SUPPLIES THE PARAMETERS OF THE ATOMS IN THE ASYMMETRIC UNIT. THE THIRD CLASS OF DATA ARE THOSE WHICH GIVE INFORMATION ABOUT THE REFINEMENT OF THE STRUCTURE IN TERMS OF THE PARAMETERS. THIS LAST CATEGORY IS ALSO TREATED BY THE REFINEMENT PROGRAMS AND IS OPTIONAL AT PARAMETER LOADING. THE PROGRAM IS CODED TO CHECK FOR ATOMS IN SPECIAL POSITIONS AND TO ADJUST THE POPULATION PARAMETER FOR THEM CORRECTLY. IF A VALUE DIFFERENT THAN 1.0 IS SUPPLIED FOR AN ATOM IN A SPECIAL POSITION IT SUPERSEDES THE VALUE CALCULATED BY THE PROGRAM AND IS ACCEPTED AS SUPPLIED.

THE OVERALL PLAN IS SUCH, THAT AT AN A PRIORI START ALL ATOMIC QUANTITIES WILL BE TAKEN FROM CARDS AND BE PLACED IN THE BINARY DATA FILE. AT AN UPDATE, QUANTITIES FROM CARDS WILL TAKE PRECEDENCE, BUT NO INFORMATION FROM THE FILE WILL BE LOST. THE POSSIBILITY FOR INSERTION, DELETION AND REPLACEMENT ALL EXIST. THE WHOLE METHOD DEPENDS UPON THE ATOM IDENTIFICATION. THIS IS A SIX CHARACTER CODE WHICH MUST UNIQUELY IDENTIFY EACH ATOM. THESE SIX CHARACTERS CONSIST OF TWO SUB-FIELDS, ONE A4 AND THE OTHER A2. THE A4 FIELD MUST BE IDENTICAL TO THE A4 DESIGNATION SUPPLIED AT DATA REDUCTION TIME FOR ONE OF THE SCATTERING FACTORS. THE A2 FIELD THEN SERVES TO DISTINGUISH AMONG ATOMS OF A GIVEN ATOMIC SPECIES. NOTE WELL.... ONE MUST EXERCISE GREAT CARE TO ALWAYS PUNCH THESE DESIGNATIONS EXACTLY THE SAME WAY WITH RESPECT TO BOTH CHARACTERS AND SPACES.

NOTE THAT THIS LINK SERVES ALL THE STRUCTURE FACTOR CALCULATING PROGRAMS. THESE PROGRAMS CAN NOT LOAD ATOMIC COORDINATES. THEY CAN, HOWEVER, SELECT NAMED ATOMS OR CLASSES OF ATOMS FROM THE BINARY DATA FILE PREPARED BY =LOADAT=.

MODIFICATION OF THE BINARY DATA FILE

THIS PROGRAM WAS WRITTEN BY J.M.STEWART. THE PURPOSE OF THIS LINK OF THE X-RAY SYSTEM IS TO PROVIDE A MECHANISM FOR MAKING INSERTIONS AND REPLACEMENTS OF QUANTITIES IN THE BINARY DATA FILE. A ''QUANTITY'' MIGHT BE THE PHASE OF SELECTED REFLECTIONS, NEW VALUES OF THE STANDARD DEVIATION OF UNIT CELL PARAMETERS OR ANY OTHER QUANTITIES STORED IN THE DATA FILE. THE INPUT DECK PERMITS REPLACEMENT OR ADDITION ON THREE BASES, ONE THROUGH THE USE OF 'MODFIL' CARDS, ONE BY MEANS OF 'MODREF' CARDS AND ONE WHICH PRODUCES F RELATIVES OF CONTROLLED ERROR. THIS IS DONE BY REPLACING EVERY RELATIVE STRUCTURE FACTOR WITH THE CURRENT VALUE OF CALCULATED STRUCTURE FACTOR MULTIPLIED BY AN ARBITRARY SCALE AND MODIFIED TO HAVE A STIPULATED AMOUNT OF 'RANDOM' ERROR.

THE 'MODFIL' CARD GIVES THE USER THE DIRECT ABILITY TO SPECIFY AND REPLACE ANY WORD OF ANY PHYSICAL RECORD OF ANY LOGICAL RECORD IN HIS BINARY DATA FILE.

THE 'MODREF' CARD PERMITS THE USER TO REPLACE ANY SPECIFIED QUANTITY FOR ANY SPECIFIED REFLECTION IN THE BINARY DATA FILE.

THE REPLACEMENT OF F RELATIVE IS CARRIED OUT WHEN IT IS SIGNALED IN THE 'MODIFY' CARD. THIS FUNCTION IS PROVIDED FOR EXPERIMENTAL AND TEST CALCULATIONS TO PROVIDE CONTROLLED DATA OF KNOWN RANDOM ERROR.

THE MAIN RESTRICTIONS IN THE USE OF THIS PROGRAM ARE- 1. THE 'MODFIL' AND 'MODREF' CARDS MUST COME IN EXACTLY THE SAME ORDER AS THE DATA COMES IN THE FILE (SEE 1.DATRDN OR THE COMMENTS IN PROGRAM =NUON= FOR A DESCRIPTION OF THE BINARY DATA FILE) 2. 'MODFIL' CARDS WHICH CALL TO MODIFY THE REFLECTION RECORD CAN NOT BE USED AT THE SAME TIME AS 'MODREF' CARDS - ALL 'MODFIL' CARDS MUST COME BEFORE ANY 'MODREF' CARD.

EACH CARD FOR MODIFICATION PROVIDES FOR THE INPUT OF TWO QUANTITIES, ONE FIXED POINT, THE OTHER FLOATING POINT. IF THE FIXED POINT QUANTITY IS ZERO THE FLOATING POINT QUANTITY IS STORED, IF BOTH ARE ZERO, ZERO IS STORED. IN NEITHER CASE IS THE MODE CHANGED. IT IS ESSENTIAL THAT ONE TAKE CARE IN USING THIS LINK SINCE NO RESTRICTION IS PLACED ON THE QUANTITIES WHICH MAY BE REPLACED AND THIS COULD LEAD TO VERY STRANGE ERRORS IN SUBSEQUENT RUNS FROM THE MODIFIED DATA FILE.

PROBABLY THE MOST COMMON WAY IN WHICH THIS PROGRAM WILL BE USED IS TO PLACE PHASES IN THE DATA FILE FOR REFLECTIONS DETERMINED BY THE SYMBOLIC ADDITION PROCEEDURE OF KARLE AND KARLE. IN THIS CASE A 'MODIFY' CARD WITH THE COMPOUND IDENTITY IS PREPARED, THEN A BUNDLE OF 'MODREF' CARDS EACH WITH H, K,L, THE WORD CATALOG NUMBER AND A PHASE ANGLE IN CYCLES PUNCHED IN THEM. THESE MUST BE SORTED IN EXACTLY THE SAME ORDER AS THE ORGINAL DATA REDUCTION REFLECTIONS - ONLY THOSE REFLECTIONS TO BE MODIFIED NEED BE PRESENT. THE CATALOG NUMBER INDICATES THE RELATIVE POSITION IN EACH REFLECTION RECORD WHERE

THE ESTIMATED PHASE BELONGS. IN THE FLOATING POINT FIELD OF EACH CARD ONE PLACES A ZERO FOR PHASES OF ZERO, A 0.5 FOR PHASES OF PI RADIANS. THUS THE PHASE ANGLE ALPHA IS INSERTED IN UNITS OF CYCLES BETWEEN -0.9999 AND +0.9999. FINALLY THE DECK IS CONCLUDED WITH AN END CARD.

IF ONE WISHES TO REPLACE MORE THAN ONE QUANTITY FOR THE SAME RECORD OR REFLECTION APPROPRIATE 'MODFIL' AND 'MODREF' CARDS ARE PLACED RIGHT NEXT TO ONE ANOTHER WITH THE VARIOUS WORD DESIGNATIONS SET PROPERLY. IT SHOULD BE NOTED THAT HKL CARDS OF DATA REDUCTION ALSO ALLOW FOR THE STORING OF PHASE INFORMATION.

IT SHOULD BE OBVIOUS THAT THIS PROGRAM IS INTENDED ONLY FOR LIMITED AND SPECIAL MODIFICATION OF THE BINARY DATA FILE. WHEN EXTENSIVE CHANGES NEED TO BE MADE =DATRDN=, =LOADAT=, ETC. ARE DESIGNED FOR THESE PURPOSES.

=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 EXTENSIVELY MODIFIED TO CONFORM WITH THE X-RAY SYSTEM BY J.M.STEWART AND F.A.KUNDELL. 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, 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 SYSTEM. THE NUMBER OF OBSERVATIONS IS LIMITED ONLY BY THE NUMBER OF REFLECTIONS THAT MAY BE STORED IN ONE BINARY DATA FILE.

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 FILE FOR EACH COMPOUND THAT REQUIRES SPECIAL PATCHING. AN IMPORTANT CHANGE WITH RESPECT TO PATCHING INVOLVES THE SUBROUTINES =TWPH=, =TRRX=, AND =TRRB=, WHOSE CALLING SEQUENCES ARE NOW -

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CALL XRY047(IMSYM,I,TJ,HJ,HHJ,IREJKT,ATOM(I))
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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.

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CALL XRY050(XYZ,ATOM,NA)

CALL XRY051(BETA,ATOM,NA)
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THE SYSTEM VERSION OF =ORFLS= PERMITS A NUMBER OF VARIABLES, PARAMETERS, AND ATOMS IN THE ASYMMETRIC UNIT WHICH DEPENDS UPON THE STORAGE AVAILABLE IN EACH MACHINE. THIS MUST BE SET AT EACH COMPUTER INSTALLATION AT THE TIME THE PROGRAMS ARE COMPILED. DETAILS FOR THE SETTING OF THESE LIMITS ARE GIVEN IN PROGRAM =XYOR=. FIXED ATOM CALCULATIONS ARE POSSIBLE SO THAT

ANY RESTRICTIONS MAY BE MITIGATED BY LARGE BLOCK REFINEMENT.

THE LIST OF CONTROL CARDS REQUIRED HAS BEEN REDUCED SINCE THE MAIN CELL, ATOMIC PARAMETERS, AND REFLECTION INFORMATION IS READ FROM THE SYSTEM BINARY DATA FILE =NFILEA= AND AN UPDATE FILE IS GENERATED AT THE END OF THE SPECIFIED NUMBER OF CYCLES ON =NFILEB= FOR SUBSEQUENT USE.

THE BINARY DATA FILE HAS STORED IN IT ALL SCATTERING FACTOR, CELL, SYMMETRY, REFLECTION, AND PREVIOUS ATOM PARAMETER INFORMATION. =ONPR= OF THE SYSTEM INITIALIZES THE PARAMETER REFINEMENT INDICATOR TO REFINE ON F RELATIVE SCALE FACTORS, X, Y, Z, AND THE TEMPERATURE FACTORS OF ALL ATOMS IN THE ASYMMETRIC UNIT. 'NOREF' AND 'REF' CARDS MAY BE USED TO CHANGE THESE INDICATORS AS DESIRED. THE ATOM PARAMETERS ARE LOADED BY =LOADAT= AND =ORFLS= PERMITS THE SELECTION OF ANY SPECIFIED ATOMS OR ALL ATOMS FROM THE BINARY DATA FILE.

SUBROUTINES =TWFN= AND =TWWT= HAVE BEEN ADDED TO THE ORIGNAL PROGRAM. =TWFN= IS ANALOGOUS TO =FBFN= OF THE FOURIER PROGRAM IN THAT IT UTILIZES THE SYMMETRY INFORMATION OF =RDGN= OF DATA REDUCTION TO MAKE POSSIBLE THE GENERATION OF EQUIVALENT REFLECTIONS BY MEANS OF COMPUTED =GO TO='S. THUS THE FOURIER CODES SERVE FOR STRUCTURE FACTOR AND DERIVATIVE CALCULATIONS. =TWWT= CAUSES THE LATEST RESULTANT PARAMETERS AND THEIR STANDARD DEVIATIONS TO BE WRITTEN IN THE OUTPUT BINARY DATA FILE =NFILEB= TO SERVE AS INPUT TO SUBSEQUENT CYCLES. 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. IN THE EVENT OF SUCH SINGULARITIES THE MATRIX IS DUMPED FOR INSPECTION.

1. NUMBER OF CYCLES (MAXIMUM 9 PER 'ORFLS' CARD). NOTE THAT AN R ((SUM DELTA F)/(SUM FO) 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 OR ANY MIXTURE OF THE TWO FORMS MAY BE REFINED. 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. NOTE THAT THE PRELIMINARY OF LISTING PARAMETERS REFERS TO B'S NOT BETA'S THUS ALLOWING MORE DIRECT INTERCOMPARISON OF ISOTROPIC AND ANISOTROPIC VALUES.

3. REFINEMENT MAY BE BASED ON F OR F**2.

4. F RELATIVE SCALE FACTORS MAY BE LOADED FROM CARDS OR SPECIFIED TO BE TAKEN FROM THE SCALE OR RESCALE STORAGE OF THE BINARY DATA FILE (SEE 1.FC). 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 DATA FILE ARE TO BE USED. 'SCALE' CARDS MAY BE USED TO SUPERSEDE OR ALTER THE BAND AS USUAL. A 'NOREF' CARD WITH SCALE IN COLS 8-12 CAUSES SCALE FACTOR REFINEMENT TO BE STOPPED.

5. EITHER THE WEIGHTS STORED ON =NFILEA= OR UNIT WEIGHT MAY BE SPECIFIED.

6. THE PUNCHING OF 'SCALE', 'ATOM', 'B', AND 'BIJ' (IF ANISTROPIC) CARDS AT THE END OF EACH CYCLE MAY BE SPECIFIED. REMEMBER THAT IN THIS CASE THESE CARD IMAGES WILL APPEAR ON =NFILEC=.
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. THE DIAGONAL TERM VALUES OF THE ESTIMATED ERROR ARE PUNCHED FOR X, Y, AND Z IN THE 'ATOM' CARDS. THESE MAY THEN BE USED WITH =BONDLA=. =BONDLA= OF COURSE WILL USUALLY OBTAIN THESE QUANTITIES DIRECTLY FROM THE BINARY DATA FILE.

7. 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. CERTAIN OTHER LISTING FEATURES OF THE PROGRAM HAVE BEEN CHANGED TO CONFORM WITH THE SYSTEM (E.G.- TITLE HANDLING, PARAMETER LISTING, ETC.).

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

9. 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 (A AND B) ON THE BINARY DATA FILE =NFILEA= ARE TO BE USED AND THEIR VALUES ESTABLISHED AS THE FUTURE =FIXED ATOM= CONTRIBUTION FOR FUTURE FC'S.

IN ORDER TO FACILITATE THE USE OF ''FIXED ATOMS'' A BRIEF OUTLINE OF THE METHOD USED WILL BE FOUND USEFUL. THE VERY LIMITED NUMBER OF PARAMETERS THAT FULL MATRIX LEAST SQUARES IS CAPABLE OF HANDLING MAKES THE USE OF FIXED ATOMS A NECESSITY FOR MOST COMPOUNDS. THE STRUCTURE FACTOR PROGRAM CAN BE UTILIZED TO CALCULATE STRUCTURE FACTORS FOR A PORTION OF THE ATOMS IN THE ASSYMETRIC UNIT OF A GIVEN UNIT CELL. THESE ARE ATOMS WHOSE PARAMETERS ARE NOT TO BE VARIED. THE RESULTING STRUCTURE FACTORS MAY THEN BE

USED AS ''FIXED ATOM'' CONTRIBUTIONS TO THE STRUCTURE FACTORS CALCULATED FOR THE WHOLE CELL, OR THAT PORTION DETERMINED SO FAR IN THE STRUCTURE ANALYSIS. THE STORAGE RESTRICTION ON THE FC PROGRAM IS SUCH THAT IT CAN HANDLE MORE THAN 1000 ATOMS IN THE UNIT CELL SO THAT BY JUDICIOUS USE OF THE ATOM LIMITATION OF THE FULL MATRIX LEAST SQUARES PROGRAM A NUMBER OF LARGE BLOCK REFINEMENTS MAY BE CARRIED OUT. THIS PROCEDURE WILL RESULT IN THE REFINEMENT OF THE WHOLE STRUCTURE. SOME ''OVERLAP'' OF PARAMETERS MAY BE DESIREABLE. THE BINARY DATA FILE HAS QUANTITIES STORED, AMONG OTHERS, FOR EACH REFLECTION FOR A, B, AND FIXED CONTRIBUTION TO A AND B (WHERE A AND B REFER TO THE REAL AND IMAGINARY PARTS OF THE STRUCTURE FACTOR). DATA REDUCTION INITIALIZES ALL FOUR TO ZERO. AFTER AN FC CALCULATION A AND B HAVE BEEN GIVEN A VALUE AND THIS IS WRITTEN ON =NFILEB=. THE FILE ON UNIT =NFILEB= IS NOW SWITCHED TO BE A =NFILEA= AND THIS BINARY FILE BECOMES INPUT INFORMATION FOR THE NEXT CALCULATION OF STRUCTURE FACTORS (FOR LEAST SQUARES OR OTHER STRUCTURE FACTOR TYPE PROGRAMS). AT THIS POINT THE STRUCTURE FACTOR TYPE PROGRAM IS KEYED TO ESTABLISH AND APPLY THE PREVIOUS FC AS A FIXED ATOM CALCULATION. THIS RESULTS IN THE A AND B ON THE NEW =NFILEA= BEING PLACED IN THE FIXED ATOM A AND B ON =NFILEB= AND THE STRUCTURE FACTOR TYPE PROGRAM USING THESE VALUES INSTEAD OF ZEROS TO START THE STRUCTURE FACTOR SUMMATIONS. THE =NFILEB= AT THE END OF THE RUN THEN HAS A SET OF FIXED ATOM CONTRIBUTIONS STORED UPON IT AND MAY BE USED AS AN =NFILEA= IN SUBSEQUENT RUNS AND CODED EITHER TO USE PREVIOUS FC TO ESTABLISH AND APPLY AS FIXED ATOM CONTRIBUTION OR SIMPLY TO APPLY THE FIXED ATOM CONTRIBUTION NOW ESTABLISHED. NOTE THAT IN THE FIRST CASE CASCADING OCCURS AND IN THE SECOND THE SET ALREADY ESTABLISHED IS CONTINUED AS THE FIXED ATOM SET. LARGE TIME SAVINGS MAY RESULT FROM THE USE OF THE FIXED ATOM FACILITY, ESPECIALLY IN THE CASE OF FULL MATIRX LEAST SQUARES REFINEMENT OF A FEW PARAMETERS OF A SMALL PORTION OF A LARGE NUMBER OF ATOMS IN A UNIT CELL.

10. THE OPTION OF REFINING NEUTRON SCATTERING FACTOR DATA IS LOST.

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

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

13. 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.

14. THE NEED FOR PATCHING MAY BE SIGNALED.

THE PATCHING OF ORFLS FOR ATOMS IN SPECIAL POSITIONS REQUIRES CAREFUL CONSIDERATION. IN THE X-RAY SYSTEM 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. 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) AND THE ATOM PARAMETER LOADING LINK

(LOADAT) 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.

LEAST SQUARES REFINEMENT OF LATTICE PARAMETERS

THE PROGRAM FOR THE LEAST SQUARES REFINEMENT OF LATTICE PARAMETERS WAS WRITTEN BY RICHARD A. ALDEN. IT WAS ADAPTED TO THE =SYSTEMS= AND SLIGHTLY MODIFIED BY HERMAN L. AMMON AND F. MAUER.

THE REFINEMENT IS ACCOMPLISHED BY MINIMIZATION OF THE QUANTITY =R=.

D = ARCSIN(((SIN THETA CALC)**2)**0.5) - THETA OBS.

R = SUM OVER J OBSERVATIONS OF (D(J)/SIGMA(2 THETA))**2

NECESSARY DATA FOR THE REFINEMENT CONSISTS OF THE RADIATION WAVELENGTH USED, LATTICE TYPE, CRUDE LATTICE PARAMETERS, TWO THETA VALUES FOR SEVERAL REFLECTIONS (AT LEAST TEN SHOULD BE USED) AND THEIR STANDARD DEVIATIONS. IT IS RECOMMENDED THAT AXIAL REFLECTIONS BE AVOIDED. THE STANDARD DEVIATIONS ARE USED ONLY TO WEIGHT THE SEVERAL TWO THETA'S. =PARAM= WILL SET ALL UNSPECIFIED STANDARD DEVIATIONS TO 0.01, A CASE IN WHICH ALL TWO THETA'S HAVE EQUAL WEIGHT. IF SIN (THETA) IS GREATER THAN 1.0 FOR ANY REFLECTION, IT WILL BE OMITTED FROM THE REFINEMENT.

THE REFINEMENT WILL STOP WHEN ANY ONE OF THE FOLLOWING THREE CONDITIONS IS MET -

1. FIVE CYCLES HAVE BEEN CALCULATED
2. NO CHANGE IN A LATTICE DIMENSION CALCULATED DURING THE LAST CYCLE WAS GREATER THAN .0005 ANGSTROMS
3. NO CHANGE IN A LATTICE ANGLE CALCULATED DURING THE LAST CYCLE WAS GREATER THAN .005 DEGREES

OUTPUT FOR EACH CYCLE CONSISTS OF OLD AND NEW PARAMETERS, PARAMETER CHANGES, ESTIMATED PARAMETER STANDARD DEVIATIONS, THE ERROR OF FIT AND CORRELATION COEFFICIENTS. FOLLOWING THE LAST CYCLE, A SUMMARY OF INPUT TWO THETA'S, CALCULATED FROM THE NEW LATTICE PARAMETERS AND THE DIFFERENCE BETWEEN THESE TWO VALUES IS GIVEN. A RAPID SCAN OF THE ''DIFFERENCE'' COLUMN WILL SERVE TO SPOT ANY UNUSUALLY ''BAD'' OBSERVED TWO THETA'S AND IS WELL WORTH THE MINUTE REQUIRED TO DO SO.

EQUATIONS FOR SOME OF THE QUANTITIES CALCULATED ARE -

ERROR OF FIT = E = (N-K)**-0.5 SUM D(K)/SIGMA(2 THETA)

ESTIMATED STANDARD DEVIATION = S - (M**-1)E

N=NUMBER OF OBSERVATIONS
K=NUMBER OF PARAMETERS

M=MATRIX OF NORMAL EQUATIONS ADJUSTED

CORRELATIONS COEFFICIENT = C(N,M) = M(N,M)**-1/((M(N)**-1(M(M)**-1))**0.5

AN ALGORITHM FOR FINDING A SET OF PHASES DIRECTLY FROM SIGMA TWO RELATIONSHIPS (CENTROSYMMETRIC CASE)

THIS PROGRAM WAS WRITTEN BY R.V. CHASTAIN.

ALL SIGMA TWO RELATIONSHIPS OF THE E'S ABOVE AN ARBITRARY VALUE (USUALLY E IS GREATER THAN OR EQUAL TO 1.5 DEPENDING ON COMPUTER SPEED AND TIME) ARE GENERATED. THESE ARE REFERRED TO AS SIGMA TWO RELATIONSHIPS OF THE FIRST KIND AND EXPRESS THEM

SE(H)SE(K)SE(L) = PI(J), P(J) (FIRST KIND)

WHERE J IS THE RELATIONSHIP CATALOG NUMBER, H, K, AND L ARE CATALOG NUMBERS OF THE E'S, SE(H) IS THE SIGN OF E(H), PI IS THE SYMMETRY SIGN (E.G. FOR P ONE BAR ALL PI(J) ARE (+), AND P(J) IS PROBABILITY THAT THE J-TH RELATIONSHIP IS VALID.

SIGMA TWO RELATIONSHIPS OF THE SECOND KIND ARE NEXT FORMED AS PRODUCTS BETWEEN RELATIONSHIPS OF THE FIRST KIND WHICH HAVE A COMMON SIGN FACTOR. WE EXPRESS THESE AS
SE(H)SE(K)SE(L)SE(H')SE(K')SE(L') = PI(I)PI(K), P(I) OR P(K) WHICHEVER IS SMALLER

WHICH REDUCES TO

SE(H)SE(K)SE(H')SE(K') = PI(J), P(J) (SECOND KIND)

IN ORDER TO MAINTAIN A HIGH CONFIDENCE LEVEL WITH THE RELATIONSHIPS OF THE SECOND KIND, E(L) IN THE ABOVE EXPRESSION IT IS NECESSARY TO HAVE A VALUE EQUAL TO OR GREATER THAN SOME ARBITRARY LEVEL. (NOTE 1) THE COMBINED SET OF RELATIONSHIPS OF THE FIRST AND SECOND KIND IS REFERRED TO AS THE EXTENDED SET OF SIGMA TWO RELATIONSHIPS.

E(1) TO E(M), IN DECREASING VALUE OF E, ARE DEFINED AS ''GENERATORS'', THAT IS, THEIR PHASES WILL BE SOLVED FOR DIRECTLY. E(M+1) TO E(N) ARE REFERRED TO AS THE ''GENERATED'' BECAUSE THEIR PHASES WILL BE GENERATED IN TERMS OF THE PHASES OF THE ''GENERATORS''. THE EXTENDED SET OF RELATIONSHIPS IS NOW LIMITED TO THOSE RELATIONSHIPS INVOLVING OMLY THE GENERATORS AND HAVING P-J GREATER THAN SOME ARBITRARY VALUE. FOR OPTIMIZATION, THE LIMITED SUBSET OF RELATIONSHIPS IS SORTED IN THE ORDER OF DECREASING P(J).

THE LIMITED SUBSET OF SIGMA TWO RELATIONSHIPS IS NOW SOLVED (BY ASSUMING THAT EVERY RELATIONSHIP IN THE LIMITED SUBSET IS CORRECT) FOR THE SIGNS OF THE GENERATORS IN TERMS OF THE SYMMETRY SIGNS TO GIVE THE SET OF RELATIONSHIPS. (NOTE 2)

SE(H) = O(H) H = 1,2,3,...., M

THE FUNCTION O(H) IS A PRODUCT OF PI'S FROM THE EQUATIONS USED IN THE INVERSION, AND THE ARBITRARY PHASES PERMITTED BY THE SPACE GROUP. THIS SET OF SIGNS FOR THE GENERATORS MAY BE A GOOD FIRST APPROXIMATION TO THE CORRECT SET OF PHASES.
(NOTE 3)

NOT ONLY DOES THE PRODUCT OF PI'S IN O(H) SERVE TO DEFINE THE SIGN OF E(H), IT ALSO SHOWS EACH PI UPON WHICH THE SIGN OF E(H) IS DEPENDENT. FOR THIS REASON O(H) IS REFERRED TO AS THE PEDIGREE OF SE(H). THROUGH THE SET OF THE M O'S IT IS POSSIBLE TO FIND ALL SE'S WHICH ARE EFFECTED BY A CHANGE IN ANY GIVEN PI.

THE INVERSION PROCESS REQUIRED ONLY M RELATIONSHIPS OF THE COMPLETE LIMITED SUBSET OF SIGMA TWO RELATIONSHIPS. THE REMAINDER OF THE RELATIONSHIPS CAN BE USED TO CHECK THE REASONABLENESS OF THE APPROXIMATE SOLUTION. SOME NUMBER OF THE RELATIONSHIPS MAY BE FOUND DISCREPANT, THAT IS

SE(H)SE(K)SE(L) NOT EQUAL TO PI(J) OR SE(H)SE(K)SE(H')SE(K') NOT EQUAL TO PI(J)

WHILE THE OTHER RELATIONSHIPS WILL BE FOUND ACCORDANT, THAT IS

SE(H)SE(K)SE(L) = PI(J) OR SE(H)SE(K)SE(H')SE(K') = PI(J)

THE PROGRAM IS DESIGNED TO MODIFY THE APPROXIMATE SOLUTION TO REDUCE THE TOTAL NUMBER OF DISCREPANT RELATIONSHIPS. TO ACCOMPLISH THIS, A SECOND KIND OF PEDIGREE IS INTRODUCED - THE PEDIGREE OF A RELATIONSHIP. THE ELEMENTS OF THIS PEDIGREE ARE FOUND AS THE RESULTANT FACTORS GIVEN BY THE PRODUCTS OF THE SYMMETRY SIGN AND THE PEDIGREE OF THE SE'S INVOLVED IN THE RELATIONSHIPS, THAT IS

O(H)O(K)O(L)PI(J) OR O(H)O(K)O(H')O(K')PI(J)

THE PEDIGREE OF THE RELATIONSHIP SHOWS EACH PI WHICH WILL INFLUENCE WHETHER THIS RELATIONSHIP IS ACCORDANT OR DISCREPANT.

THE ALGORITHM USED FOR MODIFYING THE APPROXIMATE SOLUTION EMPLOYS TWO COUNTS FOR EACH OF THE PI'S INVOLVED IN THE INVERSION PROCESS. ONE COUNT, D(J), IS THE NUMBER OF TIMES PI(J) APPEARS IN PEDIGREES OF DISCREPANT RELATIONSHIPS, THE OTHER COUNT, A(J), IS THE NUMBER OF TIMES PI(J) APPEARS IN THE PEDIGREES OF ACCORDANT RELATIONSHIPS. WHEN THE COUNTING IS COMPLETED FOR THE LIMITED SUBSET OF SIGMA TWO RELATIONSHIPS, THE DISCREPANCY DIFFERENCES, DELTA(J), ARE FORMED.

DELTA(J) = D(J) - A(J)

THE LIST OF DELTA'S IS SCANNED FOR THE LARGEST POSITIVE DELTA(J), AND THE PI(J) ASSOCIATED WITH IT IS ESTABLISHED AS THE VILLAIN. (NOTE 4)

AT THIS POINT EACH SE WHICH CONTAINS THE VILLAIN PI(J) IN ITS PEDIGREE IS CHANGED TO PRODUCE A NEW APPROXIMATION TO THE PHASES THAT WILL YIELD FEWER DISCREPANCIES. THE PROCESS CAN BE CARRIED OUT REPEATEDLY BY SUBSTITUTING THE NEW APPROXIMATION OF THE PHASES INTO THE LIMITED SET OF SIGMA TWO RELATIONSHIPS

UNTIL NO POSITIVE DELTA'S REMAIN. THE SET OF PHASES WHICH GIVES NO POSITIVE DELTA'S IS ACCEPTED AS A SOLUTION FOR A SET OF GENERATOR PHASES.

TO DETERMINE THE VALUES OF THE ''GENERATED'' PHASES THE SIGMA TWO RELATIONSHIPS ARE LIMITED TO THE SIGMA TWO RELATIONSHIPS OF THE FIRST KIND WHICH CONTAIN TWO GENERATOR PHASES AND ONE GENERATED PHASE. IF SE(L) IS THE PHASE TO BE GENERATED AND SE(H) AND SE(K) ARE KNOWN GENERATOR PHASES, THEN THE REARRANGED RELATIONSHIP

SE(L) = PI(J)SE(H)SE(K)

SERVES TO DEFINE THE PHASES SE(L). SINCE ANY PARTICULAR SE(L) MAY BE DETERMINED MANY TIMES, SOMETIMES RESULTING IN CONFLICTING PHASE VALUES, THE CURRENT CODE SIMPLY USES THE PHASE VALUE GIVEN MOST FREQUENTLY, AND LEAVES EQUAL BUT OPPOSITE AS UNDETERMINED.

NOTES

NOTE 1. THIS MINIMUM E VALUE IS USUALLY THE VALUE OF THE SMALLEST E TO HAVE ITS PHASE GENERATED.

NOTE 2. SOMETIMES IT IS FOUND THAT NOT ALL SE CAN BE SOLVED FOR UNIQUELY. THIS IS USUALLY REMEDIED BY EITHER LOWERING THE ESTABLISHED CONFIDENCE LEVELS OR REDUCING THE NUMBER PHASES TO BE USED AS GENERATORS. SOMETIMES IT IS EXPEDIENT MERELY TO WITHDRAW THE FEW TROUBLESOME SE'S FROM THE LINE OF GENERATORS.

NOTE 3. THIS IS BECAUSE MOST RELATIONSHIPS INVOLVING SIGNS OF LARGE E'S AND HAVING HIGH PROBABILITIES ARE EXPRESSING THE ''TRUTH''.

NOTE 4. EXCEPT FOR THE ACCORDANT SIGMA TWO RELATIONSHIPS THAT BY COINCIDENCE ARE DEPENDENT ON AN EVEN NUMBER OF INCORRECT PI'S, ALL RELATIONSHIPS DEPENDING ON A VILLAIN PI WILL BE DISCREPANT AND NO ACCORDANT RELATIONSHIPS WILL BE DEPENDENT ON A VILLAIN PI. WITH GOOD DATA AND BY ESTABLISHING A SUFFICIENTLY HIGH CONFIDENCE LEVEL FOR THE RELATIONSHIPS USED, A(J) IN GENERAL WILL BE MUCH SMALLER THAN D(J) FOR A VILLAIN.

ALSO, A CONDITION COULD EXIST IN WHICH TWO OR MORE DELTA'S COULD BE THE LARGEST NON-NEGATIVE DISCREPANCY DIFFERENCES. THIS CONDITION CAN USUALLY BE REMOVED BY RAISING THE CONFIDENCE LEVEL OF THE RELATIONSHIPS USED.

PROGRAM FOR THE CALCULATION OF R VALUES

THIS LINK WAS WRITTEN BY WILLIAM KEEFE IN COLLABORATION WITH J.M. STEWART.

THIS LINK IS DESIGNED TO EXPLORE ON SEVERAL BASES THE AGREEMENT BETWEEN CALCULATED AND OBSERVED STRUCTURE FACTORS. IT IS DESIGNED TO SEPARATE THE REFLECTION DATA INTO A NUMBER OF GROUPINGS - SOME AS STANDARD FEATURES OF THE PROGRAM, THE REST AS SPECIFIED BY THE USER. THE STANDARD CLASSIFICATIONS ARE-- H00, 0K0, 00L, HK0, H0L, 0KL, HKL (ALL INDICES NON ZERO), THE LEVEL SCALE GROUPS, AND UP TO 15 USER SPECIFIED CATEGORIES. THESE CATEGORIES MAY SPECIFY CLASSES OF REFLECTIONS, RANGES OF SIN THETA OVER LAMBDA, RANGES OF F OBSERVED, OR RANGES OF INTENSITY. THE OUTPUT IS THEN IN THE FORM OF COUNTS OF THE VARIOUS TYPES OF REFLECTION IN EACH CATEGORY, AND A NUMBER OF R VALUES. THESE ''R'' VALUES TAKE THE FOLLOWING FORM....

1. THE 'CONVENTIONAL' R, THAT IS THE SUM OF DELTA F OVER THE SUM OF F OBSERVED FOR THE OBSERVED REFLECTIONS. (DELTA F IS F0-FC)

2. AN R VALUE FOR THE ''LESS-THANS'' DELTA F IS SET EQUAL TO ZERO FOR THOSE REFLECTIONS FOR WHICH IT IS MINUS.

3. THE SQUARE ROOT OF THE RATIO OF THE SUM OF THE LEAST SQUARES WEIGHTED DELTA F SQUARED OVER THE SUM OF THE WEIGHTED F'S OBSERVED SQUARED.

4. THE 'CONVENTIONAL' R INCLUDING REFLECTION MULTIPLICITY.

5. THE 'CONVENTIONAL' R INCLUDING CORRECTION FOR DISPERSION.

6. THE SLOPE OF LN(F0/FC) VERSUS SIN THETA OVER LAMBDA ALL SQUARED. THIS IS A TEST OF TEMPERATURE FACTOR FIT.

7. THE RESCALE FACTOR RATIO WHICH IS THE SUM OF F CALCULATED OVER THE SUM OF F OBSERVED.

ONE MAY SELECT UP TO 15 CATEGORIES PER RUN BY MEANS OF 'CATEGO' CARDS. THESE CARDS ALLOW FOR A 12 CHARACTER NAME FOR THE CATEGORY WHICH IS TO BE SUPPLIED BY THE USER FOR THE OUTPUT LISTING. A 'MATCH' TEST FOR H, K, AND OR L IS ESTABLISHED IF ANY OR ALL OF THESE FIELDS IS LEFT BLANK THEN ALL REFLECTIONS ARE TESTED FURTHER. IF HOWEVER A NUMBER IS PUNCHED THEN ONLY REFLECTIONS WITH THE VALUE(S) PUNCHED WILL BE INCLUDED IN THE CATEGORY. FOR EXAMPLE, IF ONE PUNCHES 1 IN THE H FIELD THEN THE CATEGORY APPLIES ONLY TO 1KL REFLECTIONS. NEXT ONE MAY SPECIFY IF THE CATEGORY IS TO BE BASED ON AN ADDITIVE COMBINATION OF THE MILLER INDICES HAVING A SPECIFIED VALUE. FOR EXAMPLE ONE PUNCHES A 4 TO INDICATE THE CATEGORY IS BASED ON H+K AND A 2 TO INDICATE THAT H+K MUST BE EVEN. THE FINAL ALTERNATIVES FOR CATEGORIES ARE BASED UPON RANGES OF VALUES

FOR THREE POSSIBLE CRYSTALLOGRAPHIC QUANTITIES - SIN THETA/LAMBDA, INTENSITY, OR F OBSERVED.

THESE POSSIBILITIES SHOULD PERMIT THE EVALUATION OF STRUCTURES WITH VERY SPECIAL CATEGORIES OF REFLECTIONS.

THE UPDATE PROGRAM

THE =UPDATE= PROGRAM ENABLES ONE TO (1) MAKE SPECIFIC CHANGES ON THE SYMBOLIC TAPE, (2) PRINT A SPECIFIC ROUTINE (OR THE ENTIRE SYSTEM), (3) PUNCH A SPECIFIC ROUTINE (OR THE ENTIRE SYSTEM), (4) END OF FILE THE TAPE BEFORE A SPECIFIC SUBROUTINE OR BEFORE ALL SUBROUTINES, AND (5) COPY THE SYMBOLIC TAPE. IT WAS WRITTEN BY F.A. KUNDELL IN COLLABORATION WITH J.M. STEWART.

WHEN ERRORS ARE FOUND IN THE X-RAY SYSTEM CORRECTIONS WILL BE SENT OUT IN THE FORM OF AN UPDATE DECK OR LISTING. THE UPDATE PROGRAM RELIES ON THE CARD NUMBER AND LABEL WHICH MAY BE CHANGED AT EACH UPDATING. CONSEQUENTLY, THE USER MUST BE VERY CAREFULLY WHEN AN UPDATE IS TO BE CARRIED OUT. ALL CORRECTIONS MUST BE MADE IF SUBSEQUENT CORRECTIONS ARE TO HAVE MEANING. THIS IS BECAUSE WITH EACH UPDATE THE SEQUENCE NUMBERS OF THE DECK WILL BE REASSIGNED DURING THE UPDATE PROCESS. CORRECTIONS WILL REFER TO THE SEQUENCE NUMBERS OF THE MOST RECENT RUN. FURTHERMORE, THE CORRECTIONS MUST BE MADE IN THE ORDER IN WHICH THEY ARE MAILED.

SIFTING ROUTINE

THE =USIFT= PROGRAM IS THE SIFTING ROUTINE OF THE X-RAY SYSTEM. IT WAS WRITTEN BY F.A. KUNDELL IN COLLABORATION WITH J.M. STEWART.

THE ROUTINE WILL CORRECT ALL CARDS WHICH FULFILL THE STATED REQUIREMENTS. THERE ARE THREE TYPES OF CORRECTIONS POSSIBLE (ALTERATIONS, DELETION, AND INSERTION). ALTERATION IS ACCOMPLISHED BY MEANS OF THE 'SETCHK' CARD WHICH ENABLES ONE TO CHANGE A WORD OR SYMBOL THROUGHOUT THE DECK. THUS THE 'SETCHK' CARD CAN BE USED TO CHANGE THE REREAD STATEMENT (READ (NCDBUF,$),LIST) WHICH IS USED ON MOST MACHINES TO THE CDC DECODE STATEMENT (DECODE (NCDBUF,$), LIST) WHERE $ REPRESENTS THE FORMAT NUMBER.

DELETION IS ACCOMPLISHED BY THE 'SKIP' CARD. THUS ALL CARDS WITH A SPECIFIED SIGNAL NMEMONIC OR CHARACTER WILL BE SKIPPED. IF ALL REWINDS ARE TO BE DELETED THEN THE SKIP CARD WOULD BE USED.

INSERTION IS ACCOMPLISHED WITH THE 'ADD' CARD. THIS IS PARTICULARLY USEFUL IN INSERTING NEW CONTROLL CARDS IN THE SYSTEM PROGRAM DECKS.

TABLE OF CONTENTS PART II

THE WRITE-UP OF EACH PROGRAM LINK IS GIVEN IN TWO PARTS. THE FIRST IS DESCRIPTIVE THE SECOND IS A CARD ORDER SUMMARY, FILE HANDLING SUMMARY AND CARD FORMAT DESCRIPTION. IN EACH CASE THE WRITE-UP APPEARS ALPHABETICALLY BY PROGRAM CARD CALLING MNEMONIC.

BLOKLS ATOMIC PARAMETER REFINEMENT BY BLOCK LEAST SQUARES.

BONDLA DETERMINATION OF CONTACT AND BOND DISTANCES AND ANGLES WITH ESTIMATED ERRORS.

DATCO3 TREATMENT OF CARD CONTROLLED XRD-6 OUTPUT.

DATFIX PRELIMINARY DATA SCALING CALCULATION OF QUASINORMALIZED STRUCTURE FACTORS (E) AND ESTIMATION OF OVERALL TEMPERATURE FACTOR.

DATRDN PREPARATION OF BINARY DATA FILE AND PRELIMINARY TREATMENT OF DATA AND SYMMETRY.

DIAGLS ATOMIC PARAMETER REFINEMENT BY DIAGONAL LEAST SQUARES.

DIFOPP PROCESS DIFFRACTOMETER OUTPUT DATA.

DIFSET GENERATE SETTINGS FOR GATHERING DATA ON A AUTOMATED DIFFRACTOMETER.

DUMCOP DUMP OR COPY THE BINARY DATA FILE.

FC STRUCTURE FACTOR CALCULATION.

FOURR FOURIER TRANSFORMATIONS TO GIVE PATTERSON, VECTOR, ELECTRON DENSITY, DIFFERENCE OR E MAPS.

GENERL GENERAL SYSTEM OPERATION CARD DESCRIPTION

LOADAT LOAD ATOMIC PARAMETERS INTO THE BINARY DATA FILE.

MODIFY BINARY DATA EDITING AND GENERATION OF PSEUDO DATA.

ORFLS ATOMIC PARAMETER REFINEMENT BY FULL MATRIX LEAST SQUARES.

PARAM LEAST SQUARES REFINEMENT OF CELL PARAMETER FROM TWO THETA DATA.

PHASE SEARCH OF SIGMA TWO RELATIONSHIPS FOR A SET OF POSSIBLE PHASES.

RLIST LIST R VALUES FOR VARIOUS ZONES AND OTHER REFLECTIONS CLASSES.

SIGMA2 GENERATION OF SIGMA TWO RELATIONSHIPS.

UPDATE UPDATE SYMBOLIC PROGRAMS ON TAPE.

USIFT CONVERT SYMBOLIC DECKS OF THE SYSTEM FROM ONE FORTRAN TO ANOTHER.

WRITEU FORM WRITE-UP FROM PUNCHED CARDS.

APENDX-1 CONTRIBUTORS TO THE SYSTEM.

APENDX-2 DESCRIPTION OF THE X-RAY SYSTEM BINARY DATA FILE.

A. CARD ORDER SUMMARY FOR =BLOKLS= PROGRAM

BLOKLS	CALLING CARD FOR BLOCK-DIAGONAL-LEAST-SQUARES
*SCALE	SCALE CARD FOR F RELATIVE DATA
*ATOM	ATOM SELECTION CARD
*REF	TURN ON REFINEMENT OF SPECIFIED PARAMETERS
*NOREF	SHUT OFF REFINEMENT OF SPECIFIED PARAMETERS
*DAMP	SPECIAL DAMPING LIMITS FOR SHIFTS
END	END CARD

* THESE CARDS ARE OPTIONAL.

NOTE 1 - THIS PROGRAM DOES NOT TREAT THE OVERALL TEMPERATURE FACTOR.

NOTE 2 - IF NO ATOM CARDS ARE PRESENT ALL THE ATOMS IN THE BINARY FILE ARE USED. IF ANY ATOMS ARE SPECIFIED BY CARDS ONLY THOSE SPECIFIED ON THE CARDS ARE SELECTED FROM THE BINARY FILE. IF THERE ARE TOO MANY ATOMS IN THE FILE FOR THE STORAGE CAPACITY, SELECTION CARDS WILL BE EXPECTED.

NOTE 3 - IF ALL REFINEMENT RESTRICTION CARDS ARE LEFT OUT REFINEMENT WILL BE ON ALL POSITIONAL AND TEMPERATURE PARAMETERS. HOWEVER, NO SCATTERING FACTORS OR POPULATION FACTORS WILL BE SET TO REFINE.

***** READS =NFILEA= AND WRITES =NFILEB= *****

IF THE PROGRAM IS SET TO PUNCH CARDS (COLS 32-34 OF =BLOKLS= CARD) THE PROGRAM WRITES THESE IMAGES ON =NFILEC=, THE PUNCH FILE.

B. CARD FORMATS FOR =BLOKLS= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

BLOKLS - CALLING CARD FOR BLOCK-DIAGONAL-LEAST-SQUARES PROGRAM.
FORMAT (A2,A4,1X,A4,A2,11I3,3F4.3,I3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	BLOKLS
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-16	NUMBER OF CYCLES TO BE CALC. (NC)
17-19	(1)/(2)/(3) FOR (ISOTROPIC)/(ANISOTROPIC)/(MIXED) PROGRAM CONVERTS IF REQUIRED. AVERAGE DIAGONAL ELEMENT USED IN ANISOTROPIC CONVERSION. NO CONVERSION MADE UNLESS SPECIFIED BY A =REF= CARD IN MIXED MODE. (ITF)
20-22	(BLANK)/(1) FOR REFINEMENT BASED ON (F)/(F**2) (IFSQ)
23-25	(BLANK)/(1) FOR USE (SCALE)/(RESCALE) FACTORS FROM TAPE (IRESC)
26-28	(BLANK)/(1) FOR (DO)/(DO NOT) HALT IF CONVENTIONAL R INCREASES BY 0.1 IN ANY CYCLE.
29-31	(BLANK)/(1) FOR (WEIGHTS FROM TAPE)/(ALL WEIGHTS EQUAL 1.0) (IW)
32-34	(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	(BLANK)/(1) FOR (DO NOT)/(DO) LIST THE REFLECT. INFO. DURING LAST CYCLE (ILIST)
38-40	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	(BLANK)/(1)/(2) FOR (NO)/(USE)/(USE PREVIOUS FC) FIXED ATOM CONTRIB. (IP)
44-46	(BLANK)/(1) FOR (X-RAY)/(NEUTRON) (INEU)
47-50	DAMPING OR ENHANCING FACTOR FOR PARAMETER SHIFTS (BLANK OR 0.0 = 1.0)
51-54	RR TO CONTROL LIST (BLANK = 2.0)
55-58	REJECT FROM CONSIDERATION IN SHIFTS REFLECTIONS WHOSE WEIGHTED DELTA-F IS LARGER. (BLANK = 10**8)
59-61	(BLANK)/(1) (NO)/(SPECIAL) SYMMETRY PATCH REQUIRED.
62-72	BLANK

SCALE - SCALE CARD FOR F RELATIVE DATA.
FORMAT (A2,A4,F10.4,I4,F10.4,I2,3F10.4)

```
 COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
 1-5   SCALE
 6     BLANK
 7-16  SCALE FACTOR TO APPLY TO F REL.
 17-20 GROUP IDENTIFICATION (1-64)
 21-72 BLANK

ATOM   - ATOM SELECTION CARD.
    FORMAT (A2,A4,1X,A4,A2)

 COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
 1-4   ATOM
 5-7   BLANK
 8-13  ATOM NAME - CONSISTS OF TWO PARTS. THE FIRST FOUR COLUMNS MUST BE THE
       ATOM-TYPE NAME (SEE FORMFX).  THE REST MUST BE IDENTIFICATION OF THE
       PARTICULAR ATOM OF THE SPECIFIED TYPE.  IF THE SECOND FIELD IS LEFT
       BLANK ALL ATOMS OF THE SCATTERING FACTOR TYPE SPECIFIED WILL BE LOADED.
 14-72 BLANK

REF OR NOREF - SET PARAMETER REFINEMENT IF IT IS TO BE DIFFERENT THAN THAT
        ALREADY SET IN THE DATA FILE.
    FORMAT (A2,A4,1X,A4,A2,13A3)

 COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
 1-5   REF OR NOREF
 6-7   BLANK
 8-11  SCATTERING FACTOR TYPE (EXACTLY AS SHOWN IN FORMFX CARDS).
 12-13 ATOM IDENTITY FOR THIS SCATTERING FACTOR TYPE.
       (NOTE.... IF 12-13 IS BLANK CARDS APPLY TO ALL ATOMS OF NAMED TYPE.
       IF 8-11 IS BLANK CARD APPLIES TO ALL ATOMS.)
       (IF =SCALE= IS PUNCHED IN 8-12 THEN COMMAND APPLIES TO F-RELATIVE SCALE
       FACTOR REFINEMENT)
 14-16 EACH FIELD MAY CONTAIN BLANKS OR ONE OF THE FOLLOWING LEFT JUSTIFIED
       SYMBOLS.  X, Y, Z, B, B11, B22, B33, B12, B13, B23, M, S, D (M IS THE
       POPULATION PARAMETER, S THE NEUTRON SCATTERING FACTOR AND D THE
       DISPERSION CORRECTION)  IF ALL FIELDS ARE LEFT BLANK ALL QUANTITIES
       ARE ACTED UPON.  IF ANY FIELD IS PUNCHED ONLY THE PARAMETERS NAMED ARE
       ACTED UPON.
 17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43, 44-46, 47-49,
 50-52 (SYMBOL FROM ABOVE LIST)
 53-72 BLANK

DAMP   - DAMP PARAMETER SHIFTS ABOVE A GIVEN LEVEL.
    FORMAT (A2,A4,1X,13F5.3)

 COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
 1-4   DAMP
 5-7   BLANK
 8-12  MAXIMUM X SHIFT IN ANGSTROM UNITS
 13-17 MAXIMUM Y SHIFT IN ANGSTROM UNITS
 18-22 MAXIMUM Z SHIFT IN ANGSTROM UNITS
 23-27 MAXIMUM B SHIFT IN UNITS OF B
 28-32 MAXIMUM B11 SHIFT IN UNITS OF B
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  33-37 MAXIMUM B22 SHIFT IN UNITS OF B
  38-42 MAXIMUM B33 SHIFT IN UNITS OF B
  43-47 MAXIMUM B12 SHIFT IN UNITS OF B
  48-52 MAXIMUM B13 SHIFT IN UNITS OF B
  53-57 MAXIMUM B23 SHIFT IN UNITS OF B
  58-62 POPULATION PARAMETER SHIFT
  63-67 F-RELATIVE SCALE FACTOR SHIFT
  68-72 NEUTRON SCATTERING FACTOR SHIFT

END     - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =BONDLA= PROGRAM

BONDLA	PROGRAM CALLING CARD.
*CELL	CELL DIMENSION.
*CELLSD	STANDARD DEVIATIONS OF CELL PARAMETERS.
*LATICE	LATTICE TYPE.
*SYMTRY	SYMMETRY OPERATION.
*ATOM	ATOM PARAMETERS.
*BOND	PRODUCE A SPECIFIC BOND DISTANCE.
*ANGLE	PRODUCE A SPECIFIC BOND ANGLE.
END	END CARD

* THESE CARDS ARE OPTIONAL

****READS =NFILEA= AND WRITES =NFILEB= UNLESS SIGNALED IN 'BONDLA' CARD THAT WHOLE CALCULATION IS FROM CARDS ONLY.****

B. CARD FORMATS FOR =BONDLA= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

BONDLA - CALLING CARD.
FORMAT (A2,A4,1XA4,A2,1X11,3F10.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	BONDLA
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14	BLANK
15	(BLANK)/(1) (ALL)/(SOME) INFORMATION FROM CARDS, I.E. (NO)/(YES) BINARY DATA FILE REQUIRED
16-25	MAXIMUM CONTACT DISTANCE (BLANK = 2.50)
26-35	MAXIMUM BOND DISTANCE (BLANK = 1.80)
36-45	MINIMUM BOND DISTANCE (BLANK = 0.03)

CELL - CELL CONSTANT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5,F7.0)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	CELL
5-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-21	A CELL DIMENSION OR A* RECIPROCAL CELL DIMENSION
22-29	B CELL DIMENSION OR B* RECIPROCAL CELL DIMENSION
30-37	C CELL DIMENSION OR C* RECIPROCAL CELL DIMENSION
38-46	COS ALPHA OR ALPHA IN DEGREES OR COS ALPHA* OR ALPHA* IN DEGREES
47-55	COS BETA OR BETA IN DEGREES OR COS BETA* OR BETA* IN DEGREES
56-64	COS GAMMA OR GAMMA IN DEGREES OR COS GAMMA* OR GAMMA* IN DEGREES
65-71	F(0,0,0)

NOTE... QUANTITIES MUST BE EITHER ALL IN DIRECT SPACE OR ALL IN RECIPROCAL SPACE.

CELLSD - STANDARD DEVIATION OF UNIT CELL PARAMETERS.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	CELLSD
7	BLANK

8-13 COMPOUND IDENTIFICATION CODE
14-21 STANDARD DEVIATION IN A CELL DIMENSION (ANGSTROMS)
22-29 STANDARD DEVIATION IN B CELL DIMENSION (ANGSTROMS)
30-37 STANDARD DEVIATION IN C CELL DIMENSION (ANGSTROMS)
38-46 STANDARD DEVIATION IN COS ALPHA CELL DIMENSION (ANGSTROMS)
47-55 STANDARD DEVIATION IN COS BETA CELL DIMENSION (ANGSTROMS)
56-64 STANDARD DEVIATION IN COS GAMMA CELL DIMENSION (ANGSTROMS)

LATICE - CENTRICITY IDENTIFICATION CARD.
FORMAT (A2,A4,2X,A1,2X,A1)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 LATICE =LATTICE= SPELLING ALSO ACCEPTED
7-8 BLANK
9 C = CENTRIC CELL, A = ACENTRIC CELL.
10-11 BLANK
12 DESIGNATION OF LATTICE TYPE P,A,B,C,R,I,F ONE OF THE FOREGOING MUST BE PUNCHED.
13-72 BLANK

SYMTRY - SYMMETRY OPERATION CARD.
FORMAT (12(A2,A4))

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 SYMTRY
7-72 GENERAL EQUIVALENT POSITION. 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.

NOTE... DO NOT PUNCH ANY OPERATIONS THROUGH THE CENTER IF SPACE GROUP IS CODED CENTRIC ON LATICE CARD.

(SEE STATEMENT ON SYMMETRY IN 1.GENERL)

ATOM - ATOM PARAMETER CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.4,F6.3,F5.2,3F8.5)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4 ATOM
5-7 BLANK
8-11 SCATTERING FACTOR TYPE (EXACTLY AS ON FORMFX CARDS)
12-13 ATOM IDENTITY FOR GIVEN SCATTERING FACTOR TYPE
14-21 X FRACTIONAL COORDINATE. DECIMAL POINT MUST BE PUNCHED IN ORDER TO SUPERSEDE FORMAT.
22-29 Y
30-37 Z
38-43 INDIVIDUAL ISOTROPIC TEMPERATURE FACTOR. MAY BE ZEROS OR BLANK IF APPLYING OVERALL TEMPERATURE FACTOR OR IF A SEPARATE TEMPERATURE

```
        FACTOR CARD IS USED, SINCE THIS WORD IS THEN IGNORED.
  44-48 INDIVIDUAL ATOM SCALE FACTOR.  MUST BE ZEROS OR BLANK TO BE IGNORED.
  49-56 STANDARD DEVIATION IN X (REQUIRED ONLY IF REQUIRED BY PROGRAM BEING
        USED.)
  57-64 STANDARD DEVIATION IN Y.
  65-72 STANDARD DEVIATION IN Z.

BOND   - CALCULATE A SPECIFIED =BOND= DISTANCE.
     FORMAT (A2,A4,2(1X,A4,A2))

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   BOND
  5-7   BLANK
  8-13  ATOM ID FOR FIRST ATOM.
  14    BLANK
  15-20 ATOM ID FOR BONDED ATOM.
  21-72 BLANK

ANGLE  - CALCULATE A SPECIFIED =BOND= ANGLE.
     FORMAT (A2,A4,4(1X,A4,A2))

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   ANGLE
  6-7   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 BLANK

NOTE - IF THE FIRST THREE FIELDS ARE SPECIFIED, THE CENTRAL ATOM MUST BE
       SECOND.  IF FOUR FIELDS ARE SPECIFIED, THE FIRST AND SECOND DEFINE ONE
       LINE, THE THIRD AND FOURTH THE SECOND AND ATOMS TWO AND THREE ARE
       PRESUMED TO BE TOWARD THE APEX OF THE ANGLE TO BE CALCULATED.

END    - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-76  BLANK
```

A. CARD ORDER SUMMARY FOR =DATC03= PROGRAM

DATC03	CALLING CARD
W99999	MODEL XRD-6 OUTPUT CARD
------	DECK OF CARDS FROM XRD-6
END	END CARD

****READS CARDS FROM 'NTIN'

****WRITES CARDS ON 'NFILEC' OPTIONALLY

B. CARD FORMATS FOR =DATC03= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DATC03 - PROGRAM CALLING CARD.
FORMAT (A2,A4,1XA4,A2,I2,4F10.2,4XA1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DATC03
8-13	COMPOUND IDENTIFICATION CODE
15	(BLANK)/(1)/(2) (DO NOT)/(HKL INTENSITY)/(X-RAY-63 F) PUNCH CARDS ON NFILEC
16-25	MULTIPLE OF INTENSITY STANDARD DEVIATIONS TO ESTABLISH THRESHOLD OF OBSERVABILITY. IF THE INTENSITY IS LESS THAN THIS FACTOR TIMES THE STANDARD DEVIATION IN THE INTENSITY THE REFLECTION WILL BE CODED A 'LESS-THAN' AND THE VALUE OF INTENSITY SET TO THIS FACTOR TIMES THE STANDARD DEVIATION.
26-35	BACKGROUND COUNT TIME IN SECONDS (ONE SIDE ONLY - EXACTLY THE PRESET TIME SET IN THE SCALER)
36-45	SCALE FACTOR FOR INTENSITIES. MAY BE USEFUL AS A FILTER FACTOR.
46-55	MULTIPLE OF BACKGROUND STANDARD DEVIATION WHICH IS TO BE USED TO FLAG REFLECTIONS WHERE THE DIFFERENCE BETWEEN BACKGROUNDS IS GREATER THAN THIS FACTOR TIMES THE STANDARD DEVIATION.
60	ANY CHARACTER DESIRED TO DELIMIT STANDARD REFLECTION ESTIMATED STANDARD DEVIATION ON SUMMARY PLOT (USUALLY LEFT BLANK)

W999999999 - MODEL DIFFRACTOMETER OUTPUT CARD.
FORMAT (80A1)

(SEE SECTION 1.DATC03 FOR GENERAL DISCUSSION.)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-80	CHARACTERS EXACTLY AS ANTICIPATED FOR DIFFRACTOMETER OUTPUT CARDS WHICH FOLLOW. USE 9 IN ANY COLUMN WHERE ANY NUMERIC PUNCH IS ACCEPTIBLE (I.E. ANGLE AND COUNT FIELDS) CARDS AS OUTPUT FROM THE XRD-6. (REMEMBER THAT THERE IS A POSSIBILITY THAT THESE CARDS HAVE SOME ''INVALID'' COLUMNS. THAT IS COLUMNS IN WHICH THE PUNCHING IS SUCH THAT THE CARD CAN NOT BE LOADED INTO THE MACHINE. IN THIS CASE TRY TO GET THE OPERATOR TO SKIP THESE CARDS NOT REJECT THE WHOLE JOB. DATC03 WILL SORT OUT WHAT REMAINS.)

END - END CARD.

B. CARD FORMATS FOR =DATC03= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DATC03 - PROGRAM CALLING CARD.
FORMAT (A2,A4,1XA4,A2,I2,4F10.2,4XA1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DATC03
8-13	COMPOUND IDENTIFICATION CODE
15	(BLANK)/(1)/(2) (DO NOT)/(HKL INTENSITY)/(X-RAY-63 F) PUNCH CARDS ON NFILEC
16-25	MULTIPLE OF INTENSITY STANDARD DEVIATIONS TO ESTABLISH THRESHOLD OF OBSERVABILITY. IF THE INTENSITY IS LESS THAN THIS FACTOR TIMES THE STANDARD DEVIATION IN THE INTENSITY THE REFLECTION WILL BE CODED A 'LESS-THAN' AND THE VALUE OF INTENSITY SET TO THIS FACTOR TIMES THE STANDARD DEVIATION.
26-35	BACKGROUND COUNT TIME IN SECONDS (ONE SIDE ONLY - EXACTLY THE PRESET TIME SET IN THE SCALER)
36-45	SCALE FACTOR FOR INTENSITIES. MAY BE USEFUL AS A FILTER FACTOR.
46-55	MULTIPLE OF BACKGROUND STANDARD DEVIATION WHICH IS TO BE USED TO FLAG REFLECTIONS WHERE THE DIFFERENCE BETWEEN BACKGROUNDS IS GREATER THAN THIS FACTOR TIMES THE STANDARD DEVIATION.
60	ANY CHARACTER DESIRED TO DELIMIT STANDARD REFLECTION ESTIMATED STANDARD DEVIATION ON SUMMARY PLOT (USUALLY LEFT BLANK)

W999999999 - MODEL DIFFRACTOMETER OUTPUT CARD.
FORMAT (80A1)

(SEE SECTION 1.DATC03 FOR GENERAL DISCUSSION.)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-80	CHARACTERS EXACTLY AS ANTICIPATED FOR DIFFRACTOMETER OUTPUT CARDS WHICH FOLLOW. USE 9 IN ANY COLUMN WHERE ANY NUMERIC PUNCH IS ACCEPTIBLE (I.E. ANGLE AND COUNT FIELDS) CARDS AS OUTPUT FROM THE XRD-6. (REMEMBER THAT THERE IS A POSSIBILITY THAT THESE CARDS HAVE SOME ''INVALID'' COLUMNS. THAT IS COLUMNS IN WHICH THE PUNCHING IS SUCH THAT THE CARD CAN NOT BE LOADED INTO THE MACHINE. IN THIS CASE TRY TO GET THE OPERATOR TO SKIP THESE CARDS NOT REJECT THE WHOLE JOB. DATC03 WILL SORT OUT WHAT REMAINS.)

END - END CARD.

FORMAT (A2,A4)

	COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
	1-3	END
6	4-72	BLANK

A. CARD ORDER SUMMARY FOR =DATFIX= PROGRAM

DATFIX	PROGRAM CALLING CARD
*EPSILON	ZONE WEIGHTING FACTORS
CELCON	UNIT CELL CONTENTS (ONE PER ATOM TYPE)
*BRANGE	SPECIFIES TEMPERATURE FACTOR RANGE
*XRANGE	SPECIFIES (SINE THETA/LAMBDA) EXPONENT RANGE
*K(I)/K	SPECIFIES GROUP SCALE FACTOR RATIO RANGE
END	END CARD. SIGNALS END OF DATA AND INITIATES CALCULATION.

* THESE CARDS ARE OPTIONAL.

***** READS =NFILEA= AND WRITES =NFILEB= *****

B. CARD FORMATS FOR =DATFIX= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DATFIX - CALLING CARD FOR DATA MANIPULATION PROGRAM.
FORMAT (A2,A4,1X,A4,A2,2I2,F6.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DATFIX
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-15	(0)/(1) FOR (DO NOT)/(DO) LIST E VALUES PLACED IN FILE
16-17	(0)/(1)/(2) FOR PLACE CALCULATED SCALE AND TEMPERATURE FACTOR DATA IN (LOGICAL RECORD 7)/(LOGICAL RECORD 16)/(BOTH)
18-23	MINIMUM F RELATIVE TO BE INCLUDED IN E SCALING PROCESS (BLANK = 0.0)
24-72	BLANK

EPSILON- ZONE WEIGHTS CARD.
FORMAT (A2,A4,1X,6F3.0)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-7	EPSILON
8-10	EPSILON FOR H00 (BLANK = 1) RATIO OF SYSTEMATICALLY ABSENT REFLECTIONS FOR REFLECTION CLASS (E.G. H0L ABSENT FOR L ODD IMPLIES 2 IN COLS 22)
11-13	0K0
14-16	00L
17-19	0KL
20-22	H0L
23-25	HK0
26-72	BLANK

CELCON - CELL CONTENTS CARD.
FORMAT (A2,A4,1X,A4,2X,F4.0,F7.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	CELCON
7	BLANK
8-11	ATOM TYPE (EXACTLY AS IN FORMFX CARDS)
12-13	BLANK
14-17	NUMBER OF ATOMS OF SPECIFIED TYPE IN WHOLE UNIT CELL
18-24	ATOMIC WEIGHT OF THE SPECIES

25-72 BLANK

BRANGE - SPECIFIES TEMPERATURE FACTOR RANGE.
FORMAT (A2,A4,I3,2F6.0)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 BRANGE
7-9 NUMBER OF VALUES OF B TO BE USED IN SEARCH FOR MINIMUM (IF BLANK THIS IS SET TO SIX.)
10-15 LOWER LIMIT OF B (BLANK IMPLIES ZERO)
16-21 INTERVAL IN B (BLANK IMPLIES 1.0)
22-72 BLANK

XRANGE - SPECIFIES SINE THETA/LAMBDA EXPONENT RANGE.
FORMAT (A2,A4,I3,2F6.0)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 XRANGE
7-9 NUMBER OF VALUES OF X TO BE USED IN SEARCH FOR MINIMUM (BLANK IMPLIES 1)
10-15 LOWER LIMIT OF X (BLANK IMPLIES 2.0)
16-21 INTERVAL IN X (BLANK IMPLIES 0.25)
22-72 BLANK

K(I)/K - SPECIFIES GROUP SCALE FACTOR RATIO RANGE.
FORMAT (A2,A4,2F6.0)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 K(I)/K
7-12 MINIMUM PERMISSIBLE RATIO FOR AN ESTIMATED LEVEL SCALE FACTOR TO THE OVERALL ESTIMATED SCALE FACTOR (BLANK = 1.0, I.E NO VARIATION)
13-18 MAXIMUM PERMISSIBLE RATIO FOR A LEVEL SCALE FACTOR TO THE OVERALL SCALE FACTOR (BLANK = 1.0)
19-72 BLANK
NOTE... IF NO K(I)/K CARD IS SUPPLIED, EACH LEVEL SCALE FACTOR IS SET EQUAL TO OVERALL SCALE FACTOR.

END - END CARD.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3 END
4-72 BLANK

NOTE... IF NEITHER A BRANGE NOR XRANGE CARD IS SUPPLIED 6 VALUES OF B ARE USED STARTING AT 0.0 IN INTERVALS OF 1.0. X IS SET EQUAL TO 2.0.

A. CARD ORDER SUMMARY FOR =DATRDN= PROGRAM

DATRDN PROGRAM CALLING CARD

*LABEL FILE HEADING. FILE IDENTIFICATION INFORMATION OR ABSTRACT (MAXIMUM OF 16 CARDS)

CELL UNIT CELL PARAMETERS.

*CELLSD STANDARD DEVIATION OF UNIT CELL PARAMETERS

*MAXHKL TO ESTABLISH LIMITS ON H, K, L, OR SIN THETA.

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.

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).

*GRID ONE MAY SPECIFY A DESIRED GRID INTERVAL TO BE USED LATER BY THE FOURIER PROGRAM. IF IT IS LEFT OUT THE DATA REDUCTION PROGRAM CALCULATES A SET OF INTERVALS BASED

UPON THE CELL DIMENSIONS.

*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 PRECEDING, THEN =CONDIT= AND/OR =FORMAT= CARDS WILL BE NECESSARY.

*REFIN USE THE 'REFIN' CARD WITH CARE. THE SPECIAL REFLECTION DECK SPECIFIED MUST FOLLOW NEXT AFTER THE 'REFIN' CARD OR CONTROL WILL BE LOST.

*HKL REFLECTION CARDS.

END END 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 =NFILEA= IF REFLECTION DATA IS TO BE UPDATED FROM THE BINARY FILE. *****

***** INITIATES OR EDITS A BINARY DATA FILE WHICH IS THEN WRITTEN ON

=NFILEB= *****

B. CARD FORMATS FOR =DATRDN= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DATRDN - CALLING CARD FOR DATA REDUCTION PROGRAM.
FORMAT (A2,A4,1X,A4,A2)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DATRDN
7	BLANK
8-13	SIX COLUMNS OF HOLLERITH PUNCHING OR BLANKS TO IDENTIFY COMPOUND. THIS IDENTIFICATION IS CHECKED BY VARIOUS PROGRAMS FOR CONSISTANCY, SO CHOOSE CAREFULLY AND REMEMBER YOUR CHOICE. TAKE GREAT CARE TO LOCATE BLANKS IN THE SAME WAY EVERY SUCCEEDING TIME THE COMPOUND I.D. IS PUNCHED.
14	BLANK
15	(BLANK)/(1) (NO)/(YES) AN OLD DATA FILE ON NFILEA
16	BLANK
17	(BLANK)/(1) (DO)/(DO NOT) LIST REFLECTION INFORMATION
18	BLANK
19	(BLANK)/(1) (DO NOT)/(DO) EXPECT TO EDIT REFLECTIONS (FORCES THE NEED FOR PREVIOUS DATA FILE ON NFILEA)
20-21	MAXIMUM NUMBER OF SCALE GROUPS IF DIFFERENT THAN 1 (UP TO 64 ALLOWED)
22-72	BLANK

LABEL - TAPE LABELING CARD. USED TO IDENTIFY BINARY TAPE.
FORMAT (A2,A4,16A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	LABEL
6	BLANK
7-70	ALPHANUMERIC INFORMATION TO BE USED AS TAPE LABEL.
71-72	BLANK

CELL - CELL CONSTANT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5,F7.0)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	CELL
5-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-21	A CELL DIMENSION OR A* RECIPROCAL CELL DIMENSION

22-29 B CELL DIMENSION OR B* RECIPROCAL CELL DIMENSION
30-37 C CELL DIMENSION OR C* RECIPROCAL CELL DIMENSION
38-46 COS ALPHA OR ALPHA IN DEGREES OR COS ALPHA* OR ALPHA* IN DEGREES
47-55 COS BETA OR BETA IN DEGREES OR COS BETA* OR BETA* IN DEGREES
56-64 COS GAMMA OR GAMMA IN DEGREES OR COS GAMMA* OR GAMMA* IN DEGREES
65-71 F(0,0,0)

NOTE... QUANTITIES MUST BE EITHER ALL IN DIRECT SPACE OR ALL IN RECIPROCAL SPACE.

CELLSD - STANDARD DEVIATION OF UNIT CELL PARAMETERS.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 CELLSD
7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-21 STANDARD DEVIATION IN A CELL DIMENSION (ANGSTROMS)
22-29 STANDARD DEVIATION IN B CELL DIMENSION (ANGSTROMS)
30-37 STANDARD DEVIATION IN C CELL DIMENSION (ANGSTROMS)
38-46 STANDARD DEVIATION IN COS ALPHA CELL DIMENSION (ANGSTROMS)
47-55 STANDARD DEVIATION IN COS BETA CELL DIMENSION (ANGSTROMS)
56-64 STANDARD DEVIATION IN COS GAMMA CELL DIMENSION (ANGSTROMS)

MAXHKL - LIMITS FOR FOURIER SUMMATION.
FORMAT (A2,A4,7X,3I4,2F8.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 MAXHKL
7-13 BLANK
14-17 MAXIMUM H TO BE USED
18-21 MAXIMUM K TO BE USED
22-25 MAXIMUM L TO BE USED
26-33 MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
34-41 MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
42-72 BLANK

FORMFX - ATOMIC FORM FACTORS FOR X-RAYS.
FORMAT (A2,A4,1X,A4,2X,F7.5,F8.3,6(A2,A4),A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 FORMFX
7 BLANK
8-11 ONE TO FOUR CHARACTERS TO IDENTIFY THE ATOM-TYPE. TO AVOID ERRORS LEFT JUSTIFICATION IS RECOMMENDED.
12-13 BLANK
14-20 SIN(THETA)/LAMBDA
21-28 ATOMIC SCATTERING FACTOR
29-72 SOURCE REFERENCE CONTINUED FROM CARD TO CARD

FORMFN - ATOMIC FORM FACTORS FOR NEUTRONS.
FORMAT (A2,A4,1X,A4,2X,F8.3,8(A2,A4),A1)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD

```
  1-6    FORMFN
  7      BLANK
  8-11   ATOM TYPE NAME (SEE COLS. 8-11 OF FORMFX).
  12-13  BLANK
  14-21  COHERENT ATOMIC SCATTERING FACTOR
  22-72  SOURCE REFERENCE

LATICE - CENTRICITY IDENTIFICATION CARD.
     FORMAT (A2,A4,2X,A1,2X,A1)

  COLS   SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6    LATICE      =LATTICE= SPELLING ALSO ACCEPTED
  7-8    BLANK
  9      C = CENTRIC CELL,  A = ACENTRIC CELL.
  10-11  BLANK
  12     DESIGNATION OF LATTICE TYPE P,A,B,C,R,I,F   ONE OF THE FOREGOING MUST
         BE PUNCHED.
  13-72  BLANK

SYMTRY - SYMMETRY OPERATION CARD.
     FORMAT (12(A2,A4))

  COLS   SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6    SYMTRY
  7-72   GENERAL EQUIVALENT POSITION.  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.

         NOTE... DO NOT PUNCH ANY OPERATIONS THROUGH THE CENTER IF SPACE GROUP
                 IS CODED CENTRIC ON LATICE CARD.

         (SEE STATEMENT ON SYMMETRY IN 1.GENERL)

DISPER - TEMPLETON DISPERSION CORRECTION CARD.
     FORMAT (A2,A4,1X,A4,2X,2F10.3)

  COLS   SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6    DISPER
  7      BLANK
  8-11   ATOM TYPE NAME (SEE COLS. 8-11 OF FORMFX).
  12-13  BLANK
  14-23  DELTA FJ PRIME
  24-33  DELTA FJ DOUBLE PRIME
  34-72  BLANK

CONDIT - CONDITION CARD. SETS-UP CALCULATIONS CODES.
     FORMAT (A2,A4,1X,A4,A2,2F8.5,8X,9I3,F8.5)
```

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 CONDIT
7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-21 WAVELENGTH IN ANGSTROM UNITS
22-29 MAXIMUM VALUE OF SIN THETA FOR THE CONDITIONS OF OBSERVATION. THIS IS THE ACCURATE VALUE OF SIN MU FOR THE PRECESSION METHOD.
30-37 BLANK
38-40 (1)/(2) (X-RAY)/(NEUTRON) DIFFRACTOMETER DATA.
41-43 1/LP SWITCH, VALUES FROM 1 TO 9.
IF 1 - POWDER SPECTROMETER
IF 2 - SPECTROMETER WITH EULERIN CRADLE GEOMETRY AND TWO THETA SCAN
IF 3 - EQUI-INCLINATION WEISSENBERG
IF 4 - PRECESSION
IF 5 - NORMAL BEAM
IF 6 - FLAT CONE
IF 7 - EQUAL CONE
IF 8 - OSCILLATION
IF 9 - DO NOT APPLY A 1/LP CORRECTION
44-46 (1)/(2) FOR (DO)/(DO NOT) TAKE SQUARE ROOT OF INTENSITY
47-49, 50-52, 53-55 REQUIRE MILLER INDICES OF THE PLANE NORMAL TO THE BEAM AXIS AT ZERO DEGREES MU. FOR THE PRECESSION METHOD, 4 ABOVE. FOR 3,5,6,7 OR 8 ABOVE THESE MUST BE THE GENERAL ROTATION AXIS DEFINED BY U,V,W, WHERE U,V, AND W ARE INDICES OF THE ZONE AXIS PARALLEL TO THE ROTATION AXIS. FOR EXAMPLE, CORRECTION FOR WEISSENBERG DATA FROM A CRYSTAL MOUNTED TO ROTATE ABOUT THE B CELL AXIS USE 010.

FOR EXAMPLE IN THE PRECESSION METHOD FOR A MONOCLINIC CRYSTAL -

```
                          **
                        ** * -- 010 PLANE
                      **   *
                      *    *
-------}   --------*--   *
 BEAM       ''B''  *   **
            AXIS   * **
                   **
```

(E.G. IF BEAM IS COMING ALONG ''B'' AXIS, THEN THIS PLANE IS THE 010 PLANE)
56-58, 59-61, 62-64 REQUIRE THE MILLER INDICES OF THE PLANE NORMAL TO THE SPINDLE AXIS. (NOT NEEDED FOR WEISSENBERG METHOD)

FOR EXAMPLE IN THE PRECESSION METHOD -

```
                C*        /
               I         / A*
               I        /
               I       /
          *****.*.*** /
          *         *.
          *    . . .*
          *      .(-.---- 100 REFLECTION
```

```
--()-----------*    .  . *
               *   ) .   *
               * /       *
               * /       *
               */********
               /
              /
             / BEAM
            / ''B'' AXIS
```

(PARENTHESISES MEAN ROTATION)

PICK ONE OF THE HOL RECIPROCAL LATTICE POINTS ON THE MOST NEARLY HORIZONTAL AXIS PASSING THROUGH THE CENTER OF THE FILM. (IN THIS CASE THE 100 REFLECTION ON THE A* AXIS) THE MILLER INDICES OF THE PLANE NORMAL TO A* ARE 100 - THE INDICES OF THAT POINT.

65-72 REQUIRE SIGMA, THE ANGLE BETWEEN THE MOST NEARLY HORIZONTAL AXIS (A*) AND THE HORIZONTAL OF THE FILM, MEASURED IN A RIGHT HANDED SYSTEM LOOKING ALONG THE X-RAY BEAM (FROM SOURCE TO CRYSTAL, CLOCKWISE IS POSITIVE)

CONDIT - CONDITION CARD FOR CHANGE OF DATA.
FORMAT (A2,A4,1X,A4,A2,2F8.5,8X,9I3,F8.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	CONDIT
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-72	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.

FILTER - FILTER CARD. FOR USE WITH SPECTROMETER DATA.
FORMAT (A2,A4,1X,I2,F10.8)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	FILTER
7	BLANK
8-9	ID NUMBER OF FILTER (1 TO 99)
10-19	TRANSMITTANCY OF FILTER
20-72	BLANK

ABSORB - ABSORPTION CORRECTION CARD. (REQUIRES ONE CARD FOR EACH ENTRY IN TABLE. TOTAL = 19 CARDS)
FORMAT (A2,A4,1X,I1,I4,F4.0,2X,F10.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	ABSORB
7	BLANK
8	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	GROUP NUMBER OF DATA ALONG THE AXIS OF ROTATION.
13-16	TYRTA. THETA, OR UPSILON/2 (BUERGERS NOTATION). 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 ABSORPTION CORRECTION AS LISTED IN TABLE
29-72 BLANK

GRID - FOURIER GRID CARD.
FORMAT (A2,A4,1X,A4,A2,3I4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4 GRID
5-7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-17 NUMBER OF GRID INTERVALS ALONG THE X AXIAL DIRECTION.
18-21 GRID INTERVALS ALONG Y AXIAL DIRECTION
22-25 GRID INTERVALS ALONG Z AXIAL DIRECTION
26-72 BLANK

SCALE - SCALE CARD FOR INTENSITY DATA.
FORMAT (A2,A4,F10.4,I4,F10.4,I2,5F5.3)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 SCALE
6 BLANK
7-16 SCALE FACTOR TO APPLY TO INPUT INTENSITY, FREL, OR FREL**2
17-20 GROUP IDENTIFICATION (ONE NUMBER PER GROUP FROM 01 TO MAX OF 64).
21-72 MAY BE BLANK OR AS FOLLOWS
21-30 MINIMUM OBSERVED INTENSITY
31-32 WEIGHT ROUTINE SWITCH (0 OR 1)/(2)/(3) FOR (NO WEIGHTS)/(APPLY U. OF W. WEIGHTING SCHEME)/(USE PATCH SUBROUTINE TO CALCULATE WEIGHTS BY SPECIAL PROGRAMMING)
U. OF W. SCHEME IS (WEIGHT = Q1/MAX1F(SIGMA,Q2*FREL+Q3,Q4*FRELM+Q5)
(REFER TO SECTION 1.DATRDN FOR DETAILED EXPLANATION OF NEXT FIVE FIELDS, F5.3)
33-37 Q1
38-42 Q2
43-47 Q3
48-52 Q4
53-57 Q5
58-72 BLANK

FORMAT - DEFINES BCD REFLECTION DATA.
FORMAT (12(A2,A4))

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 FORMAT
7-72 THE FORMAT OF THE BCD REFLECTION DATA, AS IF A STANDARD FORTRAN CARD (E.G.- =USUAL= FORMAT IS (A2,A4,1X,A4,A2,4I4,F10.2) WHICH IS SUPPLIED IF NO CARD IS READ.)

REFIN - INSTRUCTION CARD FOR UNUSUAL REFLECTION INPUT.
FORMAT (A2,A4,I3,2I6,3I3,14(1X,A2))

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD

1-5 REFIN — 9 ≠ 0 if out same file
6-9 BLANK
10-15 NUMBER OF REFLECTIONS TO SKIP BEFORE PROCESSING FIRST REFLECTION RECORD
16-21 MAXIMUM NUMBER OF REFLECTIONS TO PROCESS USING INFORMATION FROM THE LAST PRECEDING =SCALE= CARD
22-24 VALUE OF H FOR LAST REFLECTION TO BE PROCESSED USING INFORMATION FROM LAST PRECEEDING =SCALE= CARD
25-27 VALUE OF K FOR LAST REFLECTION
28-30 VALUE OF L FOR LAST REFLECTION

NOTE - THERE ARE TWO WAYS TO TERMINATE USE OF INFORMATION FROM THE PRECEDING =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 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 REFLECTION 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 FLOATING OR FIXED FUNCTION OF INTENSITY
FW OR IW FOR FLOATING OR FIXED WEIGHT OR STANDARD DEVIATION OF THE INTENSITY
FD OR ID FOR FLOATING OR FIXED LESS-THAN INDICATOR
FI OR II FOR FLOATING 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.

ENDOBS - SIGNALS THAT FOLLOWING REFLECTIONS ARE SYSTEMATICALLY ABSENT.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 ENDOBS
7-72 BLANK

HKL - STANDARD X-RAY SYSTEM REFLECTION INPUT OR REFLECTION EDITING CARD.
FORMAT (A2,A4,1X,A4,A2,6I3,2F9.0,F5.0,F4.4,F4.3,I2,F5.4,I3)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3 HKL
4-7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-16 H
17-19 K
20-22 L
23-25 FUNCTION OF CARD SIGNAL

(0 OR BLANK)/(1)/(2)/(3) FOR (CAUSES THE HKL CARD TO BE A REFLECTION INPUT CARD . ALSO USED FOR AN A-PRIORI START WHEN NO BINARY FILE EXISTS.)/(SIGNALS THAT THE BINARY DATA FILE IS TO BE PROCESSED DOWN TO THE REFLECTION SPECIFIED IN THE HKL CARD AND THEN ALL VALUES ON THE CARD ARE TO REPLACE THE VALUES ON THE FILE.)/(PROCESS DOWN TO SPECIFIED HKL IN DATA FILE AND DELETE THE REFLECTION FROM THE BINARY FILE.)/(COPY THE BINARY DATA FILE DOWN TO AND INCLUDING THE DESIGNATED H, K, AND L. THIS IS A POSITIONING FUNCTION.

26-28 REFLECTION TYPE
(1)/(2)/(3)/(4)/(5) FOR (OBSERVED)/(LESS-THAN)/(EXTINCT)/(TO BE IGNORED)/(SYSTEMATICALLY EXTINCT)

29-31 DATA GROUP FOR SCALING PURPOSES

32-40 REFLECTION INTENSITY

40-48 BACKGROUND INTENSITY

49-52 STANDARD DEV IN INTENSITY
(MAY ALSO BE WEIGHT IF SIGNALED IN SCALE CARD)

52-55 PHASE IN CYCLES IF KNOWN

55-58 NORMALIZED STRUCTURE FACTOR

59-60 EPSILON, THE E WEIGHT

61-65 ABSORPTION CORRECTION

66-68 NUMBER OF TIMES INTENSITY WAS INDEPENDENTLY OBSERVED

NOTE.... IN EVERY CASE ONCE AN HKL CARD FUNCTION IS FULFILLED CONTROL RETURNS TO THE CARD INPUT STREAM. AN END CARD CAUSES THE BINARY FILE TO BE DRAINED OF REFLECTION DATA WHENEVER ANY EDITING IS BEING DONE.

IF AT ANY TIME DURING EDITING THE BINARY FILE IS EXHAUSTED A FAULT IS IS SIGNALED AND THE WHOLE RUN ABORTED AT THAT POINT.

THE ORDER OF H, K, AND L ON THE INPUT EDITING CARDS MUST BE EXACTLY THE SAME AS THOSE IN THE BINARY DATA FILE.
IF THEY ARE NOT IN THE SAME ORDER A FAULT WILL OCCUR.

END - END CARD.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3 END
4-72 BLANK

A. CARD ORDER SUMMARY FOR =DIAGLS= PROGRAM

DIAGLS	CALLING CARD FOR DIAGONAL LEAST-SQUARES
*SCALE	SCALE CARD FOR F RELATIVE DATA
*ATOM	ATOM SELECTION CARD
*REF	TURN ON REFINEMENT OF SPECIFIED PARAMETERS
*NOREF	SHUT OFF REFINEMENT OF SPECIFIED PARAMETERS
*DAMP	SPECIAL DAMPING LIMITS FOR SHIFTS
END	END CARD

* THESE CARDS ARE OPTIONAL.

NOTE 1 - THIS PROGRAM DOES NOT TREAT THE OVERALL TEMPERATURE FACTOR.

NOTE 2 - IF NO ATOM CARDS ARE PRESENT ALL THE ATOMS IN THE BINARY FILE ARE USED. IF ANY ATOMS ARE SPECIFIED BY CARDS ONLY THOSE SPECIFIED ON THE CARDS ARE SELECTED FROM THE BINARY FILE. IF THERE ARE TOO MANY ATOMS IN THE FILE FOR THE STORAGE CAPACITY, CARDS WILL BE EXPECTED.

NOTE 3 - IF ALL REFINEMENT RESTRICTION CARDS ARE LEFT OUT REFINEMENT WILL BE ON ALL POSITIONAL AND TEMPERATURE PARAMETERS. HOWEVER, NO SCATTERING FACTORS OR POPULATION FACTORS WILL BE SET TO REFINE.

***** READS =NFILEA= AND WRITES =NFILEB= *****

IF THE PROGRAM IS SET TO PUNCH CARDS (COLS 32-34 OF =DIAGLS= CARD) THE PROGRAM WRITES THESE IMAGES ON =NFILEC=, THE PUNCH FILE.

B. CARD FORMATS FOR =DIAGLS= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DIAGLS - CALLING CARD FOR DIAGONAL LEAST-SQUARES PROGRAM.
FORMAT (A2,A4,1X,A4,A2,11I3,3F4.3,I3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DIAGLS
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-16	NUMBER OF CYCLES TO BE CALC. (NC)
17-19	(1)/(2)/(3) FOR (ISOTROPIC)/(ANISOTROPIC)/(MIXED) PROGRAM CONVERTS IF REQUIRED. AVERAGE DIAGONAL ELEMENT USED IN ANISOTROPIC CONVERSION. NO CONVERSION MADE UNLESS SPECIFIED BY A =REF= CARD IN MIXED MODE. (ITF)
20-22	(BLANK)/(1) FOR REFINEMENT BASED ON (F)/(F**2) (IFSQ)
23-25	(BLANK)/(1) FOR USE (SCALE)/(RESCALE) FACTORS FROM TAPE (IRESC)
26-28	(BLANK)/(1) FOR (DO)/(DO NOT) HALT IF CONVENTIONAL R INCREASES BY 0.1 IN ANY CYCLE.
29-31	(BLANK)/(1) FOR (WEIGHTS FROM TAPE)/(ALL WEIGHTS EQUAL 1.0) (IW)
32-34	(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	(BLANK)/(1) FOR (DO NOT)/(DO) LIST THE REFLECT. INFO. DURING LAST CYCLE (ILIST)
38-40	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	(BLANK)/(1)/(2) FOR (NO)/(USE)/(USE PREVIOUS FC) FIXED ATOM CONTRIB. (IP)
44-46	(BLANK)/(1) FOR (X-RAY)/(NEUTRON) (INEU)
47-50	DAMPING OR ENHANCING FACTOR FOR PARAMETER SHIFTS (BLANK OR 0.0 = 1.0)
51-54	RR TO CONTROL LIST (BLANK = 2.0)
55-58	REJECT FROM CONSIDERATION IN SHIFTS REFLECTIONS WHOSE WEIGHTED DELTA-F IS LARGER. (BLANK = 10**8)
59-61	(BLANK)/(1) (NO)/(SPECIAL) SYMMETRY PATCH REQUIRED.
62-72	BLANK

SCALE - SCALE CARD FOR F RELATIVE DATA.
FORMAT (A2,A4,F10.4,I4,F10.4,I2,3F10.4)

```
  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   SCALE
  6     BLANK
  7-16  SCALE FACTOR TO APPLY TO F REL.
  17-20 GROUP IDENTIFICATION (1-64)
  21-72 BLANK

ATOM   - ATOM SELECTION CARD.
     FORMAT (A2,A4,1X,A4,A2)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   ATOM
  5-7   BLANK
  8-11  SCATTERING FACTOR TYPE (EXACTLY AS ON FORMFX CARDS)
  12-13 ATOM IDENTITY FOR GIVEN SCATTERING FACTOR TYPE
  14-72 BLANK

REF OR NOREF - SET PARAMETER REFINEMENT IF IT IS TO BE DIFFERENT THAN THAT
         ALREADY SET IN THE DATA FILE.
     FORMAT (A2,A4,1X,A4,A2,13A3)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   REF OR NOREF
  6-7   BLANK
  8-11  SCATTERING FACTOR TYPE (EXACTLY AS SHOWN IN FORMFX CARDS).
  12-13 ATOM IDENTITY FOR THIS SCATTERING FACTOR TYPE.
        (NOTE.... IF 12-13 IS BLANK CARDS APPLY TO ALL ATOMS OF NAMED TYPE.
        IF 8-11 IS BLANK CARD APPLIES TO ALL ATOMS.)
        (IF =SCALE= IS PUNCHED IN 8-12 THEN COMMAND APPLIES TO F-RELATIVE SCALE
        FACTOR REFINEMENT)
  14-16 EACH FIELD MAY CONTAIN BLANKS OR ONE OF THE FOLLOWING LEFT JUSTIFIED
        SYMBOLS.  X, Y, Z, B, B11, B22, B33, B12, B13, B23, M, S, D (M IS THE
        POPULATION PARAMETER, S THE NEUTRON SCATTERING FACTOR AND D THE
        DISPERSION CORRECTION)  IF ALL FIELDS ARE LEFT BLANK ALL QUANTITIES
        ARE ACTED UPON.  IF ANY FIELD IS PUNCHED ONLY THE PARAMETERS NAMED ARE
        ACTED UPON.
  17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43, 44-46, 47-49,
  50-52 (SYMBOL FROM ABOVE LIST)
  53-72 BLANK

DAMP   - DAMP PARAMETER SHIFTS ABOVE A GIVEN LEVEL.
     FORMAT (A2,A4,1X,13F5.3)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   DAMP
  5-7   BLANK
  8-12  MAXIMUM X SHIFT IN ANGSTROM UNITS
  13-17 MAXIMUM Y SHIFT IN ANGSTROM UNITS
  18-22 MAXIMUM Z SHIFT IN ANGSTROM UNITS
  23-27 MAXIMUM B SHIFT IN UNITS OF B
  28-32 MAXIMUM B11 SHIFT IN UNITS OF B
  33-37 MAXIMUM B22 SHIFT IN UNITS OF B
  38-42 MAXIMUM B33 SHIFT IN UNITS OF B
```

```
43-47 MAXIMUM B12 SHIFT IN UNITS OF B
48-52 MAXIMUM B13 SHIFT IN UNITS OF B
53-57 MAXIMUM B23 SHIFT IN UNITS OF B
58-62 POPULATION PARAMETER SHIFT
63-67 F-RELATIVE SCALE FACTOR SHIFT
68-72 NEUTRON SCATTERING FACTOR SHIFT

END     - END CARD.
    FORMAT (A2,A4)

COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3   END
4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =DIFOPP= PROGRAM

FOR FUNCTIONS OF THESE CARDS SEE SECTION B --- CARD FORMATS FOR =DIFOPP=

```
  DIFOPP
  CELL
  ORIENT
* ANGMX
* BAKSET/EQNCON
* BALFLT/FILTER
 (SCAN AND SRCTAB)/(PEAK AND PTITAB)
* TEST
  REFLEC
*$ SCALE
*$ TLRNCE
 $(RDCARD AND DIFFRACTOMETER DATA CARDS AND BREAK) AND/OR (RDTAPE WITH
 $    DIFFRACTOMETER DATA ON NFILEE)
  END
```

* CARDS ON ANY LINE MARKED WITH AN ASTERISK MAY BE OMITTED.

( ) CARDS ENCLOSED IN PARENTHESES MUST BE TREATED AS A GROUP.

A/B MEANS CARD A OR CARD B.

$ CARDS ON LINES MARKED WITH A DOLLAR SIGN MAY BE REPEATED AS A GROUP

AS MANY TIMES AS DESIRED AS, FOR EXAMPLE, IN READING MULTIPLE FILES FROM NFILEE OR IN READING SEVERAL BATCHES OF CARDS WITH DIFFERENT SCALE FACTORS AND/OR TOLERANCES.

****READS	NTIN	CARD INPUT
****READS	NFILEE	DIFFRACTOMETER OUTPUT ON MAGNETIC TAPE (OPTIONAL)
****WRITES	NTOUT	PRINTER OUTPUT
****WRITES	NFILEB	INPUT TO DATA REDUCTION
****WRITES	NFILEA	SETTINGS FOR REFLECTIONS THAT ARE TO BE REMEASURED

B. CARD FORMATS FOR =DIFOPP= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DIFOPP - CALLING CARD FOR AUTOMATIC DIFFRACTOMETER OUTPUT PROCESSOR.
FORMAT (A2,A4,1X,A4,A2,7X,2F10.6,F10.0)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DIFOPP
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE.
14-20	BLANK
21-30	WAVELENGTH FOR ALPHA(1).
41-50	MAXIMUM NUMBER OF SCALER COUNTS WITHOUT EXCEEDING LINEAR RANGE. IF BLANK, 200,000 IS SUPPLIED.

CELL - CELL CONSTANT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	CELL
5-7	BLANK
8-13	SIX COLUMNS OF HOLLERITH PUNCHING OR BLANKS TO IDENTIFY COMPOUND. THIS IDENTIFICATION IS CHECKED BY VARIOUS PROGRAMS FOR CONSTANCY, SO CHOOSE CAREFULLY AND REMEMBER YOUR CHOICE.
14-21	A CELL DIMENSION
22-29	B CELL DIMENSION
30-37	C CELL DIMENSION
38-46	COS ALPHA OR ALPHA
47-55	COS BETA OR BETA
56-64	COS GAMMA OR GAMMA
65-71	BLANK

NOTE... MUST BE DIRECT CELL DIMENSIONS.

ORIENT - CRYSTAL ORIENTATION CARD.
FORMAT (A2,A4,1X,A4,A2,2X,7F8.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	ORIENT
7	BLANK

8-13 COMPOUND IDENTIFICATION CODE.
14-15 BLANK
16-23 H INDEX (MAY BE FRACTIONAL) OF THE RECIPROCAL LATTICE VECTOR LYING ALONG THE POSITIVE DIRECTION OF THE PHI AXIS.
24-31 K INDEX AS ABOVE.
32-39 L INDEX AS ABOVE.
40-47 H INDEX (MAY BE FRACTIONAL) OF A RECIPROCAL LATTICE VECTOR LYING IN THE PHI = 0 DEGREES PLANE (THIS PLANE CONTAINS THE PHI AXIS).
48-55 K INDEX AS ABOVE.
56-63 L INDEX AS ABOVE.
64-71 CORRECTION TO BE APPLIED TO ALL CALCULATED PHI'S TO OBTAIN TRUE PHI'S. THIS CORRECTION IS THE ANGLE (OF + OR - PHI) BETWEEN THE PLANE SPECIFIED ABOVE AND THE PHI = 0 PLANE.

ANGMX - TWO THETA SETTING LIMITS.
FORMAT (A2,A4,54X,F10.6)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 ANGMX
6-60 BLANK
61-70 UPPER LIMIT FOR TWO THETA.

IF NO 'ANGMX' CARD IS SUPPLIED, THE UPPER LIMIT FOR TWO THETA IS 165 DEGREES.

BAKSET - CONSTANT INCREMENT FOR CALCULATING START AND STOP ANGLES FOR TWO-THETA SCAN.
FORMAT (A2,A4,9X,F5.2)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 BAKSET
7-15 BLANK
16-20 BACK-SETTING ANGLE IN DEGREES.

EQNCON - CONSTANTS A AND B FOR CALCULATING BACKSET TABLE FROM THE EQUATION
TABLE(I) = ACON/2. + (BCON/2.)*(SINF(THETA)/COSF(THETA))
FORMAT (A2,A4,4X,2F10.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 EQNCON
7-10 BLANK
11-20 ACON.
21-30 BCON.
SUGGESTED VALUES ARE A=1.80 AND B=0.86 FOR COPPER RADIATION OR A=1.80 AND B=1.00 FOR MOLYBDENUM.
31-72 BLANK

NO CARD- IF NEITHER 'BAKSET' OR 'EQNCON' CARD IS SUPPLIED THE BACKSET ANGLE IS TAKEN FROM THE TABLE IN PROGRAM (THE SAME AS IN 'DIFSET'). SCAN RANGE IS FROM TWO THETA(LAMD1) MINUS BACKSET TO TWO THETA(LAMD2) PLUS BACKSET.

BALFLT - CAUSES BRANCHING TO PART OF PROGRAM FOR PROCESSING DATA OBTAINED BY THE BALANCED FILTER METHOD, AND SUPPLIES A NUMERICAL CONSTANT, XFIL2. SCALER READINGS OBTAINED WITH FILTER 2 (ALPHA-ABSORBING FILTER) ARE

MULTIPLIED BY THIS CONSTANT BEFORE SUBTRACTING FROM READINGS OBTAINED WITH FILTER 1.
FORMAT (A2,A4,4X,F10.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 BALFLT
7-10 BLANK
11-20 XFIL.

FILTER - ATTENUATION FILTER FACTORS (= COUNTS WITHOUT FILTER / COUNTS WITH FILTER)
FORMAT (A2,A4,1X,I5,6F10.2)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 FILTER
7 BLANK
8-12 NUMFFC, THE NUMBER OF FILTER FACTORS TO BE PUNCHED (MAXIMUM OF SIX).
13-22 FILTER FACTOR FOR FILTER CODE 0.
23-32 FILTER FACTOR FOR FILTER CODE 1.
33-42 FILTER FACTOR FOR FILTER CODE 2.
43-52 FILTER FACTOR FOR FILTER CODE 3.
53-62 FILTER FACTOR FOR FILTER CODE 4.
63-72 FILTER FACTOR FOR FILTER CODE 5.

NO CARD- IF NEITHER 'BALFLT' OR 'FILTER' CARD IS SUPPLIED, DIFFRACTOMETER DATA WILL BE TREATED AS HAVING BEEN OBTAINED BY THE SINGLE FILTER METHOD. FILTER CODE DIGITS OTHER THAN ZERO IN SCALER WORD WILL CAUSE PRINT OUT OF ERROR MESSAGE, BUT DATA WILL BE PROCESSED USING A FILTER FACTOR OF 1. IF NUMBER OF ERROR MESSAGES EXCEEDS 50, EXIT WILL BE CALLED.

SCAN - CAUSES BRANCHING TO PART OF PROGRAM FOR PROCESSING DATA OBTAINED BY THE TWO THETA SCAN METHOD, SUPPLIES TIME(SECONDS) SPENT IN COUNTING EACH BACKGROUND, AND SUPPLIES TABLE OF SCANNING SPEEDS CORRESPONDING TO SPEED CODE DIGIT OF TWO THETA WORD. IF COLS. 13-60 ARE BLANK, INTERNAL TABLE WILL BE USED. VALUES FOR SPEEDS 1-6 ARE .25, .50, 1, 2, 4, AND 0 DEGREES PER MINUTE, RESPECTIVELY. IF ANY VALUE IS TO BE READ IN, SPEED(1) MUST BE DIFFERENT FROM ZERO AND ALL SPEEDS MUST BE PUNCHED.
FORMAT (A2,A4,1X,F5.0,6F8.3)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4 SCAN
5-7 BLANK
8-12 TIME (SECONDS), EACH BACKGROUND.
13-20 SPEED(1) IN DEGREES PER MINUTE.
21-28 SPEED(2) IN DEGREES PER MINUTE.
29-36 SPEED(3) IN DEGREES PER MINUTE.
37-44 SPEED(4) IN DEGREES PER MINUTE.
45-52 SPEED(5) IN DEGREES PER MINUTE.
53-60 SPEED(6) IN DEGREES PER MINUTE.

SRCTAB - SUPPLIES A CORRECTION FOR THE COUNTS LOST BY USING A LIMITED SCAN RANGE (ALEXANDER AND SMITH, 1962). A MAXIMUM OF EIGHT OF THESE CARDS

MAY BE USED. EACH GIVES THE CORRECTION FACTOR SRC(M,N) AT 0, 10, 20, ... 170 DEGREES TWO THETA FOR THE SCAN RANGE IN COLUMN 8. BECAUSE OF LIMITED SPACE, SRC(M,N)-1. IS PUNCHED, AND 1. IS ADDED IN THE PROGRAM. PROGRAM DOES A TWO WAY INTERPOLATION FOR SCAN RANGE AND TWO THETA ANGLE.

FORMAT (A2,A4,1X,I1,18F4.4)

```
COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6   SRCTAB
7     BLANK
8     TOTAL SCAN RANGE, DEGREES (INTEGER 1-8).
9-12  SRC(M,N)-1. AT  0 DEGREES TWO THETA.
13-16 SRC(M,N)-1. AT 10 DEGREES TWO THETA.
 ---
77-80 SRC(M,N)-1. AT 170 DEGREES TWO THETA.
```

IF THE DECIMAL POINT IS NOT PUNCHED, IT WILL BE ASSUMED TO BE TO THE LEFT OF THE FOUR DIGITS IN EACH OF THESE FIELDS.

PEAK - (1) THE PRESENCE OF THIS CARD CAUSES BRANCHING TO THE PART OF THE PROGRAM FOR PROCESSING DATA OBTAINED BY THE PEAK HEIGHT METHOD.
(2) IT SUPPLIES THE COUNTING TIME IN SECONDS FOR PEAK AND EACH BACKGROUND.
(3) IT SUPPLIES AN INTEGER, CALLED =JIG= IN PROGRAM, THAT DEPENDS ON THE NUMBER OF BACKGROUND MEASUREMENTS PER REFLECTION AND CAUSES APPROPRIATE BRANCHING.
(4) IT SUPPLIES CONSTANTS FOR EQUATIONS USED TO ESTIMATE BACKGROUND IF INTEGER IN 3 ABOVE SPECIFIES LESS THAN TWO BACKGROUND MEASUREMENTS.

FORMAT (A2,A4,4X,2F5.0,4X,I1,3F10.2)

```
COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4   PEAK
5-10  BLANK
11-15 TIME IN SECONDS FOR PEAK.
16-20 TIME IN SECONDS FOR EACH BACKGROUND.
21-24 BLANK
25    1/2/3/4   INTEGER =JIG=
        1 IF BOTH BACKGROUNDS WERE MEASURED
        2 IF ONLY BACKGROUND(LOW) WAS MEASURED
        3 IF ONLY BACKGROUND(HIGH) WAS MEASURED
        4 IF NEITHER BACKGROUND WAS MEASURED
26-35 XBG
```

IF THE INTEGER IN COL. 25 IS 2 OR 3, THE BACKGROUND THAT WAS MEASURED IS MULTIPLIED BY XBG TO OBTAINED AN ESTIMATED VALUE FOR ONE THAT WAS NOT.

```
36-45 BKGRND
46-55 XPK
```

IF THE INTEGER IN COL. 25 IS 4, THE CONSTANTS BKGRND AND XPK ARE USED IN THE EXPRESSION-

```
          XXI=XPK*(SC12-BKGRND)                SINGLE FILTER CASE
     OR   XXI=XPK*(SC12-XFIL2*SC22-BKGRND)     BALANCED FILTER CASE
```

TO ESTIMATE NET COUNTS (XXI) FROM THE NUMBER OF COUNTS (SC12 OR SC12 AND SC22)

AT THE PEAK POSITION. XFIL2 IS A CONSTANT SUPPLIED ON =BALFLT= CARD.

PTITAB - TABLE OF CORRECTION FACTORS FOR CONVERTING PEAK HEIGHT INTENSITIES TO INTEGRATED INTENSITIES (ALEXANDER AND SMITH, 1962). VALUES TABULATED ARE PTI(M)=(I(INTEGRATED)/I(PEAK))-1. AT 0, 10, 20, ... 170 DEGREES TWO THETA.
FORMAT (A2,A4,2X,18F4.4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	PTITAB
7-8	BLANK
9-12	PTI(1) AT 0 DEGREES TWO THETA.
13-16	PTI(2) AT 10 DEGREES TWO THETA.

77-80	PTI(18) AT 170 DEGREES TWO THETA.

IF THE DECIMAL POINT IS NOT PUNCHED, IT WILL BE ASSUMED TO BE TO THE LEFT OF THE FOUR DIGITS IN EACH OF THESE FIELDS.

TEST - CRITERIA FOR SELECTION OF REFLECTIONS TO BE TREATED AS UNOBSERVABLE, AND FOR ASSIGNING AN INTENSITY TO THESE. REFLECTIONS WILL BE TAGGED AS UNOBSERVABLE (LESTH=2) IF THE NET NUMBER OF COUNTS IS LESS THAN OR EQUAL TO A TEST QUANTITY DEFINED AS XXIMIN, OR XSIG*STANDARD DEVIATION OF NET COUNTS, WHICHEVER IS LARGER. THE NUMBER OF NET COUNTS FOR THESE REFLECTIONS WILL BE SET EQUAL TO XTEST*TEST QUANTITY.
FORMAT (A2,A4,4X,3F10.2)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	TEST
5-10	BLANK
11-20	XXIMIN
31-40	XTEST

NO CARD - IF NO 'TEST' CARD IS INCLUDED, REFLECTIONS FOR WHICH THE NET NUMBER OF COUNTS IS LESS THAN OR EQUAL TO 2.*SIGMA (NET COUNTS) WILL BE TAGGED AS UNOBSERVABLE (LESTH=2) AND WILL BE ASSIGNED THE VALUE NET COUNTS = SIGMA (NET COUNTS)

REFLEC - THIS CARD CAUSES THE PROGRAM TO CHECK INPUT DATA FOR COMPLETENESS, PRINT OUT INITIAL REMARKS, AND PREPARE TO PROCESS REFLECTION DATA (DIFFRACTOMETER OUTPUT).
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	REFLEC
7-80	BLANK

SCALE - CAUSES THE INTENSITY DATA THAT FOLLOW TO BE MULTIPLIED BY THE FACTOR IN COLS. 14-23
FORMAT (A2,A4,7X,F10.4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	SCALE

6-13 BLANK
14-23 SCALE FACTOR.

IF NO 'SCALE' CARD IS INCLUDED A SCALE FACTOR OF 1. IS USED.

TLRNCE - TOLERANCES.

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
FORMAT (A2,A4,4X,3F10.2)
1-6 TLRNCE
7-10 BLANK
11-20 CHI TOLERANCE, + OR -, IN DEGREES.
21-30 PHI TOLERANCE, + OR -, IN DEGREES.
31-40 TWO THETA TOLERANCE, + OR -, IN DEG.

IF NO 'TLRNCE' CARD IS SUPPLIED, THE TOLERANCES ON PHI, CHI AND TWO THETA ARE + OR - .05 DEGREES. AS MANY 'SCALE' AND 'TLRNCE' CARDS AS DESIRED MAY BE USED AFTER THE 'REFLEC' CARD AND BEFORE THE 'END' CARD.

RDCARD - CAUSES TRANSFER TO SUBROUTINE THAT READS DIFFRACTOMETER OUTPUT FROM CARDS.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 RDCARD

- DIFFRACTOMETER OUTPUT DATA CARDS (NO IDENTIFICATION FIELD).
FORMAT (80A1)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-80 OUTPUT DATA IN TEN-CHARACTER WORDS EACH BEGINNING WITH A BEGIN WORD CODE. SEE ITAB IN XRY323 FOR LEGAL BEGIN WORD CODES.

BREAK - CAUSES TRANSFER BACK TO THE PART OF PROGRAM THAT READS 'TLRNCE', 'SCALE' AND 'END' CARDS. ONE OF THESE MUST COME AT END OF DIFFRACTOMETER OUTPUT CARD DECK.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 BREAK

RDTAPE - CAUSES TRANSFER TO SUBROUTINE THAT READS DIFFRACTOMETER DATA FROM MAGNETIC TAPE PREPARED BY DIGI-DATA PAPER TAPE TO MAG TAPE CONVERTER.
FORMAT (A2,A4,4X,3I4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 RDTAPE
7-10 BLANK
11-14 H INDEX
15-18 K INDEX
19-22 L INDEX
(WHEN THE HKL WORD FOR THIS REFLECTION IS READ FROM THE MAGNETIC TAPE (NTAPEE), CONTROL IS RETURNED TO SUBROUTINE XRY321 SO THAT ANY OF THE FOLLOWING CARDS MAY BE READ --- TLRNCE, SCALE, RDTAPE,

RDCARD, END. IF THE DESIGNATED HKL IS NOT READ, THE END-OF-FILE MARK ON NTAPEE WILL CAUSE THE RETURN.

END - END CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	END
4-72	BLANK

C. OUTPUT FORMATS FOR =DIFOPP= PROGRAM

NTAPEB - INPUT TO DATA REDUCTION.
FORMAT (7X,A2,A4,I2,3I4,F10.2,F10.4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-15	LESS-THAN INDICATOR 1/2 FOR OBSERVABLE/UNOBSERVABLE
16-19	H INDEX
20-23	K INDEX
24-27	L INDEX
28-37	F (OBSERVED)
38-47	STANDARD DEVIATION OF F (OBSERVED)

LAST RECORD ONLY

1-9 'TAPES N'
WHERE N IS THE LOGICAL NUMBER OF NTIN AS DEFINED IN NUSY (NUC006).
WHEN NFILEB IS READ BY DATA REDUCTION THIS RECORD CAUSES SUBSEQUENT READING TO BE FROM THE NORMAL CARD INPUT UNIT, NTIN.

NTAPEA - SETTING CARDS FOR REFLECTIONS THAT ARE TO BE RE-MEASURED.
FORMAT (A2,A4,3I4,5F9.2)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	COMPOUND IDENTIFICATION CODE
7-10	H INDEX
11-14	K INDEX
15-18	L INDEX
19-27	CHI SETTING
28-36	PHI SETTING
37-45	TWO THETA SETTING FOR BACKGROUND (LOW)
46-54	TWO THETA SETTING FOR PEAK
55-63	TWO THETA SETTING FOR BACKGROUND (HIGH)
64-72	TIME (SECONDS) FOR TWO THETA SCAN

A. CARD ORDER SUMMARY FOR =DIFSET= PROGRAM

DIFSET CALLS PROGRAM. GIVES COMPOUND IDENTIFICATION, WAVELENGTH, SCANNING SPEED, AND OPTIONS TO SUPPRESS PUNCHING OF SETTING CARDS.

CELL OR PARAMC - FURNISHES CELL CONSTANTS.

ORIENT ORIENTATION.

*ANGMX LIMITS OF PHI, CHI, AND TWO-THETA RANGES.

*INDEX LIMITS OF H, K, AND L INDICES.

*BAKSET OR *EQNCON - METHOD OF COMPUTING SCAN RANGE.

*SYSABS SYSTEMATIC ABSENCES.

PREP CAUSES PROGRAM TO CHECK INPUT, PRINT SPECIFICATIONS, AND PREPARE TO COMPUTE SETTINGS.

* (OPTIONAL AUTOMATIC DIFFRACTOMER CONTROL DECK - SEE BELOW)

*HKL INDICES OF REFLECTION TO BE ADDED TO OUTPUT.

*------ (SETTING CARD - COMPOUND IDENTIFICATION IN COLS 1 - 6) SETTINGS OF REFLECTION TO BE ADDED TO OUTPUT.

*GENHKL CAUSES GENERATION OF MILLER INDICES.

END CAUSES END-OF-FILE AND REWIND OF ANY TAPES USED AND PRINTING OF NUMBER OF REFLECTIONS PROCESSED.

* THESE CARDS ARE OPTIONAL

AUTOMATIC DIFFRACTOMETER CONTROL DECK

INSERT AS INDICATED ABOVE IF CONTROL TAPE OR CARD DECK IS REQUIRED

XRUC TYPE OF DIFFRACTOMETER, OUTPUT REQUIRED, SCANNING SPEED, NUMBER OF CHARACTERS PER OUTPUT RECORD.

XRUFMT FORMAT OF DIFFRACTOMETER COMMAND WORDS FOR DATA.

TTYFMT FORMAT OF TELETYPE OUTPUT FOR DATA (NBS ONLY).

$STDREF DESIGNATES THE REFLECTION ON THE NEXT HKL OR 'SETTING CARD' AS A STANDARD REFLECTION, GIVES ITS IDENTIFICATION NUMBER, AND SPECIFIES HOW OFTEN IT IS TO BE INSERTED IN OUTPUT.

$XRDFMT FORMAT FOR DIFFRACTOMETER COMMAND WORDS FOR STANDARD REFLECTION.

$TTYFMT FORMAT FOR TELETYPE OUTPUT FOR STANDARD REFLECTION (NBS ONLY).

$HKL OR 'SETTING CARD' - DEFINES THE STANDARD REFLECTION.

$ THESE CARDS ARE OPTIONAL AS A GROUP WITHIN THE OPTIONAL CONTROL DECK. THE WHOLE GROUP IS REPEATED FOR EACH STANDARD REFLECTION. STANDARD REFLECTIONS MUST BE NUMBERED SEQUENTIALLY 2 - 10. THE CARDS 'STDREF', 'XRDFMT', AND 'TTYFMT' MUST BEAR THE SEQUENCE NUMBER FOR THE STANDARD DEFINED BY THE 'HKL' OR 'SETTING CARD' FOR EACH STANDARD REFLECTION.

****READS	NTIN	CARD READER
****WRITES	NTOUT	PRINTER
****WRITES	NFILEH	SETTING CARDS (OPTIONAL)
****WRITES	NFILEC	DIFFRACTOMETER CONTROL CARD DECK (OPTIONAL)
****WRITES	NFILEI	MAGNETIC TAPE FOR PUNCHING DIFFRACTOMETER CONTROL TAPE (OPTIONAL)

B. CARD FORMATS FOR =DIFSET= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DIFSET - CALLING CARD FOR DIFFRACTOMETER SETTING PROGRAM.
FORMAT (A2,A4,1X,A4,A2,7X,3F10.6,2I10)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DIFSET
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE.
14-20	BLANK
21-30	WAVELENGTH FOR ALPHA(1). 1.54051 ANGSTROMS USED IF BLANK.
31-40	WAVELENGTH FOR ALPHA(2). 1.54433 ANGSTROMS USED IF BLANK. NOTE - IF ALPHA(1) IS SUPPLIED BUT ALPHA(2) IS BLANK, THE ALPHA(1) WAVELENGTH GIVEN WILL ALSO BE USED FOR ALPHA(2).
41-50	TWO THETA SCAN RATE IN DEGREES PER MINUTE.
51-60	(BLANK)/(1) FOR (DO)/(DO NOT) PUNCH SETTING CARDS. IF BLANK, CARD IMAGES WILL BE WRITTEN ON NTAPEH.
61-70	(BLANK)/(1) FOR (DO)/(DO NOT) PUNCH SETTINGS CARDS FOR THOSE REFLECTIONS WHICH ARE SYSTEMATICALLY ABSENT. THIS FIELD HAS NO EFFECT UNLESS COLUMNS 51-60 ARE BLANK.
71-72	BLANK

CELL - CELL CONSTANT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	CELL
5-7	BLANK
8-13	SIX COLUMNS OF HOLLERITH PUNCHING OR BLANKS TO IDENTIFY COMPOUND. THIS IDENTIFICATION IS CHECKED BY VARIOUS PROGRAMS FOR CONSISTANCY, SO CHOOSE CAREFULLY AND REMEMBER YOUR CHOICE.
14-21	A CELL DIMENSION
22-29	B CELL DIMENSION
30-37	C CELL DIMENSION
38-46	COS ALPHA ..... ALPHA
47-55	COS BETA . OR . BETA
56-64	COS GAMMA ..... GAMMA
65-71	BLANK

PARAMC - CELL CONSTANTS CALCULATED BY A PREVIOUS =PARAM=.

FORMAT (A2,A4,72X)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 PARAMC
7-72 BLANK

ORIENT - CRYSTAL ORIENTATION CARD.
FORMAT (A2,A4,1X,A4,A2,2X,7F8.3)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 ORIENT
7 BLANK
8-13 COMPOUND IDENTIFICATION CODE.
14-15 BLANK
16-23 H INDEX (MAY BE FRACTIONAL) OF THE RECIPROCAL LATTICE VECTOR LYING ALONG THE POSITIVE DIRECTION OF THE PHI AXIS.
24-31 K INDEX AS ABOVE.
32-39 L INDEX AS ABOVE.
40-47 H INDEX (MAY BE FRACTIONAL) OF A RECIPROCAL LATTICE VECTOR LYING IN THE PHI = 0 DEGREES PLANE (THIS PLANE CONTAINS THE PHI AXIS).
48-55 K INDEX AS ABOVE.
56-63 L INDEX AS ABOVE.
64-71 CORRECTION TO BE APPLIED TO ALL CALCULATED PHI'S TO OBTAIN TRUE PHI'S. THIS CORRECTION IS THE ANGLE (OF + OR - PHI) BETWEEN THE PLANE SPECIFIED ABOVE AND THE PHI = 0 PLANE.

ANGMX - DIFFRACTOMETER AND GONIOSTAT ANGLE LIMITS.
FORMAT (A2,A4,4X,6F10.6)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 ANGMX
6-10 BLANK
11-20 LOWER LIMIT FOR PHI.
21-30 UPPER LIMIT FOR PHI.
31-40 LOWER LIMIT FOR CHI.
41-50 UPPER LIMIT FOR CHI.
51-60 LOWER LIMIT FOR TWO THETA.
61-70 UPPER LIMIT FOR TWO THETA.
71-72 BLANK

INDEX - INDEX GENERATION LIMITS.
FORMAT (A2,A4,4X,6(1X,I4))

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 INDEX
6-11 BLANK
12-15 LOWER LIMIT FOR H INDEX.
16-20 UPPER LIMIT FOR H INDEX.
21-25 LOWER LIMIT FOR K INDEX.
26-30 UPPER LIMIT FOR K INDEX.
31-35 LOWER LIMIT FOR L INDEX.
36-40 UPPER LIMIT FOR L INDEX.
41-72 BLANK

BAKSET - CONSTANT INCREMENT FOR CALCULATING TWO-THETA SETTINGS FOR BACKGROUND READINGS OR FOR BEGINNING AND END OF SCAN RANGE.
FORMAT (A2,A4,9X,F5.2)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 BAKSET
7-15 BLANK
16-20 INCREMENT IN DEGREES.
21-72 BLANK

EQNCON - CONSTANTS FOR EQUATION USED IN CALCULATING TWO-THETA SETTINGS FOR BACKGROUND READINGS OR FOR BEGINNING AND END OF SCAN RANGE.
FORMAT (A2,A4,4X,2F10.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 EQNCON
7-10 BLANK
11-20 A IN DEGREES.
21-30 B IN DEGREES.
SUGGESTED VALUES ARE A=1.80 AND B=0.86 FOR COPPER RADIATION OR A=1.80 AND B=1.00 FOR MOLYBDENUM.
31-72 BLANK

SYSABS - SYSTEMATIC ABSENCES CARD.
FORMAT (A2,A4,1X,A4,A2,7X,23I1)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 SYSABS
7 BLANK
8-13 COMPOUND IDENTIFICATION CODE.
14-20 BLANK
21-43 VALUE OF 'X' FOR APPLICATION OF SYSTEMATIC ABSENCES TEST. ONLY THOSE COLUMNS CORRESPONDING TO TESTS TO BE APPLIED SHOULD BE NON-ZERO.
21 HKL ABSENT IF H+K=XN+1
22 HKL ABSENT IF H+L=XN+1
23 HKL ABSENT IF K+L=XN+1
24 HKL ABSENT IF ALL H+K, H+L, K+L=XN+1
25 HKL ABSENT IF H+K+L=XN+1
26 HKL ABSENT IF -H+K+L=XN+1
27 HHL ABSENT IF H=XN+1
28 HHL ABSENT IF L=XN+1
29 HHL ABSENT IF H+L=XN+1
30 HHL ABSENT IF 2H+L=XN+1
31 0KL ABSENT IF K=XN+1
32 0KL ABSENT IF L=XN+1

33 0KL ABSENT IF K+L=XN+1
34 H0L ABSENT IF H=XN+1
35 H0L ABSENT IF L=XN+1
36 H0L ABSENT IF H+L=XN+1
37 HK0 ABSENT IF H=XN+1
38 HK0 ABSENT IF K=XN+1

```
39     HK0 ABSENT IF H+K=XN+1
40     HH0 ABSENT IF H=XN+1
41     H00 ABSENT IF H=XN+1
42     0K0 ABSENT IF K=XN+1
43     00L ABSENT IF L=XN+1
```

PREP - CAUSES PROGRAM TO PREPARE TO COMPUTE SETTINGS BY CHECKING INPUT DATA, COMPUTING CONSTANTS AND PRINTING OUT SPECIFICATIONS.

FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	PREP

HKL - MILLER INDICES OF A REFLECTION THAT IS TO BE INSERTED IN THE OUTPUT. THE SETTINGS ARE COMPUTED, THE INDEX AND ANGLE LIMITS ARE CHECKED, AND THE PHI-ANGLE CORRECTION, IF ANY, IS APPLIED.

FORMAT (A2,A4,7X,3I3)

COLS	FUNCTION OF FIELD
1-3	HKL
4-13	BLANK
14-16	H INDEX
17-19	K INDEX
20-22	L INDEX

------ - 'SETTING CARDS'. MILLER INDICES AND SETTING ANGLES FOR A REFLECTION THAT IS TO BE INSERTED IN THE OUTPUT. NO CHECK IS MADE ON THE INDICES AND ANGLES. THESE CARDS MAY BE GENERATED BY THIS PROGRAM FOR SORTING, AND THEN READ BY IT TO CREATE A CONTROL TAPE OR CARD DECK.

FORMAT (A2,A4,3I4,6F9.2,A2,A4)

COLS	FUNCTION OF FIELD
1-6	(COMPOUND IDENTIFICATION CODE). MUST AGREE WITH =DIFSET= CARD COLS. 8-13.
7-10	H INDEX
11-14	K INDEX
15-18	L INDEX
19-27	CHI SETTING
28-36	PHI SETTING
37-45	START TWO-THETA SETTING
46-54	PEAK TWO-THETA SETTING
55-63	STOP TWO-THETA SETTING
64-72	SCANNING TIME
73-78	BLANK OR 'ABSENT'

GENHKL - STARTS GENERATION OF MILLER INDICES AND SPECIFIES ORDER. THE RECIPROCAL AXIS THAT LIES ALONG THE PHI AXIS SHOULD BE INCREMENTED MOST FREQUENTLY SO THAT PHI DOES NOT CHANGE OFTEN.

FORMAT (A2,A4,I4,10X,5I5)

COLS	FUNCTION OF FIELD
1-6	GENHKL
7-10	2 FOR USE SUBROUTINE XRY271

11-20 BLANK
21-25 1/2/3 FOR H/K/L INDEX INCREMENTED MOST FREQUENTLY
26-30 1/2/3 FOR H/K/L INDEX INCREMENTED NEXT
31-35 1/2/3 FOR H/K/L INDEX INCREMENTED LAST
36-40 +1/-1 FOR THE INCREMENT TO BE APPLIED TO THE INDEX SPECIFIED IN COLS. 26-30 WHEN THE INDEX SPECIFIED IN COLS. 31-35 IS POSITIVE OR ZERO. THIS DETERMINES THE DIRECTION IN WHICH PHI SETTINGS WILL PROGRESS.
41-45 =1 IF ALL POSITIVE VALUES OF THE INDEX SPECIFIED IN COLS. 31-35 ARE TO BE SCANNED, FOLLOWED BY ALL NEGATIVE VALUES. PHI WILL PROGRESS IN ONE DIRECTION, THEN JUMP BACK WHEN THIS INDEX IS INCREMENTED.
=0 IF FOR EACH VALUE, N, OF THE INDEX SPECIFIED IN COLS. 31-35 LAYERS FOR BOTH +N AND -N ARE SCANNED BEFORE THE INDEX IS INCREMENTED. IN THIS CASE, PHI SETTING PROGRESS AROUND THE CIRCLE AND START OVER AGAIN WHEN THE INDEX IS INCREMENTED.

END - END CARD.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3 END
4-72 BLANK

THE FOLLOWING CARDS ARE USED ONLY IF AN AUTOMATIC DIFFRACTOMETER CONTROL TAPE OR CARD DECK IS TO BE MADE.

XRDC - SPECIFICATIONS FOR AUTOMATIC DIFFRACTOMETER CONTROL TAPE OR CARD DECK.
FORMAT (A2,A4,1X,7I5)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4 XRDC
5-7 BLANK
8-12 TYPE OF DIFFRACTOMETER
1 FOR DATEX
13-17 TYPE OF INPUT REQUIRED BY DIFFRACTOMETER
1 FOR PAPER TAPE (DATEX)--- OUTPUT ON NTAPEI
2 FOR PAPER TAPE (NBS) --- OUTPUT ON NTAPEI
3 FOR CARDS --- OUTPUT ON NTAPEC

1/2/3/4/5/6 FOR .25/.50/1.0/2.0/4.0/SLEW SPEED IN DEG/MIN. THIS IS USED TO COMPUTE SCAN TIME ONLY. IT IS INDEPENDENT OF ACTUAL SCAN SPEED SELECTED, WHICH IS CONTROLLED BY 'XRDFMT' CARD. IF BLANK, SCAN TIME WILL BE COMPUTED FOR A SPEED OF 1 DEG/MIN. THIS OVER-RIDES SCAN RATE ON 'DIFSET' CARD.
23-27 MAXOUT. THIS IS THE NUMBER OF CHARACTERS THAT MUST BE ACCUMULATED IN THE OUTPUT BUFFER BEFORE OUTPUT OF A DIFFRACTOMETER CONTROL CARD OR A BLOCK OF MAG TAPE WILL OCCUR. IF NECESSARY, CARDS WILL BE FILLED WITH BLANKS TO MAKE 80 COLUMNS AND MAG TAPE RECORDS WILL BE FILLED WITH BLANKS TO MAKE A BLOCK OF 120 CHARACTERS. BLANKS ARE SKIPPED IN PUNCHING PAPER TAPE FROM THE MAG TAPE. MAXOUT MUST NOT EXCEED 80 FOR CARDS, 120 FOR DATEX TAPE OR ABOUT 90 FOR NBS DIFFRACTOMETER TAPE. IF COL 23-27 ARE BLANK MAXOUT=80.

XRDFMT - FORMAT FOR AS MANY AS TWELVE DIFFRACTOMETER COMMAND WORDS.
ONE OF THESE CARDS IS REQUIRED FOR DATA AND ONE FOR EACH STANDARD

REFLECTION.
FORMAT(A2,A4,I2,A1,5X,11(5A1,I1))

```
COLS  FUNCTION OF FIELD
1-6   XRDFMT
7-8   SEQUENCE NUMBER.  =1 FOR DATA REFLECTION,  =2 FOR FIRST STANDARD
      REFLECTION --- =10 FOR NINETH STANDARD REFLECTION.  THIS NUMBER
      MUST AGREE WITH THE SEQUENCE NUMBER ON THE CORRESPONDING =STDREF=
      AND =TTYFMT= CARDS, IF ANY.
9     BEGIN-WORD CODE FOR WORD 1, WHICH MUST BE AN HKL WORD.
10-14 BLANK
15    WORD 2 - BEGIN WORD CODE FOR AXIS COMMAND
16    WORD 2 - MODE CODE
17    WORD 2 - STEP CODE
18    WORD 2 - FILTER CODE
19    WORD 2 - SPEED CODE
20    WORD 2 - DIGIT TO DESIGNATE THE ANGLE TO BE INSERTED AS CHARACTER
      6-10 OF THE COMMAND WORD.  THE OPTIONS ARE=
             1    CHI SETTING
             2    PHI SETTING
             3    START TWO-THETA SETTING
             4    PEAK TWO-THETA SETTING
             5    STOP TWO-THETA SETTING
             6    ZERO  DEGREES
             7    FIVE BLANKS (CARD OUTPUT ONLY)
             8    (CLOSE UP ANGLE FIELD)
      6, 7 , AND 8 ARE NOT ORDINARILY USED.
21-26 WORD 3 - SAME FORMAT AS WORD 2
27-32 WORD 4 - SAME FORMAT AS WORD 2
33-38 WORD 5 - SAME FORMAT AS WORD 2
39-44 WORD 6 - SAME FORMAT AS WORD 2
45-50 WORD 7 - SAME FORMAT AS WORD 2
51-56 WORD 8 - SAME FORMAT AS WORD 2
57-62 WORD 9 - SAME FORMAT AS WORD 2
63-68 WORD 10 - SAME FORMAT AS WORD 2
69-74 WORD 11 - SAME FORMAT AS WORD 2
75-80 WORD 12 - SAME FORMAT AS WORD 2
```

TTYFMT - FORMAT FOR TELETYPE OUTPUT (NBS ONLY). ONE OF THESE IS REQUIRED FOR DATA, AND ONE FOR EACH STANDARD REFLECTION.
FORMAT (A2,A4,I2,2X,I2,1X,I1,11(5X,I1))

```
COLS  FUNCTION OF FIELD
1-6   TTYFMT
7-8   SEQUENCE NUMBER.  COPY FROM CORRESPONDING =XRDFMT= CARD.
9-10  BLANK
11-12 N, THE NUMBER OF SPACES OR ASTERISKS AT BEGINNING OF EACH LINE OF
      OUTPUT AFTER THE FIRST FOR EACH REFLECTION.  THIS PEMITS INDENTING,
      AND MARKING STANDARD REFLECTIONS.  THIS NUMBER SHOULD NOT EXCEED
      ELEVEN.
13    BLANK
14    WORD 1 PREFIX - 0/1/2/3 DESIGNATES THE TELETYPE CONTROL CHARACTERS TO
      BE INSERTED BEFORE THE CORRESPONDING COMMAND WORD.  ALLOW FOR A
      DIFFRACTOMETER OUTPUT WORD WHENEVER THE MODE CODE CALLS FOR ONE.
```

```
            0 - SPACE
            1 - SPACE, CARRIAGE RETURN, LINE FEED
            2 - SPACE, CARRIAGE RETURN, LINE FEED, N SPACES
            3 - SPACE, CARRIAGE RETURN, LINE FEED, N ASTERISKS
15-19 BLANK
20    WORD 2 PREFIX   (SEE WORD 1)
21-25 BLANK
26    WORD 3 PREFIX   (SEE WORD 1)
27-31 BLANK
32    WORD 4 PREFIX   (SEE WORD 1)
33-37 BLANK
38    WORD 5 PREFIX   (SEE WORD 1)
39-43 BLANK
44    WORD 6 PREFIX   (SEE WORD 1)
45-49 BLANK
50    WORD 7 PREFIX   (SEE WORD 1)
51-55 BLANK
56    WORD 8 PREFIX   (SEE WORD 1)
57-61 BLANK
62    WORD 9 PREFIX   (SEE WORD 1)
63-67 BLANK
68    WORD 10 PREFIX   (SEE WORD 1)
69-73 BLANK
74    WORD 11 PREFIX   (SEE WORD 1)
75-79 BLANK
80    WORD 12 PREFIX   (SEE WORD 1)
```

STDREF - DESIGNATES THE REFLECTION ON THE NEXT 'HKL' OR 'SETTING' CARD AS A STANDARD REFLECTION AND SPECIFIES HOW FREQUENTLY IT IS TO BE INSERTED IN THE CONTROL TAPE OR CARD DECK.

FORMAT (A2,A4,I2,2X,3I5)

```
COLS  FUNCTION OF FIELD
 1-6  STDREF
 7-8  SEQUENCE NUMBER, 2/3/4..../10 FOR FIRST/SECOND/THIRD..../NINETH
      STANDARD REFLECTION.  THIS NUMBER MUST AGREE WITH THAT ON CORRES-
      PONDING 'XRDFMT' AND 'TTYFMT' CARDS.
 9-10 BLANK
11-15 MINIMUM NUMBER OF REFLECTIONS BETWEEN MEASUREMENTS ON THIS STANDARD.
      ALL DATA REFLECTIONS PRINTED (EVEN THOSE THAT ARE SYSTEMATICLY ABSENT)
      ARE COUNTED.  STANDARD REFLECTIONS ARE NOT.  AFTER MINIMUM COUNT IS
      EXCEEDED, STANDARD IS INSERTED AFTER MOST-FREQUENTLY-INCREMENTED INDEX
      REACHES ZERO, UNLESS MAXIMUM NUMBER IS REACHED FIRST.
16-20 MAXIMUM NUMBER OF REFLECTIONS BETWEEN MEASUREMENTS ON THIS STANDARD.
21-25 INITIAL COUNT OF REFLECTION.  IF THIS IS THE SAME AS THE MAXIMUM, THE
      STANDARD WILL BE INSERTED AFTER THE FIRST DATA REFLECTION.
```

HKL - MILLER INDICES OF THE STANDARD REFLECTION. THE FORMAT IS THE SAME AS FOR THE 'HKL' CARD DESCRIBED ABOVE.

------ - 'SETTING CARD'. HKL AND SETTINGS FOR THE STANDARD REFLECTION. THE FORMAT IS THE SAME AS FOR 'SETTING CARDS' DESCRIBED ABOVE.

C. OUTPUT FORMATS FOR =DIFSET= PROGRAM

NTAPEH - SETTING CARD.
FORMAT (A2,A4,3I4,6F9.2,A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	COMPOUND IDENTIFICATION CODE
7-10	H INDEX
11-14	K INDEX
15-18	L INDEX
19-27	CHI SETTING
28-36	PHI SETTING
37-45	TWO THETA SETTING FOR BACKGROUND (LOW)
46-54	TWO THETA SETTING FOR PEAK
55-63	TWO THETA SETTING FOR BACKGROUND (HIGH)
64-72	TIME (SECONDS) FOR TWO THETA SCAN
73-78	BLANK OR 'ABSENT'

A. CARD ORDER SUMMARY FOR =DUMCOP= PROGRAM

DUMCOP	PROGRAM CALLING CARD
END	END CARD

****READS NFILEA****

****OPTIONAL WRITES NFILEB AND/OR NFILEC (THE CARD PUNCH FILE)****

B. CARD FORMATS FOR =DUMCOP= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

DUMCOP - PROGRAM CALLING CARD.
FORMAT (A2,A4,1X,A4,A2,1X,I1,2(4XI1),I5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DUMCOP
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE.
14	BLANK
15	(0)/(1) (DO NOT)/(DO) COPY THE BINARY FILE
16-19	BLANK
20	(0)/(1) (DO NOT)/(DO) PRINT A DUMP OF THE BINARY FILE
21-24	BLANK
25	(0)/(1) (DO NOT)/(DO) PUNCH A DECK OF CARDS WITH THE INFORMATION OF THE BINARY FILE. (USE FOR PROGRAM CHECK-OUT)
26-30	THE MAXIMUM NUMBER OF PHYSICAL RECORDS OF ANY GIVEN LOGICAL RECORD WHICH SHOULD BE PRINTED. (BLANK OR ZERO SET EQUAL TO FIVE) THIS IS TO PROTECT AGAINST HUGE PRINTED OUTPUT. USUALLY 5 PHYSICAL RECORDS OF ANY ONE LOGICAL RECORD SUFFICE TO DISCOVER ERRORS.

END - END CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	END
4-72	BLANK

A. CARD ORDER SUMMARY FOR =FC= PROGRAM

FC CALLING CARD FOR STRUCTURE FACTOR PROGRAM.

*EDIT EDIT CARD FOR MODIFYING REFLECTIONS. (MAXIMUM OF 14 AT ONE TIME).

*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 TO ESTABLISH LIMITS ON H, K, L, OR SIN THETA.

*ATOM ATOM CARD FOR SELECTING ATOMS FROM FILE.

* THESE CARDS ARE OPTIONAL.

NOTE 1 - IF AN =END= CARD APPEARS WITH NO ATOM CARDS, STRUCTURE FACTORS WILL BE CALCULATED FROM PARAMETERS STORED IN THE DATA FILE. IF ANY ATOMS ARE NAMED ON CARDS. ONLY PARAMETERS FOR NAMED ATOMS WILL BE TAKEN FROM THE FILE. IF THE COLS 12,13 ARE LEFT BLANK ALL ATOMS OF THE SPECIFIED SCATTERING FACTOR TYPE WILL BE LOADED. REMEMBER TO USE EXACTLY THE SAME JUSTIFICATION AND SYMBOLS THROUGHOUT.

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

**** READS =NFILEA= WRITES =NFILEB= ****

B. CARD FORMATS FOR =FC= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

FC - SET-UP CARD FOR STRUCTURE FACTOR CALCULATION.
FORMAT (A2,A4,1X,A4,A2,8X,8I4,F6.0,I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-2	FC
3-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-21	BLANK
22-25	RESCALE CODE. (1)/(2) FOR USE (OLD)/(NEW) F RELATIVE SCALE FACTORS.
26-29	FIXAT. (1)/(2)/(3) FOR (NO PARTIAL CONTRIBUTION)/(PARTIAL CONTRIBUTION)/ (USE PREVIOUS FC AS PARTIAL CONTRIB.)
30-33	(1)/(2) FOR (DO NOT)/(DO) MAKE A SURVEY OF REFLECTION STATISTICS PRELIMINARY TO FINAL FC LISTING.
34-37	DISPERSION CORRECTION. (1)/(2) FOR (DO NOT APPLY)/(APPLY WHERE NECESSARY)
38-41	TYPE OF TEMPERATURE FACTOR (1)/(2)/(3)/(4) (OVERALL ISTROPIC)/ (INDIVIDUAL ISTROPIC)/(INDIVIDUAL ANISTROPIC)/(INDIVIDUAL MIXED)
42-45	(1)/(2) FOR (NORMAL)/(CRIPPLE AUTOMATIC SCALING OF ATOMS AT SYMMETRY CENTERS FOR CENTRIC ONLY)
46-49	FC SCALE FACTOR. (1)/(2) FOR (NORMAL)/ (SPECIAL).
50-53	(1)/(2) FOR (DO NOT)/(DO) CORRECT OVERALL B BY AMOUNT STORED IN DATA FILE FROM PREVIOUS FC RUN.
54-59	SPECIAL FC SCALE FACTOR. (NUMBER OF ASYMMETRIC UNITS OR MOLES, IF OTHER THAN THAT DETERMINED BY LATTICE TYPE.)
60-63	(1)/(2) (DO NOT)/(DO) LIST STRUCTURE FACTORS REFLECTION BY REFLECTION.
64-72	BLANK

EDIT - EDIT CARD FOR MODIFYING REFLECTIONS AT FC TIME.
FORMAT (A2,A4,1X,5I5,2F10.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	EDIT
5-7	BLANK
8-12	H OF REFLECTION NEEDING CHANGE.
13-17	K OF REFLECTION NEEDING CHANGE.
18-22	L OF REFLECTION NEEDING CHANGE.

(NOTE.. LEAVING ANY ONE OF THE FIELDS IN COLS 23-52 BLANK WILL CAUSE FCALC TO USE OLD VALUES.

```
  23-27 NEW JCODE STATUS 1/2/3/4/5 FOR OBSERVED/ UNOBSERVED/ EXTINCT/ IGNORE/
        SYSTEMATICALLY EXTINCT.
  28-32 NEW LEVEL INDICATOR (1 TO 64 ALLOWED)
  33-42 NEW FRELATIVE
  43-52 NEW LEAST SQUARES WEIGHT
  53-72 BLANK

SCALE  - SCALE CARD FOR F RELATIVE DATA.
     FORMAT (A2,A4,F10.4,I4,F10.4,I2,3F10.4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   SCALE
  6     BLANK
  7-16  SCALE FACTOR TO APPLY TO F REL.
  17-20 GROUP IDENTIFICATION (1-64)
  21-72 BLANK

MAXHKL - LIMITS FOR FOURIER SUMMATION.
     FORMAT (A2,A4,7X,3I4,2F8.4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   MAXHKL
  7-13  BLANK
  14-17 MAXIMUM H TO BE USED
  18-21 MAXIMUM K TO BE USED
  22-25 MAXIMUM L TO BE USED
  26-33 MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
  34-41 MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
  42-72 BLANK

ATOM   - ATOM SELECTION CARD.
     FORMAT (A2,A4,1X,A4,A2)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   ATOM
  5-7   BLANK
  8-13  ATOM NAME - CONSISTS OF TWO PARTS. THE FIRST FOUR COLUMNS MUST BE THE
        ATOM-TYPE NAME (SEE FORMFX). THE REST OF THE FIELD MUST BE IDENTIFI-
        CATION OF THE PARTICULAR ATOM OF THE SPECIFIED TYPE. IF THE SECOND
        FIELD IS LEFT BLANK ALL ATOMS OF THE SPECIFIED SCATTERING FACTOR TYPE
        WILL BE LOADED.
  14-72 BLANK

END    - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =FOURR= 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 TIME).
*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', AND 'LAYOUT' IS OPTIONAL. 'END' MUST FOLLOW AFTER THESE CARDS.

***** READS =NFILEA=
***** OPTIONALLY WRITES A BINARY COPY OF MAP IN =NFILEB= *****

NOTE 1 - 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 =FOURR= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

FOURR - CALLING CARD FOR FOURIER PROGRAM.
FORMAT (A2,A4,1X,A4,A2,3X,4I3,F9.5,8F4.1,A2,I1,A1,I1)

```
COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5   FOURR
6-7   BLANK
8-13  COMPOUND IDENTIFICATION CODE
14-18 BLANK
19    (BLANK)/(1)  (DO NOT)/(DO)  WRITE OUTPUT BINARY DATA FILE ON NFILEB.
20-22 (BLANK)/(1)  FOR (NO)/(YES) LIST FC.
23-25 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).  (RESULTS OF
         =DATFIX= MUST BE ON INPUT TAPE.)
        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 WEIGHING 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 (BLANK)/(1)  USE (OLD)/(NEW) F RELATIVE SCALE FACTORS.
29-37 ELECTRON DENSITY SCALE FACTOR.  BLANKS GIVES OUTPUT AS 10*(2/V)*SIGMA
      F. FACTOR PUNCHED REPLACES  10.
38-41 REJECTION RATIO USED BY CRITERIA TESTS OF (4) AND (8). IF LEFT BLANK
      RR SET EQUAL TO ZERO TO INCLUDE ALL REFLECTIONS. THE FOLLOWING
      QUANTITIES ARE USED IF AND ONLY IF THE LAYOUT CARD IS LEFT OUT.  SEE
      NOTE ON NEXT PAGE.
42-45 SCALE OF THE FOURIER IN INCHES/ANGSTROM. (BLANK=0.5)
```

46-49 LOWER LIMIT OF X IN FRACTIONS OF A CELL. (BLANK=0)
50-53 LOWER LIMIT OF Y IN FRACTIONS OF A CELL. (BLANK=0)
54-57 LOWER LIMIT OF Z IN FRACTIONS OF A CELL. (BLANK=0)
58-61 UPPER LIMIT OF X IN FRACTIONS OF A CELL. (BLANK=1.0)
62-65 UPPER LIMIT OF Y IN FRACTIONS OF A CELL. (BLANK=1.0)
66-69 UPPER LIMIT OF Z IN FRACTIONS OF A CELL. (BLANK=1.0)
70-71 PAGE TO PAGE AXIS AS $A, $B, OR $C PROJECTIONS (REGARDLESS OF DATA) AS PA, PB, OR PC.
72 NUMBER OF TYPE WHEELS/FOURIER GRID COLUMN ONLY 2 OR 4 ALLOWED. (BLANK=2)
73 CARRIAGE CONTROL CHARACTER WHICH WILL PREVENT AUTOMATIC OVERFLOW OF PAGES ON LINE PRINTER (IF IN DOUBT LEAVE BLANK).
74 (BLANK)/(1) (DO)/(DO NOT) AUTOMATICALLY CORRECT FOR INTERAXIAL ANGLE WITHIN LAYERS.

NOTE..... IF NO PAGE TO PAGE AXIS OR FOURIER MAP (MAP HERE HAS NOTHING TO DO WITH =MAP= CARD) BOUNDARY LIMITS ARE SPECIFIED AND NO LAYOUT CARD IS INCLUDED AFTER THIS CARD, THE PROGRAM WILL SUM OVER THE SHORTEST AXIS FIRST, THUS GIVING THE FEWEST LAYERS POSSIBLE EACH LAYER BEING SPACED 0.3 ANGSTROMS FROM THE NEXT. WITHIN EACH LAYER THE SCALE WILL BE 1.0 INCHES/ANGSTROM CORRECTED FOR ANY INTERAXIAL ANGLE. ONE HALF OF CENTRIC CELLS WILL BE MAPPED WHILE WHOLE ACENTRIC CELLS ARE PLOTTED. FOUR TYPE-WHEELS/GRID COLUMN WILL BE UTILIZED. THIS METHOD MAY RESULT, FOR HIGH SYMMETRY CELLS WITH AXIS GREATER THAN 20.0 ANGSTROM UNITS, IN A STORAGE OVERFLOW. IN THIS CASE IT WILL BE NECESSARY TO RESORT TO THE USE OF A LAYOUT CARD. ....NOTE WELL THAT IT IS ALWAYS A GOOD PRECAUTION TO CAREFULLY CHECK THE SYMMETRY OF THE MAP PRODUCED.... IF LAYOUT CARD IS LEFT OUT, GRID CARD IS IGNORED.

MAXHKL - LIMITS FOR FOURIER SUMMATION.
FORMAT (A2,A4,1X,A4,A2,3I4,2F8.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 MAXHKL
7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-17 MAXIMUM H TO BE USED
18-21 MAXIMUM K TO BE USED
22-25 MAXIMUM L TO BE USED NOTE..... CARE MUST BE EXERCISED IN USE OF THESE QUANTITIES FOR HIGH SYMMETRY SYSTEMS.
26-33 MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
34-41 MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
42-72 BLANK

FZERO - PUT IN ANY VALUE OF F(000) DESIRED.
FORMAT (A2,A4,7X,F9.5)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 FZERO
6-13 BLANK
14-22 VALUE OF F(000) DESIRED.
23-72 BLANK

LAYOUT - DESCRIPTION OF MAP FOR FOURIER, PATTERSON,ETC..
FORMAT (A2,A4,1X,A4,A2,9I4,1X,3I1,I4,2I2,F7.5,A1)

```
COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6   LAYOUT
7     BLANK
8-13  COMPOUND IDENTIFICATION CODE
14-17 NUMBER OF POINTS CALCULATED IN X DIRECTION.
18-21 ORIGIN VALUE OF X (IN GRID COORDINATES).
22-25 INCREMENT ALONG X (IN GRID COORDINATES).
26-29 NUMBER OF POINTS CALCULATED IN Y DIRECTION.
30-33 ORIGIN VALUE OF Y (IN GRID COORDINATES).
34-37 INCREMENT ALONG Y (IN GRID COORDINATES).
38-41 NUMBER OF POINTS CALCULATED IN Z DIRECTION.
42-45 ORIGIN VALUE OF Z (IN GRID COORDINATES).
46-49 INCREMENT ALONG Z (IN GRID COORDINATES).
50    BLANK
51    SCANNING INDEX FOR X DIRECTION.
52    SCANNING INDEX FOR Y DIRECTION.
53    SCANNING INDEX FOR Z DIRECTION.
54-57 LINE WIDTH.
```

THE SCANNING INDEX FOR A GIVEN DIRECTION IS ONE IF THAT COORIDINATE GOES FROM PAGE TO PAGE IN THE MAP (FIRST SUM), TWO IF IT IS DOWN THE PAGE (SECOND SUM), AND THREE IF IT IS ACROSS THE TOP OF THE PAGE (THIRD SUM).

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, 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, ALL REMAINING POINTS WILL BE PRINTED ON THIS PAGE. THE MAXIMUM PERMISSIBLE VALUE FOR W IS 30 IN THE FOUR COLUMNS MODE, 60 IN THE 2 COLUMNS MODE. IT IS HELPFUL TO ALWAYS THINK OF W AS BEING EQUAL TO THE NUMBER OF POINTS TO BE CALCULATED IN THE THIRD SUM DIRECTION OR 1/2 THAT NUMBER OR 1/4 ETC. BUT NEVER THAT NUMBER -1 AS THIS WILL CAUSE AN ADDITIONAL UNWANTED SHEET (FOR LISTING ON A 120-CHAR. PRINTER (IBM 717), MAX. W IS 27.)

AS AN EXAMPLE, IN THE FOUR COLUMN MODE 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 (OR 10-60 IN THE TWO COLUMN MODE) THE PROGRAM WILL COMPUTE AN OPTIMUM VALUE OF W.

```
58-59 SPACE CONTROL INDEX.
```

THE SPACE CONTROL INDEX MAY BE 1,2,3,4(FOR SINGLE, DOUBLE, TRIPLE, OR QUADRUPLE SPACING, RESPECTIVELY.

```
60-61 NUMBER OF TYPE COLUMNS PER FOURIER GRID COLUMN. BLANK=4. 2 OR 4 ONLY
      POSSIBLE.
62-68 COSINE OF INTER AXIAL ANGLE IN THE FOURIER PAGE. BETWEEN THE AXIS OF
      THE SECOND AND THIRD SUM DIRECTIONS.
69    CARRIAGE CONTROL CHARACTER WHICH WILL PREVENT AUTOMATIC PAGE OVERFLOW
      ON LINE PRINTER (IF IN DOUBT LEAVE BLANK).
70-72 BLANK
```

MAP - PRINT CONTROL CARD.
FORMAT (A2,A4,1X,A4,A2,4X,2I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	MAP
4-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-17	~~BLANK~~ FIRST POINTS VALUE TO SCALE MAP
18-21	UPPER LIMIT TO ESTABLISH PRINT SUPPRESSION
22-25	LOWER LIMIT WITH SIGN TO ESTABLISH PRINT SUPPRESSION (BLANKS WILL BE PRINTED AT ALL POINTS WHERE THE FOURIER VALUES FALL BETWEEN THESE VALUES.)
26-72	BLANK

GRID - FOURIER GRID CARD.
FORMAT (A2,A4,1X,A4,A2,3I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	GRID
5-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-17	NUMBER OF GRID INTERVALS ALONG THE X AXIAL DIRECTION.
18-21	GRID INTERVALS ALONG Y AXIAL DIRECTION
22-25	GRID INTERVALS ALONG Z AXIAL DIRECTION
26-72	BLANK

END - END CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	END
4-72	BLANK

LIST OF OPERATION CARDS

ENDFIL WRITES REMARK =END OF OUTPUT FILE= AND WRITES ONE END-OF-FILE MARK. REWINDS FILE =NTOUT= AND REDEFINES =NTOUT= TO =NTOUTM=. NOTE - IF (NTOUT)=(NTOUTM) THE 'ENDFIL' CARD IS IGNORED. (THESE FILE DESIGNATIONS ARE DEFINED IN 1.GENERL.)

FILES ASSIGNS FILE UNIT DESIGNATIONS.

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).

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. WILL NOT WORK ON MANY MACHINES. ONE MUST USE SHOP MONITOR FACILITY.

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

RESTART CAUSES REINITIALIZATION OF SYSTEM FILE ASSIGNMENTS, CLEARS TITLE TO BLANK, RESETS PAGE COUNT TO ZERO, ETC.

SAVE CAUSES UNLOADING OR PHYSICAL DISCONNECTION OF THE SPECIFIED LOGICAL FILES. THESE SHOULD NOT BE INCLUDED UNTIL THE END OF THE RUN. (THIS CARD SHOULD USUALLY BE PRECEDED BY A 'RESTART' CARD.)

TITLE FILLS IN PAGE TITLE. NEW =TITLE= CARD CHANGES STORED TITLE. 'RESTART' CARD INITIALIZES STORED TITLE TO BLANKS.

CARD FORMATS FOR SYSTEM OPERATION CARDS

ENDFIL - END FILE OUTPUT (FILE NTOUT).
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	ENDFIL
7-72	BLANK

FILES - SET VALUES FOR LOGICAL FILE DESIGNATION NUMBERS. A BLANK FIELD IMPLIES NO CHANGE IN GIVEN FILE DESIGNATION. REMEMBER THAT NFILEA AND NFILEB ARE INTERCHANGED AUTOMATICALLY AFTER EACH PROGRAM CALL.
FORMAT (A2,A4,12I3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	FILES

	FILE	USUAL PURPOSE
7-9	NTIN	CARD INPUT (FROM CARD READER)
10-12	NTOUT	PRINTED OUTPUT (TO LINE PRINTER)
13-15	NFILEA	INPUT BINARY X-RAY DATA FILE
16-18	NFILEB	OUTPUT BINARY X-RAY DATA FILE
19-21	NFILEC	PUNCH CARD OUTPUT (TO CARD PUNCH)
22-24	NFILED	SPARE OFFLINE PRINT OUTPUT FILE
25-27	NFILEE	SCRATCH FILE FOR VARIOUS LINKS
28-30	NFILEF	SCRATCH FILE FOR VARIOUS LINKS
31-33	NFILEG	SCRATCH FILE FOR VARIOUS LINKS
34-36	NFILEH	SCRATCH FILE FOR VARIOUS LINKS
37-39	NFILEI	SCRATCH FILE FOR VARIOUS LINKS
40-42	NFILEJ	SCRATCH FILE FOR VARIOUS LINKS
43-72	BLANK	

FINISH - RUN TERMINATION CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	FINISH
7-72	BLANK

OPRATR - OPERATOR INSTRUCTION CARD. OPERATION CARD. OCCURRENCE 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.) WILL NOT WORK ON ALL MACHINES.
FORMAT (A2,17A4,A2)

```
  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   OPRATR
  7-72  INSTRUCTION TO COMPUTER OPERATOR

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 INSTRUCTION.  WILL
         NOT WORK ON ALL MACHINES.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   PAUSE
  6-72  BLANK

REMARK - REMARK CARD.  OPERATION CARD.  A REMARK CARD IS USED TO INSERT A
         REMARK ONTO THE PRINTED OUTPUT ON NTOUT AT ANY TIME FOR INCLUSION
         ON THE OFF-LINE LISTING.  WILL NOT WORK ON ALL MACHINES.
     FORMAT (A2,17A4,A2)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   REMARK
  7-72  ALPHANUMERIC INFORMATION FOR REMARK

RESTART - REINITIALIZE SYSTEM.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-7   RESTART
  8-72  BLANK

SAVE   - PHYSICALLY REMOVE THE SPECIFIED DATA FILE FROM THE COMPUTER.  WILL
         NOT WORK FOR ALL MACHINES.
     FORMAT (A2,A4,12I3)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   SAVE
  7-9,10-12,13-15,....,40-42  NUMBERS OF LOGICAL FILES TO BE REMOVED.  FIRST
        BLANK FIELD TERMINATES SCAN OF CARD.

TITLE  - FOR HEADING PAGES ON THE PRINTER OUTPUT FILE (NTOUT).  SHOULD BE USED
         AT THE START OF EVERY RUN AND AFTER EVERY RESTART CARD.  INCLUDE DATE
         AND REASON FOR RUN.
     FORMAT (A2,17A4,A2)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   TITLE
  7-72  ALPHANUMERIC INFORMATION FOR PAGE TITLE
```

A. CARD ORDER SUMMARY FOR =LOADAT= PROGRAM

LOADAT	CALLING CARD FOR ATOM PARAMETER LOADING ROUTINE.
*LABEL	TO UPDATE FILE LABEL (MAXIMUM OF 15 CARDS).
*SCALE	TO UPDATE FILE F-RELATIVE SCALE FACTORS.
*GRID	TO ALTER GRID PARAMETERS. REQUIRED ONLY IF =ATOMG= CARDS ARE USED. THIS CARD NEED BE USED ONLY ONCE FOR ANY GIVEN GRID SPECIFICATION. IT IS THEN STORED IN THE BINARY FILE UNTIL CHANGED BY A SUBSEQUENT =GRID= CARD.
*MAXHKL	TO ESTABLISH LIMITS ON H, K, L, OR SIN THETA.
*DATOM	TO MOVE ALL ATOMS IN THE ASYMMETRIC UNIT BY A SPECIFIED AMOUNT.
**B	OVERALL TEMPERATURE FACTOR.
*ATOM	TO SUPPLY ATOM FRACTIONAL POPULATION, POSITIONAL, AND ISOTROPIC TEMPERATURE PARAMETERS.
*ATOMG	TO SUPPLY ATOM GRID POSITIONAL, POPULATION, AND ISOTROPIC TEMPERATURE PARAMETERS. THIS CARD REQUIRES A =GRID= CARD.
*ATOMD	TO DELETE ATOMS FROM THE BINARY FILE.
*B	ISOTROPIC TEMPERATURE FACTORS.
*UIJ	ANISOTROPIC TEMPERATURE FACTOR CARD. RMS AMPLITUDE OF VIBRATION IN CRUICKSHANK NOTATION.
*BIJ	ANISOTROPIC TEMPERATURE FACTOR (SAME SCALE AS B)
*BETA	ANISOTROPIC TEMPERATURE FACTORS IN THE EXPRESSION - EXP BASE E H**2 BETA(1,1) + ... + 2*H*K* BETA(1,2) + ...
*REF	TO ESTABLISH SIGNALS IN THE FILE WITH RESPECT TO WHICH PARAMETERS ARE TO BE REFINED UPON.
*NOREF	TO ESTABLISH SIGNALS IN THE FILE WITH RESPECT TO WHICH PARAMETERS ARE TO BE REFINED UPON.
END	END CARD.

* THESE CARDS ARE OPTIONAL.

** A B CARD AT THIS POINT WITH THE COMPOUND ID IN COLS 8-13 IS ENTERED AS AN OVERALL TEMPERATURE FACTOR.

**** READS =NFILEA= WRITES =NFILEB= ****

NOTE 1 - ALL LABEL, SCALE, GRID AND MAXHKL CARDS MUST COME FIRST. THEN ALL B, ATOM, ATOMD, ATOMG, BETA, BIJ, AND UIJ MUST COME NEXT EITHER ALL T.F. AND THEN ALL ATOM OR ATOM, TF, ATOM, TF,... IT MAKES NO DIFFERENCE. IF MORE THAN ONE CARD IS GIVEN THE SAME ATOM IDENTITY THE LAST SUPERCEDES ALL OTHERS. REF AND NOREF COME IN ORDER OF LOGIC JUST BEFORE THE END CARD.

NOTE 2 - FOR OVERALL TEMPERATURE FACTOR, A SINGLE 'B' 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' CARDS). 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', AND 'BETA' CARDS AND CONVERTS THEM INTERNALLY SO THAT THESE CARDS MAY BE DIFFERENT FOR EACH ATOM.

B. CARD FORMATS FOR =LOADAT= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

LOADAT - CALLING CARD FOR ATOM PARAMETER LOADING ROUTINE.
FORMAT (A2,A4,1X,A4,A2,I2,I5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	LOADAT
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-15	(BLANK)/(1) FOR (UPDATE)/(A-PRIORI) RUN
16-20	(BLANK)/(1) FOR USE (SCALE)/RESCALE) FACTORS FOR F-RELATIVE.
21-72	BLANK

LABEL - TO UPDATE FILE LABEL.
FORMAT (A2,A4,16A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	LABEL
6	BLANK
7-72	LABEL INFORMATION FOR DATA FILE.

SCALE - TO UPDATE FILE F-RELATIVE SCALE FACTORS.
FORMAT (A2,A4,F10.4,I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	SCALE
6	BLANK
7-16	F-RELATIVE MULTIPLICATIVE SCALE FACTOR
17-20	NUMBER OF SCALE GROUP AS ESTABLISHED AT DATA REDUCTION TIME.
21-72	BLANK

GRID - FOURIER GRID CARD.
FORMAT (A2,A4,7X,3I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	GRID
5-13	BLANK
14-17	NUMBER OF GRID POINTS ALONG A AXIS
18-21	NUMBER OF GRID POINTS ALONG B AXIS
22-25	NUMBER OF GRID POINTS ALONG C AXIS

26-72 BLANK

MAXHKL - LIMITS FOR FOURIER SUMMATION.
FORMAT (A2,A4,7X,3I4,2F8.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6 MAXHKL
7-13 BLANK
14-17 MAXIMUM H TO BE USED
18-21 MAXIMUM K TO BE USED
22-25 MAXIMUM L TO BE USED
26-33 MAXIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
34-41 MINIMUM SIN(THETA)/LAMBDA. (BLANK MEANS NO LIMIT)
42-72 BLANK

DATOM - ASYMMETRIC UNIT SHIFT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 DATOM
6-7 BLANK
8-13 COMPOUND IDENTIFICATION CODE
14-21 FACTOR TO BE ADDED TO ALL X PARAMETERS SUPPLIED (CARDS OR FILE)
22-29 Y PARAMETER SHIFT
30-37 Z PARAMETER SHIFT
38-72 BLANK

ATOM OR ATOMG - ATOM PARAMETER CARD.
AN ATOMG CARD IS IDENTICAL TO AN ATOM CARD SAVE THAT THE X, Y, Z ARE DIVIDED BY THE THREE PARAMETERS SUPPLIED ON A GRID CARD. - USED TO AVOID CONVERTING FOURIER MAP COORIDINATES.
FORMAT (A2,A4,1X,A4,A2,3F8.4,F6.4,F5.2)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 ATOM OR ATOMG
6-7 BLANK
8-11 SCATTERING FACTOR TYPE (EXACTLY AS ON FORMFX CARDS)
12-13 ATOM IDENTITY FOR GIVEN SCATTERING FACTOR TYPE
14-21 X PARAMETER IN FRACTIONS OF A CELL EDGE
22-29 Y PARAMETER IN FRACTIONS OF B CELL EDGE
30-37 Z PARAMETER IN FRACTIONS OF C CELL EDGE
38-43 ISOTROPIC TEMPERATURE FACTOR IF SUPPLIED IN THIS CARD.
44-48 POPULATION PARAMETER OF THIS SPECIES AT THIS POINT X, Y, Z BLANK IMPLIES 1.0
49-72 BLANK

ATOMD - TO DELETE ATOMS FROM THE BINARY FILE.
FORMAT (A2,A4,1X,A4,A2)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 ATOMD
6-7 BLANK
8-11 SCATTERING FACTOR TYPE (EXACTLY AS PUNCHED IN THE FORMFX CARDS A1 DATA REDUCTION)

12-13 ATOM IDENTITY FOR ATOM OF GIVEN SCATTERING FACTOR TYPE. (NOTE*** IF LEFT BLANK THIS CARD APPLIES TO ALL ATOMS OF THE STATED TYPE.***)
14-72 BLANK

B, BIJ, UIJ, AND BETA - TEMPERATURE FACTOR CARDS.

NOTE.. THE FORMAT OF B, BIJ, UIJ, AND BETA CARDS ARE ALL THE SAME.

FORMAT (A2,A4,1X,A4,A2,6F8.4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4 APPROPRIATE LABEL B, BIJ, UIJ, OR BETA
5-7 BLANK
8-11 SCATTERING FACTOR TYPE EXACTLY AS PUNCHED ON THE ATOM OR ATOMG CARD
12-13 ATOM IDENTITY EXACTLY AS ON ATOM OR ATOMG CARD
(OR 8-13 COMPOUND IDENTITY IF THIS IS AN OVERALL FACTOR.)
14-21 B OR B11 OR U11 OR BETA11
22-29 B22 OR EQUIVALENT
30-37 B33 OR EQUIVALENT
38-45 B12 OR EQUIVALENT
46-53 B13 OR EQUIVALENT
54-61 B23 OR EQUIVALENT
62-72 BLANK

REF OR NOREF - TO ESTABLISH SIGNALS IN THE FILE WITH RESPECT TO WHICH PARAMETERS ARE TO BE REFINED UPON.
FORMAT (A2,A4,1X,A4,A2,13A3)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5 REF OR NOREF
6-7 BLANK
8-11 SCATTERING FACTOR TYPE (EXACTLY AS SHOWN IN FORMFX CARDS).
12-13 ATOM IDENTITY FOR THIS SCATTERING FACTOR TYPE.
(NOTE.... IF 12-13 IS BLANK CARDS APPLY TO ALL ATOMS OF NAMED TYPE.
IF 8-11 IS BLANK CARD APPLIES TO ALL ATOMS.)
(IF =SCALE= IS PUNCHED IN 8-12 THEN COMMAND APPLIES TO F-RELATIVE SCALE FACTOR REFINEMENT)
14-16 EACH FIELD MAY CONTAIN BLANKS OR ONE OF THE FOLLOWING LEFT JUSTIFIED SYMBOLS. X, Y, Z, B, B11, B22, B33, B12, B13, B23, M, S, D (M IS THE POPULATION PARAMETER, S THE NEUTRON SCATTERING FACTOR AND D THE DISPERSION CORRECTION) IF ALL FIELDS ARE LEFT BLANK ALL QUANTITIES ARE ACTED UPON. IF ANY FIELD IS PUNCHED ONLY THE PARAMETERS NAMED ARE ACTED UPON.
17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43, 44-46, 47-49,
50-52 (SYMBOL FROM ABOVE LIST)
53-72 BLANK

END - END CARD.
FORMAT (A2,A4)

COLS SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3 END
4-72 BLANK

A. CARD ORDER SUMMARY FOR =MODIFY= PROGRAM

MODIFY	CALLING CARD
*MODFIL	MODIFY SPECIFIED ENTRY
*MODREF	MODIFY SPECIFIED REFLECTION
END	END CARD

* THESE CARDS ARE OPTIONAL

****READS NFILEA
****WRITES NFILEB
****OPTIONALLY PUNCHES CARDS ON NFILEC

B. CARD FORMATS FOR =MODIFY= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

MODIFY - CALLING CARD.
FORMAT (A2,A4,1X,A4,A2,I2,I5,3F10.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	MODIFY
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE.
14	BLANK
15	(BLANK)/(1)/(2)/(3) (DO NOT REPLACE F-RELATIVE WITH A VALUE DERIVED FROM FC)/(DO REPLACE F-RELATIVE WITH A VALUE DERIVED FROM FC)/(IMPLIES THAT IN ADDITION TO REPLACING F-RELATIVE THE PHASE OF FC IS TO BE STORED IN THE CALCULATED PHASE WORD(24))/(IMPLIES THAT IN ADDITION HKL REFLECTION CARDS BE PUNCHED FOR OTHER USES.)
16-20	(BLANK)/(N) (DO NOT)/(DO) LIST WORDS MODIFIED, N IS THE NUMBER OF LINES TO LIST.
21-30	PERCENTAGE RANDOM ERROR TO BE PLACED IN F
31-40	THRESHOLD INTENSITY
41-50	SCALE TO BE APPLIED TO F TO REMOVE IT FROM SCALE OF FC

MODFIL - MODIFY SPECIFIED ENTRY.
FORMAT (A2,A4,1X,A4,A2,I4,4XI4,I9,F10.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	MODFIL
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE.
14-15	BLANK
16-19	LOGICAL RECORD TO BE ALTERED
20-23	PHYSICAL RECORD TO BE ALTERED
28-31	NUMBER OF WORD TO BE REPLACED IN THE SPECIFIED RECORD.
32-40	FIXED POINT QUANTITY
41-50	FLOATING POINT QUANTITY

MODREF - MODIFY SPECIFIED REFLECTION.
FORMAT (A2,A4,1X,A4,A2,4I4,I9,F10.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	MODREF

```
7      BLANK
8-13   COMPOUND IDENTIFICATION CODE.
14-15  BLANK
16-19  H INDEX OF REFLECTION TO BE MODIFIED
20-23  K INDEX OF REFLECTION TO BE MODIFIED
24-27  L INDEX OF REFLECTION TO BE MODIFIED
28-31  NUMBER OF RELATIVE WORD IN REFLECTION RECORD TO BE REPLACED. (SEE FILE
       FORMAT)
32-40  FIXED PI
32-40  FIXED POINT QUANTITY                    THE CHOICE IS MADE ON THE BASIS
41-50  FLOATING POINT QUANTITY                 OF NON-ZERO.  IF BOTH ARE NON-
                                               ZERO, FIXED POINT IS STORED.

END    - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-76  BLANK
```

A. CARD ORDER SUMMARY FOR =ORFLS= PROGRAM

ORFLS	CALLING CARD FOR BUSING-MARTIN-LEVY LEAST-SQUARES
*SCALE	SCALE CARD FOR F RELATIVE DATA
*ATOM	ATOM SELECTION CARD
*REF	TURN ON REFINEMENT OF SPECIFIED PARAMETERS
*NOREF	SHUT OFF REFINEMENT OF SPECIFIED PARAMETERS
END	END CARD

* THESE CARDS ARE OPTIONAL.

NOTE 1 - THIS PROGRAM DOES NOT TREAT THE OVERALL TEMPERATURE FACTOR.

NOTE 2 - IF NO ATOM CARDS ARE PRESENT ALL THE ATOMS IN THE BINARY FILE ARE USED. IF ANY ATOMS ARE SPECIFIED BY CARDS ONLY THOSE SPECIFIED ON THE CARDS ARE SELECTED FROM THE BINARY FILE. IF THERE ARE TOO MANY ATOMS IN THE FILE FOR THE STORAGE CAPACITY, CARDS WILL BE EXPECTED.

NOTE 3 - IF ALL REFINEMENT RESTRICTION CARDS ARE LEFT OUT REFINEMENT WILL BE ON ALL POSITIONAL AND TEMPERATURE PARAMETERS. HOWEVER, NO SCATTERING FACTORS OR POPULATION FACTORS WILL BE SET TO REFINE.

***** READS =NFILEA= AND WRITES =NFILEB= *****

IF THE PROGRAM IS SET TO PUNCH CARDS (COLS 32-34 OF 'ORFLS' CARD) THE PROGRAM WRITES THESE IMAGES ON =NFILEC=, THE PUNCH FILE.

B. CARD FORMATS FOR =ORFLS= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

ORFLS - CALLING CARD FOR BUSING-MARTIN-LEVY LEAST-SQUARES PROGRAM.
FORMAT (A2,A4,1X,A4,A2,11I3,3F4.3,I3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	ORFLS
6-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-16	NUMBER OF CYCLES TO BE CALC. (NC)
17-19	(1)/(2)/(3) FOR (ISOTROPIC)/(ANISOTROPIC)/(MIXED) PROGRAM CONVERTS IF REQUIRED. AVERAGE DIAGONAL ELEMENT USED IN ANISOTROPIC CONVERSION. NO CONVERSION MADE UNLESS SPECIFIED BY A =REF= CARD IN MIXED MODE. (ITF)
20-22	(BLANK)/(1)/(2) FOR REFINEMENT BASED ON (F)/(F**2)/(FO CONNECTED FOR DISPERSION) (IFSQ)
23-25	(BLANK)/(1) FOR USE (SCALE)/(RESCALE) FACTORS FROM TAPE (IRESC)
26-28	(BLANK)/(1) FOR (DO)/(DO NOT) HALT IF CONVENTIONAL R INCREASES BY 0.1 IN ANY CYCLE.
29-31	(BLANK)/(1) FOR (WEIGHTS FROM TAPE)/(ALL WEIGHTS EQUAL 1.0) (IW)
32-34	(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	(BLANK)/(1) FOR (DO NOT)/(DO) LIST THE REFLECT. INFO. DURING LAST CYCLE (ILIST)
38-40	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	(BLANK)/(1)/(2) FOR (NO)/(USE)/(USE PREVIOUS FC) FIXED ATOM CONTRIB. (IP)
44-46	(BLANK)/(1) FOR (X-RAY)/(NEUTRON) (INEU)
47-50	DAMPING OR ENHANCING FACTOR FOR PARAMETER SHIFTS (BLANK OR 0.0 = 1.0)
51-54	RR TO CONTROL LIST (BLANK = 2.0)
55-58	REJECT FROM CONSIDERATION IN SHIFTS REFLECTIONS WHOSE WEIGHTED DELTA-F IS LARGER. (BLANK = 10**8)
59-61	(BLANK)/(1) (NO)/(SPECIAL) SYMMETRY PATCH REQUIRED.
62-72	BLANK

SCALE - SCALE CARD FOR F RELATIVE DATA.
FORMAT (A2,A4,F10.4,I4,F10.4,I2,3F10.4)

```
  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   SCALE
  6     BLANK
  7-16  SCALE FACTOR TO APPLY TO F REL.
  17-20 GROUP IDENTIFICATION (1-64)
  21-72 BLANK

ATOM   - ATOM SELECTION CARD.
     FORMAT (A2,A4,1X,A4,A2)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-4   ATOM
  5-7   BLANK
  8-11  SCATTERING FACTOR TYPE (EXACTLY AS ON FORMFX CARDS)
  12-13 ATOM IDENTITY FOR GIVEN SCATTERING FACTOR TYPE
  14-72 BLANK

REF OR NOREF - SET PARAMETER REFINEMENT IF IT IS TO BE DIFFERENT THAN THAT
          ALREADY SET IN THE DATA FILE.
     FORMAT (A2,A4,1X,A4,A2,13A3)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   REF OR NOREF
  6-7   BLANK
  8-11  SCATTERING FACTOR TYPE (EXACTLY AS SHOWN IN FORMFX CARDS).
  12-13 ATOM IDENTITY FOR THIS SCATTERING FACTOR TYPE.
        (NOTE.... IF 12-13 IS BLANK CARDS APPLY TO ALL ATOMS OF NAMED TYPE.
        IF 8-11 IS BLANK CARD APPLIES TO ALL ATOMS.)
        (IF =SCALE= IS PUNCHED IN 8-12 THEN COMMAND APPLIES TO F-RELATIVE SCALE
        FACTOR REFINEMENT)
  14-16 EACH FIELD MAY CONTAIN BLANKS OR ONE OF THE FOLLOWING LEFT JUSTIFIED
        SYMBOLS.  X, Y, Z, B, B11, B22, B33, B12, B13, B23, M, S, D (M IS THE
        POPULATION PARAMETER, S THE NEUTRON SCATTERING FACTOR AND D THE
        DISPERSION CORRECTION)  IF ALL FIELDS ARE LEFT BLANK ALL QUANTITIES
        ARE ACTED UPON.  IF ANY FIELD IS PUNCHED ONLY THE PARAMETERS NAMED ARE
        ACTED UPON.
  17-19, 20-22, 23-25, 26-28, 29-31, 32-34, 35-37, 38-40, 41-43, 44-46, 47-49,
  50-52 (SYMBOL FROM ABOVE LIST)
  53-72 BLANK

END    - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =PARAM= PROGRAM

PARAM	CALLING CARD FOR =PARAM=
CELL	CELL CONSTANT CARD
THETA	TWO THETA DATA CARD
END	END CARD

B. CARD FORMATS FOR =PARAM= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

PARAM - CALLING CARD FOR LEAST SQUARES CELL PARAMETER REFINEMENT PROGRAM.
FORMAT (A2,A4,1X,A4,A2,2X,2F10.7,A4,A2)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	PARAM
6-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-15	BLANK
16-25	WAVELENGTH OF RADIATION USED.
26-35	CORRECTION TO BE APPLIED TO THE TWO THETA VALUES CONTAINED ON THE =THETA= CARDS FOR CONVERSION TO TRUE TWO THETA'S.
36-41	LATTICE TYPE IDENTIFICATION CODE ACCORDING TO THE FOLLOWING -

TRICL1 - TRICLINIC
MONOCL - MONOCLINIC
ORTHOR - ORTHORHOMBIC
TETRAG - TETRAGONAL
CUBIC - CUBIC
TRIGRH - TRIGONAL (RHOMBOHEDRAL INDEXING)
HEXAGO - HEXAGONAL
TRIGHX - TRIGONAL (HEXAGONAL INDEXING)
IF THE LATTICE TYPE PROVIDED IS BLANK OR ILLEGAL, A TRICLINIC LATTICE WILL BE ASSUMED.

CELL - CELL CONSTANT CARD.
FORMAT (A2,A4,1X,A4,A2,3F8.3,3F9.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	CELL
5-7	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.
14-21	A CELL DIMENSION
22-29	B CELL DIMENSION
30-37	C CELL DIMENSION
38-46	ALPHA OR COSINE (ALPHA).
47-55	BETA OR COSINE (BETA). IF A MONOCLINIC LATTICE WITH BETA UNIQUE, DO

NOT SET BETA EQUAL TO 90.0 DEGREES (OR A COSINE OF 0.0) BECAUSE BETA IS TESTED TO DETERMINE IF IT OR GAMMA IS TO BE REFINED.

56-64 GAMMA OR COSINE (GAMMA).
65-71 F(0,0,0)

THETA - TWO THETA DATA CARD.
FORMAT (A2,A4,9X,3I4,2F10.6)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	THETA
6-15	BLANK
16-19	H INDEX.
20-23	K INDEX.
24-27	L INDEX.
28-37	TWO THETA.
38-47	STANDARD DEVIATION OF TWO THETA. IF ZERO OR BLANK, 0.01 IS SUPPLIED.

END - END CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	END
4-72	BLANK

A. CARD ORDER SUMMARY FOR =PHASE= PROGRAM

PHASE	CALLING CARD FOR PHASE PROGRAM.
*DEFINE	DEFINES THE PHASE OF SPECIFIED REFLECTION.
*IGNORE	CAUSES SPECIFIED REFLECTION TO BE IGNORED IN SOLUTION PROCESS.
*BADEQN	REMOVES A SPECIFIED EQUATION DERIVED FROM TWO SIGMA-TWO RELATIONSHIPS FROM THE SET USED IN SOLUTION PROCESS.
*BADSIG	REMOVES A SPECIFIED SIGMA-TWO RELATIONSHIP.
**HKL	PERMITS LOADING OF E VALUES FROM CARDS.
***EQN	PERMITS LOADING OF SIGMA-TWO DERIVED EQUATIONS FROM CARDS.
END	

* THESE CARDS ARE OPTIONAL.

** IF ANY HKL CARDS APPEAR NO SIGMA TWO DATA FILE IS USED.

**** SIGMA TWO RELATIONSHIPS MUST BE SUPPLIED IF HKL CARDS SUPPLIED.
=NFILEA= AND =NFILEB= ARE USED WHEN FILE UPDATING IS REQUESTED
=NFILEE= IS SIGMA-TWO RELATIONSHIPS FILE
=NFILEF= AND =NFILEG= ARE SCRATCH FILES ALWAYS USED
=NFILEH= SCRATCH FILE USED WHEN SORTING IS REQUESTED
IF PUNCH CARDS ARE SPECIFIED THEY ARE PLACED IN FILE =NFILEC=

B. CARD FORMATS FOR =PHASE= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

PHASE - CALLING CARD FOR PHASE.
FORMAT (A2,A4,1X,A4,A2,4I4,2F6.4,3I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	PHASE
6-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-17	(BLANK)/(1)/(2) (NO PUNCHED PHASES)/(PUNCH DEFINE CARDS)/(PUNCH MODREF CARDS)
18-21	(0)/(1) (DO NOT)/(DO) WRITE NEW BINARY FILE WITH DETERMINED PHASES INCLUDED
22-25	(-1)/(0)/(N) (DO NOT)/(DO) DEFINE ORIGIN REFLECTIONS IF POSSIBLE/ OR IGNORE UP TO N UNDEFINED GENERATORS AND PROCEED WITH LIMITED SOLUTION.
26-29	NUMBER OF LARGEST E VALUE REFLECTIONS TO BE ''GENERATORS''
30-35	MINIMUM PROBABILITY TO ACCEPT A RELATIONSHIP FROM SIGMA TWO
36-41	MINIMUM E VALUE FOR WHICH A PHASE IS TO BE DETERMINED
42-45	MAXIMUM NUMBER OF CYCLES OF REFINEMENT TO ATTEMPT TO PRODUCE A SOLUTION - 10 MAXIMUM (I.E. FEWER DESCREPANT THAN ACCORDANT)
46-49	(0)/(1) (DO)/(DO NOT) SORT SIGMA TWO RELATIONSHIPS BEFORE ATTEMPTING SOLUTION.

DEFINE - REFLECTIONS TO BE DEFINED WITH RESPECT TO PHASE.
FORMAT (A2,A4,1X,A4,A2,2X,4I4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	DEFINE
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-15	BLANK
16-19	H INDEX
20-23	K INDEX
24-27	L INDEX
28-31	+ OR - 1 TO INDICATE COSINE OF DEFINED PHASE.

IGNORE - REFLECTIONS TO BE IGNORED IN PROCESS OF PHASE DETERMINATION ELIMINATES ALL SIGMA TWO RELATIONSHIPS WHICH INVOLVES THIS REFLECTION.
FORMAT (A2,A4,1X,A4,A2,2X,3I4)

```
  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   IGNORE
  7     BLANK
  8-13  COMPOUND IDENTIFICATION CODE
  14-15 BLANK
  16-19 H INDEX
  20-23 K INDEX
  24-27 L INDEX

BADEQN - ELIMINATES A SPECIFIED RELATIONSHIP FROM USE DURING THE SOLUTION
         PROCESS.
     FORMAT (A2,A4,1X,A4,A2,2X,5I4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   BADEQN
  7     BLANK
  8-13  COMPOUND IDENTIFICATION CODE
  14-15 BLANK
  16-19 FIRST SYMBOLIC PHASE NUMBER
  20-23 SECOND SYMBOLIC PHASE NUMBER
  24-27 THIRD SYMBOLIC PHASE NUMBER
  28-31 FOURTH SYMBOLIC PHASE NUMBER  (IF NEEDED FOR A RELATIONSHIP OF THE
        SECOND KIND.)
  32-35 SIGN OF THE RELATIONSHIP.

BADSIG - ELIMINATES SPECIFIED SIGMA TWO RELATIONSHIPS FROM USE DURING THE
         SOLUTION PROCESS.
     FORMAT (A2,A4,1X,A4,A2,2X,4I4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   BADSIG
  7     BLANK
  8-13  COMPOUND IDENTIFICATION CODE
  14-15 BLANK
  16-19 FIRST SYMBOLIC PHASE NUMBER
  20-23 SECOND SYMBOLIC PHASE NUMBER
  24-27 THIRD SYMBOLIC PHASE NUMBER
  28-31 SIGN OF RELATIONSHIP

HKL    - HKL CARD.
     FORMAT (A2,A4,1X,A4,A2,2X,4I4,F7.4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   HKL
  4-7   BLANK
  8-13  COMPOUND IDENTIFICATION CODE
  14-15 BLANK
  16-19 H INDEX
  20-23 K INDEX
  24-27 L INDEX
  28-31 SYMBOLIC PHASE NUMBER FOR THIS E.
  32-38 E VALUE
```

```
EQN    - A SIGMA TWO RELATIONSHIP
     FORMAT (A2,A4,1X,A4,A2,2X,4I4,F7.5)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   EQN
  4-7   BLANK
  8-13  COMPOUND IDENTIFICATION CODE
  14-15 BLANK
  16-19 SYMBOLIC PHASE ONE
  20-23 SYMBOLIC PHASE TWO
  24-27 SYMBOLIC PHASE THREE
  28-31 + OR - 1 FOR SIGN OF RELATIONSHIP
  32-38 PROBABILITY OF THE RELATIONSHIP BEING TRUE.

END    - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =RLIST= PROGRAM

RLIST	CALLING CARD FOR R LISTING PROGRAM
*SCALE	F RELATIVE SCALE FACTOR CARD(S)
*CATEGO	TO OBTAIN R VALUES FOR CERTAIN SPECIFIED CATEGORIES.
END	END CARD

* THESE CARDS ARE OPTIONAL.

****READS =NFILEA=****

B. CARD FORMATS FOR =RLIST= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

RLIST - CALLING CARD FOR RLIST PROGRAM.
FORMAT (A2,A4,1X,A4,A2,2X,I3,2X,I1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	RLIST
6-7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-17	BLANK
18	(0 OR BLANK)/(1)/(2) FOR (USE SCALE FACTORS)/(USE RESCALE FACTORS)/ (SET SCALE FACTORS = 1). SCALES WILL BE SUPERSEDED BY ANY SCALE CARDS WHICH MAY BE SUPPLIED.
19-20	BLANK
21	(BLANK)/(1) FOR (DO)/(DO NOT) LIST R BY LEVELS OF H,K, AND L. NOTE.... IN ORDER TO OBTAIN THIS LISTING, THE BINARY DATA FILE MUST BE SEARCHED TWICE. IF THE USER WISHES TO SAVE TIME RATHER THAN SEE THIS LISTING, PLACE A ONE IN COLUMN 21.

SCALE - SCALE CARD FOR F RELATIVE DATA.
FORMAT (A2,A4,F10.4,I4,F10.4,I2,3F10.4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	SCALE
6	BLANK
7-16	SCALE FACTOR TO APPLY TO F REL.
17-20	GROUP IDENTIFICATION (1-64) 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	BLANK

CATEGO - CARD ALLOWING USER TO OBTAIN R VALUES FOR CERTAIN SPECIFIED CATEGORIES. (USE A SEPARATE CARD FOR EACH CATEGORY SELECTED.)
FORMAT (A2,A4,2X,3A4,6(1X,I4,2F10.5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	CATEGO
7-8	BLANK (OR RY)
9-20	USER'S NAME FOR CATEGORY SELECTED

```
---- CATEGORIES BY INDEX VALUES
  21-25 R VALUES DESIRED FOR A SPECIFIC H, BLANK IMPLIES NO SEARCH FOR A
        SPECIFIC H VALUE.
  26-30 R VALUES DESIRED FOR A SPECIFIC K, BLANK IMPLIES NO SEARCH FOR A
        SPECIFIC K VALUE.
  31-35 R VALUES DESIRED FOR A SPECIFIC L, BLANK IMPLIES NO SEARCH FOR A
        SPECIFIC L VALUE.

---- CATEGORIES BY INDEX COMBINATIONS
  36-40 CATEGORY OF INDEX COMBINATIONS
        (BLANK)/(1)/(2)/(3)/(4)/(5)/(6)/(7)  FOR  (IGNORE TEST)/(H)/(K)/(L)/
        (H+K)/(H+L)/(K+L)/(H+K+L)
  41-45 VALUE OF ABOVE INDICES TO BE INCLUDED IN R VALUES
        (1)/(2)/(3)/(4)/(5)/(6)/(ETC.)  FOR  (ODD ONLY)/(EVEN ONLY)/(MULTIPLES
        OF 3 ONLY)/(MULTIPLES OF 4 ONLY)/(MULTIPLES OF 5 ONLY)/(MULTIPLES OF 6
        ONLY)/(ANY REASONABLE NUMBER MAY BE SUPPLIED)

---- CATEGORIES BY MAGNITUDE OF OTHER QUANTITIES
  46-50 SELECT CATEGORY FOR RANGE OF-
        (1)/(2)/(3)  FOR  (SIN THETA/LAMBDA)/(INTENSITY)/(FO)
  51-60 LOWER LIMIT OF QUANTITY REQUESTED IN COLS 46-50
  61-70 UPPER LIMIT OF QUANTITY REQUESTED IN COLS 46-50

END     - END CARD.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =SIGMA2= PROGRAM

SIGMA2	CALLING CARD FOR =SIGMA2= PROGRAM
*WEIGHT	NUMBER OF ATOMS OF VARIOUS TYPES IN A UNIT CELL
END	END CARD

* THESE CARDS ARE OPTIONAL.

*****READS =NFILEA= WHEN RUN FROM DATA FILE*****

*****WRITES =NFILEE= WHEN PRODUCING EQUATIONS ON EXTERNAL FILE*****

B. CARD FORMATS FOR =SIGMA2= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

SIGMA2 - CALLING CARD FOR THE =SIGMA2= PROGRAM.
FORMAT (A2,A4,1X,A4,A2,F7.3,2I2,1X,A4,A2,I2,I4,2F7.3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	SIGMA2
7	BLANK
8-13	COMPOUND IDENTIFICATION CODE
14-20	NEG/0/BLANK EMIN=1.5 (EMIN)
21-22	0/1/2 EQS AND NO CARDS/EQS AND CARDS/CARDS AND NO EQS. (IPUNCH)
23-24	0/1 E'S FROM TAPE/CARDS (IF BOTH TAPE AND CARD INPUT, IREAD=0) (IREAD)
25	BLANK
26-31	LABEL FOR CARDS (CDLAB)
32-33	0/1 DO/DON'T WRITE BINARY TAPE (KEY)
34-37	NUMBER OF E'S TO DEFINE PHASES FOR (M)
38-44	MINIMUM E VALUE FOR WHICH TO DEFINE PHASE (FM)
45-51	ABSOLUTE CUTOFF FOR GENERATORS (BLANK = EMIN) (EMIN2)

WEIGHT - NUMBER OF ATOMS OF VARIOUS TYPES IN A UNIT CELL.
FORMAT (A2,A4,22I3)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	WEIGHT
7-9	NUMBER OF ATOMS OF TYPE 1 IN CELL (IXN(1))
10-12	ATOMIC NUMBER OF ATOMS OF TYPE 1 (IXN(2))
13-15	NUMBER OF ATOMS OF TYPE 2 IN CELL (IXN(3))
16-18	ATOMIC NUMBER OF ATOMS OF TYPE 2 (IXN(4))
19-21	ETC.
-	
-	
-	
70-72	ATOMIC NUMBER OF ATOMS OF TYPE 11 (IXN(22))

END - END CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	END
4-72	BLANK

A. CARD ORDER SUMMARY FOR =UPDATE= PROGRAM

UPDATE	CALLING CARD FOR THE =UPDATE= PROGRAM
*INSERT	INSERT A CARD OR CARDS
*DELETE	DELETE THE SPECIFIED CARD OR CARDS AND INSERT THE FOLLOWING CARDS, UP TO THE NEXT CONTROLL CARD, IN THEIR PLACE
*PRINT	WRITE OFF LINE THE SPECIFIED SUBROUTINE FROM THE SYMBOLIC TAPE
*PUNCH	PUNCH A SPECIFIED SUBROUTINE FROM THE SYMBOLIC TAPE
END	LAST CARD IN =UPDATE= DATA DECK

* THESE CARDS ARE OPTIONAL

B. CARD FORMATS FOR =UPDATE= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

UPDATE - CALLING CARD FOR THE =UPDATE= PROGRAM.
FORMAT (A2,A4,9X,5I5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	UPDATE
7-18	BLANK
19	0/1 DO NOT/DO PRINT THE ENTIRE TAPE
20-23	BLANK
24	0/1 DO NOT/DO PUNCH THE ENTIRE TAPE
25-28	BLANK
29	0/1 DO NOT/DO COPY THE TAPE (*)
30-33	BLANK
34	0/1 DO NOT/DO END OF FILE THE TAPE BEFORE EACH SUBROUTINE
35-38	BLANK
39	0/1 DO NOT/DO PRINT A TABLE OF CONTENTS OF THE TAPE

(*) =UPDATE READS =NFILEI= AND WRITES =NFILEJ=

INSERT - LOCATION WHERE THE CARD OR CARDS WHICH FOLLOW, UP TO THE NEXT CONTROLL CARD, ARE TO BE INSERTED.
FORMAT (A2,A4,14X,A4,I4,7X,3I5)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	INSERT
7-20	BLANK
21-24	DECK NAME AS NUXX OR XYXX. IF DECK NAME IS BLANK INSERTION IS MADE AT THE FRONT OF THE TAPE (BEFORE FIRST SUBROUTINE)
25-28	NUMBER OF CARD AFTER WHICH INSERTION IS TO BE MADE
29-39	BLANK
40	0/1 DO NOT/DO PRINT THIS SUBROUTINE
41-44	BLANK
45	0/1 DO NOT/DO PUNCH THIS SUBROUTINE
46-49	BLANK
50	0/1 DO NOT/DO END OF FILE THE TAPE **BEFORE** THIS SUBROUTINE

DELETE - DELETE ALL CARDS IN THE SPECIFIED RANGE. ALL CARDS WHICH FOLLOW WILL BE INSERTED UP TO THE NEXT CONTROLL CARD.
FORMAT (A2,A4,14X,A4,I4,2X,I4)

```
  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   DELETE
  7-20  BLANK
  21-24 DECK NAME
  25-28 NUMBER OF FIRST CARD TO BE DELETED
  29-30 BLANK
  31-34 NUMBER OF LAST CARD TO BE DELETED
  35-39 BLANK
  40    0/1  DO NOT/DO  PRINT THIS SUBROUTINE
  41-44 BLANK
  45    0/1  DO NOT/DO  PUNCH THIS SUBROUTINE
  46-49 BLANK
  50    0/1  DO NOT/DO  END OF FILE THE NEW TAPE BEFORE THIS SUBROUTINE

PRINT  - PRINT OFF LINE THE SPECIFIED SUBROUTINE.
     FORMAT (A2,A4,14X,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   PRINT
  6-20  BLANK
  21-24 DECK NAME
  25-44 BLANK
  45    0/1  DO NOT/DO  PUNCH THIS SUBROUTINE
  46-49 BLANK
  50    0/1  DO NOT/DO  END OF FILE THE TAPE **BEFORE** THIS SUBROUTINE

PUNCH  - PUNCH THE SPECIFIED SUBROUTINE.
     FORMAT (A2,A4,14X,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-5   PUNCH
  6-20  BLANK
  21-24 DECK NAME
  25-39 BLANK
  40    0/1  DO NOT/DO  PRINT THIS SUBROUTINE
  41-49 BLANK
  50    0/1  DO NOT/DO  END OF FILE THE TAPE **BEFORE** THIS SUBROUTINE

END    - LAST CARD OF =UPDATE= DECK.
     FORMAT (A2,A4)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-3   END
  4-72  BLANK
```

A. CARD ORDER SUMMARY FOR =USIFT= PROGRAM

USIFT	CALLING CARD FOR =USIFT= PROGRAM.
*SKIP	THE CHARACTERISTICS OF A CARD WHICH IS TO BE DELETED.
*ADD	INSERT A CARD EITHER BEFORE OR AFTER A CARD WITH A SIGNAL WORD.
*SETCHK	CHANGE A SPECIFIC WORD OR PHRASE THROUGHOUT THE DECK.
*TOC	A TABLE OF CONTENTS OF THE TAPE PRINTED.
*SYSSAV	SAVE ALL SYSTEM CARDS.
*SYSKIL	ELIMINATE ALL SYSTEM CARDS.
BEGIN	THE BEGIN CARD.

NOTE 1 - SINCE CARDS OF THE EXTERNAL SYSTEM ARE NOT IN GENERAL FORMATED IN A MANNER CONSISTENT WITH THE RULES OF FORTRAN, THEIR HANDLING IS VERY OFTEN ERRONEOUS. CONSEQUENTLY, WHEN SYSTEM CARDS ARE PRESENT ONE MUST USE EITHER THE SYSSAV OR THE SYSKIL CARD.

NOTE 2 -THE UPDATE PROCEDURE READS =NFILEI= AND WRITES =NFILEJ=.

B. CARD FORMATS FOR =USIFT= PROGRAM

OPERATION CARDS (DESCRIBED IN SECTION 2.GENERL-A. THE OPERATION CARD FORMATS ARE GIVEN IN SECTION 2.GENERL-B) MAY BE INSERTED AT ANY PLACE DESIRED BY THE USER.

USIFT - CALLING CARD FOR =USIFT= PROGRAM.
FORMAT (A2,A4,66A1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	USIFT
6	BLANK
7-13	(T/CTP)

WHERE T=TAPE,C=CARD, AND P=PRINT. THE SLASH DIVIDES THE INPUT FIELD FROM THE OUTPUT. IN THE ABOVE CASE THE INPUT IS FROM TAPE. THE INPUT COULD ALSO COME FROM CARDS. THUS (C/C) STATES THAT THE INPUT IS CARDS AND THE OUTPUT IS ONLY AS PUNCHED CARDS. THE SPECIFICATION CAN BE ANYWHERE BETWEEN COLUMNS 7 AND 72. THE ONLY RESTRICTION IS THAT NO BLANK MAY APPEAR WITHIN THE BRACKETS.

SKIP - CHARACTERISTICS OF A CARD WHICH IS TO BE DELETED.
FORMAT (A2,A4,3I3,4X,13A4,A1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-4	SKIP
5-6	BLANK
7-9	CARD COLUMN WHERE SCAN SHOULD BE INITIATED.
10-12	THE NUMBER OF LETTERS IN THE SIGNAL WORD.
13-15	THE LOCATION WHERE THE SCAN SHOULD BE TERMINATED.
20-72	THE SIGNAL WORD.

NOTE 1 - IF 7-9 AND 13-15 ARE BLANK THE ENTIRE CARD WILL BE SCANNED.

NOTE 2 - IF ALL RETURN CARDS ARE TO BE SKIPPED, THE SKIP CARD WOULD BE AS FOLLOWS,

```
00000000011111111112222222
12345678901234567890123 45
SKIP    7  6 20    RETURN
```

ADD - INSERT A CARD EITHER BEFORE OR AFTER A CARD WITH A SIGNAL WORD.
FORMAT (A2,A4,1X,I1,5I2,1X,15A4,A1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	ADD

```
4-7    BLANK
8      (ZERO)/(ONE) FOR (SUBSTITUTION TO BE BEFORE THE CARD WITH THE SIGNAL
       WORD)/(THE NEW CARD IS TO FOLLOW THE CARD WITH THE SIGNAL WORD)
9-10   LOCATION OF THE FIRST SYMBOL IN THE SIGNAL WORD.
11-12  THE NUMBER OF SYMBOLS IN THE SIGNAL WORD.
13-14  THE LOCATION OF A WORD ON THE SIGNAL CARD WHICH IS TO BE INCLUDED ON
       THE INSERTED CARD AT LOCATION ****, (****COULD BE EITHER A NUMBER OR A
       WORD).
15-16  THE MAXIMUM NUMBER OF SYMBOLS TO BE TRANSFERRED.
17-18  THE LOCATION WHERE THE SCAN IS TO BE TERMINATED.
19     BLANK
20-80  THE SIGNAL WORD.

NOTE 1 - AN * MUST BE PRESENT FOR EACH SYMBOL TRANSFERRED.

NOTE 2 - IF AN IBM 7094 $IBFTC CONTROL CARD IS TO BE INSERTED PRIOR TO EACH
         SUBROUTINE CARD USING THE DECK NAME FROM COLUMNS 73-76 OF THE
         SUBROUTINE CARD, THE INSERT CARD WOULD BE AS FOLLOWS,
             00000000011111111112222222222
             12345678901234567890123456789
             INSERT 0 71073 4   SUBROUTINE
             $IBFTC ****

SETCHK - CHANGE A SPECIFIC WORD OR PHRASE THROUGHOUT THE DECK.
    FORMAT (A2,A4,4I3,1X,13A4,A1)

  COLS  SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
  1-6   SETCHK
  7-9   THE LOCATION ON THE CARD WHERE THE COMPUTER SHOULD START CHECKING
         FOR THE WORD OR PHRASE WHICH IS TO BE REPLACED.
  10-12 THE NUMBER OF COLUMNS OCCUPIED BY THE WORD OR PHRASE (E.G. AS IT
        APPEARS STARTING IN COLUMN TWENTY OF THE SETCHK CARD).
  13-15 THE NUMBER OF COLUMNS OCCUPIED BY THE REPLACING WORD OR PHRASE (E.G.
        AS IT APPEARS ON THIS CARD).
  16-18 THE COLUMN AT WHICH THE SETCHK SCAN SHOULD BE TERMINATED.
  19    BLANK
  20-72 THE WORD OR PHRASE TO BE REPLACED FOLLOWED BY THE REPLACING WORD OR
        PHRASE.  DO NOT LEAVE BLANKS BETWEEN THE TWO WORDS OR PHRASES UNLESS
        THEY ARE SIGNIFICANT.

NOTE 1 - WHEN A NUMBER IS PRESENT IT IS SIGNIFIED BY A $.  IF THE NUMBER IS TO
         BE INCLUDED IN THE REPLACING WORD OR PHRASE, THE $ IS PLACED IN THE
         APPROPRIATE POSITION.  IF MORE THAN ONE NUMBER IS PRESENT, DENOTE
         AS $1, $2, ETC. (E.G. READ($1,$2)    ).  IF A WORD IS TO BE RETAINED
         THEN AN * IS TO BE USED, (E.G. READ(IN,9) IS READ(*,$)   ).  A
         MAXIMUM OF SIX LETTERS WILL BE ALLOWED FOR EACH *.  ALL BRACKETS,
         COMMAS, AND PERIODS (EXCEPT FOR DECIMAL POINTS) MUST BE INCLUDED.
         FOR A STRING OF WORDS USE ** (E.G.  DATA */**/ GOING TO DATA *(**)   ).
         IF MORE THAN ONE WORD OR PHRASE IS REQUIRED IN A GIVEN SETCHK
         CORRECTION, USE *1, *2, ETC. OR **1, **2, ETC.

NOTE 2 - IF COLUMNS 7-9 ARE BLANK, THE ENTIRE CARD WILL BE SCANNED.

NOTE 3 - IF ONE WISHES TO REPLACE THE FORTRAN 'READ NUM,' STATEMENT BY
```

'READ(BUFFER,NUM)', WHERE 'NUM' REPRESENTS THE FORMAT NUMBER, THE FOLLOWING CARD CAN BE USED.

```
0000000001111111111222222222233333333333
1234567890123456789012345678901234567890
SETCHK  7  6 14 45 READ$,READ(BUFFER,$)
```

TOC - THE TOC CARD CAUSES A TABLE OF CONTENTS OF THE TAPE TO BE PRINTED. THE TABLE APPEARS ON THE RIGHT SIDE OF THE OUTPUT.
FORMAT (A3,69X)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-3	TOC
-72	BLANK

SYSSAV - SAVE ALL SYSTEM CARDS.
FORMAT (A2,A4,1X,A1,I2,4X,I1)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	SYSSAV
7	BLANK
8	FLAG SYMBOL SUCH AS $ FOR THE IBM 7094 AND / FOR THE IBM 360.
9-10	COLUMN IN WHICH FLAG APPEARS.
11-14	BLANK
15	(BLANK)/(1) (DO NOT)/(DO) PUNCH A DECK OF ALL CONTROL CARDS.
16-72	BLANK

SYSKIL - ELIMINATE ALL SYSTEM CARDS.
FORMAT (A2,A4,1X,A1,I2)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-6	SYSKIL
7	BLANK
8	FLAG SYMBOL (SEE SYSSAV)
9-10	COLUMN IN WHICH FLAG APPEARS.
11-72	BLANK

BEGIN - THE BEGIN CARD.
FORMAT (A2,A4)

COLS	SPECIFIED PUNCHING OR FUNCTION OF THE FIELD
1-5	BEGIN

LIST OF CONTRIBUTORS TO THE SYSTEM

THE BURDEN OF THE CODING OF THE X-RAY SYSTEM IN FORTRAN HAS FALLEN TO F.A. KUNDELL, R.V. CHASTAIN, AND J.M. STEWART. THE FOLLOWING PEOPLE HAVE CONTRIBUTED ACTIVELY TO THE EFFORT. IN THE TEXT IN SECTION 1 IS GIVEN THE HISTORICAL AUTHORS OF THE VARIOUS PROGRAMS.

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DESCRIPTION OF THE X-RAY SYSTEM BINARY DATA FILE

EACH ARBITRARY CLASS OF CRYSTALLOGRAPHIC AND ACCOUNTING DATA HAS A PLACE IN THE FILE. THE ASSIGNMENT OF THIS PLACE IS FIXED AND THEREFORE IT IS IMPORTANT THAT THE UTMOST CAUTION BE EXERCISED IN CHANGING AND UPDATING IT. ONE BASIC TENENT, AND THE MOST IMPORTANT ONE, IS THAT NO PROGRAM OF THE SYSTEM WHICH COPIES THE FILE LOSES ANY INFORMATION. IT MAY ADD SOME OR IT MAY SUPERCEDE SOME BUT IT SAVES AND COPIES ALL THE REST.

IN ORDER TO FACILITATE THE MAINTENANCE OF THE DATA FILE, THE SYSTEM HAS FIVE SUBROUTINES, NUC009 TO NUC013. NUC009 SERVES TO SIGN ON THE READING AND WRITING OF A BINARY DATA FILE. NUC010 IS TO COPY SPECIFIED LOGICAL RECORDS OF A FILE. NUC011 IS TO READ A RECORD OF A FILE AND NUC012 TO WRITE ONE. NUC013 IS FOR UNBUFFERING PACKED LOGICAL RECORDS (E.G., ATOM PARAMETERS, REFLECTIONS). ALL READING AND WRITING IS DONE FROM A LABELED COMMON ARRAY CALLED IOBUF WITH LABEL/IO/. THIS ARRAY IS 255 WORDS LONG AND THE FIRST FOUR WORDS SERVE TO CHARACTERIZE THE RECORD. RECORDS IN THE FILE ARE ALWAYS LESS THAN 255 WORDS LONG BECAUSE OF THE LIMITATION ON IOBUF. PROVISION HAS BEEN MADE, HOWEVER, FOR ANY NUMBER OF PHYSICAL RECORDS TO FORM A LOGICAL RECORD. THE MAIN BURDEN IN ANY PROGRAM IS THE REFORMING OF LONG ARRAYS FROM IOBUF INTO THEIR PROPER PLACE IN STORAGE. IOBUF (1) TO (4) ARE EQUIVALENT TO IOBUF1 TO IOBUF4 FOR EASE OF PROGRAMMING OF IO STATEMENTS.

THE PURPOSE OF THE FIRST FOUR WORDS OF EVERY PHYSICAL RECORD.

WORD 1 IS THE COUNT OF ALL OF THE WORDS IN THE PHYSICAL RECORD. FOR EXAMPLE THE READ IN NUC011....

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READ(N)IOBUF1,(IOBUF(J),J=2,IOBUF1)
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WHILE IN NUC012 IT SAYS

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WRITE(N)(IOBUF(J),J=1,IOBUF1)
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WORD 2 IS THE SIGNAL THAT THERE ARE MORE PHYSICAL RECORDS IN THIS LOGICAL RECORD. ZERO MEANS LAST, NON-ZERO MEANS THAT THERE ARE MORE TO FOLLOW.
WHEN THERE ARE MORE THAN ONE PHYSICAL RECORD IN A LOGICAL RECORD WORD 2 IS SEQUENTIAL 1,2,3,4, ETC UNTIL THE LAST PHYSICAL RECORD WHERE WORD 2 IS ZERO AS IT IS FOR ALL SINGLE PHYSICAL RECORD PER LOGICAL RECORD CASES.

WORD 3 IS THE IDENTIFICATION OF THE LOGICAL RECORD TYPE. THIS IS CHECKED BY NUC011 AND THE QUIT FLAG SET TO 1 IF ANY GIVEN RECORD IS MISSING.
THESE ARE THE INTEGERS 1 TO MAXREC. MAXREC IS THE X-RAY END-OF-FILE MARK AND IS TREATED AS SUCH BY THE FILE HANDLING PROGRAMS.

WORD 4 IS THE NUMBER OF WORDS PER ITEM IN THE PARTICULAR LOGICAL RECORD TYPE (E.G. NUMBER OF WORDS PER REFLECTION IN LOGICAL RECORD OF TYPE 15). IN THOSE LOGICAL RECORDS WHERE IT IS NOT USED IT IS SET EQUAL TO ZERO.

WORD 5 THROUGH THE NUMBER OF WORDS SPECIFIED IN WORD 1 IS THE DATA AS DESCRIBED BELOW FOR EACH RECORD TYPE.

THE LOGICAL RECORDS OF THE X-RAY SYSTEM DATA FILE ARE....

RECORD 1 IS THE HISTORY RECORD
(EACH PROGRAM THAT COPIES THE TAPE =SIGNS ON=)
SEE FUNCTION OF NUC009

RECORD 2 IS THE LABEL RECORD (UP TO 1000 CHARACTERS)

RECORD 3 IS CELL CONSTANT INFORMATION

RECORD 4 IS SYMMETRY INFORMATION.

RECORD 5 IS AT PRESENT UNDEFINED

RECORD 6 IS FORM FACTOR AND CELL CONTENTS INFORMATION

RECORD 7 IS THE SCALE FACTOR RECORD

RECORD 8 IS THE ABSORPTION INFORMATION,CRYSTAL SIZE AND ORIENTATION

RECORD 9 IS MISCELLANEOUS INFORMATION FOR KEYING IMPORTANT PROGRAMS

RECORD 10 IS THE ATOMIC PARAMETERS

RECORD 11 IS THE STANDARD DEVIATIONS OF THE ATOMIC PARAMETERS

RECORD 12 IS REFINEMENT SIGNAL AND SPECIAL POSITION INFORMATION

RECORD 13 AND 14 ARE AT PRESENT UNDEFINED

RECORD 15 IS THE REFLECTION RECORD

RECORD 16 IS THE RESCALE FACTOR RECORD

RECORD 17 IS THE OUTPUT OF THE FOURIER

RECORD 18 IS THE RESULT OF A 'BONDLA' SEARCH FOR ATOMIC CONNECTIONS.
(COORDINATES)

RECORD 19 IS THE LEAST SQUARES MATRIX

RECORD 20, 21, 22, 23, AND 24 ARE AT PRESENT UNDEFINED

RECORD 25 IS CURRENTLY THE END OF FILE SIGNAL (MAXREC IS SET BY NUSY TO 25)

(THAT IS TO SAY, WHEN A RECORD OF TYPE TWENTY-FIVE IS ENCOUNTERED IN THE FILE IT IS TREATED AS AN X-RAY-SYSTEM END OF FILE MARK.)

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IN WHAT FOLLOWS THE FIRST FOUR WORDS ARE IN EVERY RECORD SET JUST THE SAME WAY AS SHOWN ABOVE.
GIVEN ABOVE.

STRUCTURE OF RECORD 1-IDENTITY

WORDS 5 AND 6 ARE THE COMPOUND IDENTITY CODE AS A2,A4
WORDS 7 THRU 22 FORM THE CURRENT TAPE LABEL AS 16A4
WORDS 23 TO THE END ARE THE PROGRAM IDENTITY CODES
TWO WORDS EACH AS A2,A4 (E.G. DATRDN, FC, ETC.)

STRUCTURE OF RECORD 2-LABEL OR ABSTRACT

WORD 5 IS THE NUMBER OF A4 WORDS OF LABEL INFORMATION
WORD 6 TO WORD 255 BLANKS OR LABEL INFORMATION

STRUCTURE OF RECORD 3-CELL QUANTITIES

WORD 5 METRIC TENSOR - ELEMENT 1,1 A**2
WORD 6 METRIC TENSOR - ELEMENT 1,2 A*B*COS(GAMMA)
WORD 7 METRIC TENSOR - ELEMENT 1,3 A*C*COS(BETA)
WORD 8 METRIC TENSOR - ELEMENT 2,1 A*B*COS(GAMMA)
WORD 9 METRIC TENSOR - ELEMENT 2,2 B**2
WORD 10 METRIC TENSOR - ELEMENT 2,3 B*C*COS(ALPHA)
WORD 11 METRIC TENSOR - ELEMENT 3,1 A*C*COS(BETA)
WORD 12 METRIC TENSOR - ELEMENT 3,2 B*C*COS(ALPHA)
WORD 13 METRIC TENSOR - ELEMENT 3,3 C**2
WORD 14-22 RECIPRICAL METRIC TENSOR.
WORD 23 A
WORD 24 B
WORD 25 C
WORD 26 COS(ALPHA)
WORD 27 COS(BETA)
WORD 28 COS(GAMMA)
WORD 29 A*
WORD 30 B*
WORD 31 C*
WORD 32 COS(ALPHA*)
WORD 33 COS(BETA*)
WORD 34 COS(GAMMA*)
WORD 35-43 TRANSFORMATION MATRIX FROM FRACTIONAL COORDINATES TO ORTHOGONAL ANGSTROMS COORDINATES
WORD 44-52 TRANSFORMATION MATRIX MILLER INDICES TO ORTHOGONAL PSEUDO-MILLER INDICES
WORD 53 UNUSED
WORD 54 CELL VOLUME
WORD 55 RECIPROCAL CELL VOLUME
WORD 56-61 COEFFICIENTS IN SINE THETA/ LAMBDA EQUATION

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                (H**2)*WORD(47) + ETC.
WORD  62  SIN(ALPHA)
WORD  63  SIN(BETA)
WORD  64  SIN(GAMMA)
WORD  65  SIN(ALPHA*)
WORD  66  SIN(BETA*)
WORD  67  SIN(GAMMA*)
WORD  68  ALPHA IN DEGREES
WORD  69  BETA IN DEGREES
WORD  70  GAMMA IN DEGREES
WORD  71  ALPHA*
WORD  72  BETA*
WORD  73  GAMMA*
WORDS 74-76  - STANDARD DEVIATION IN A,B, AND C
WORDS 77-79  - STANDARD DEVIATION IN COS(ANGLE)
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STRUCTURE OF RECORD 4-SYMMETRY INFORMATION

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 WORD 5  LATTICE TYPE   P  I  R  F  A  B  C
         ACENTRIC AS    1  2  3  4  5  6  7
          CENTRIC AS    8  9 10 11 12 13 14
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WORD 6 0/1 FOR ACENTRIC/CENTRIC

WORD 7 NUMBER OF SYMMETRY OPERATIONS LESS THE CENTER AND ANY LATTICE CENTERING. (N)

WORD 8 NUMBER OF ROTATION MATRICES OF IDENTICAL PATTERN OF ZEROS

WORD 9 FC MULTIPLIER

WORD 10 TO 12*(N) + 9
ARE THE ROTATION MATRICES AND TRANSLATION VECTORS.

ORDER OF THE MATRIX R11,R12,R13,R21,R22,R23,R31,R32,R33,T1,T2,T3

THERE MAY BE MORE THAN ONE PHYSICAL RECORD IN THIS LOGICAL RECORD

STRUCTURE OF RECORD 5

* TO BE SET

STRUCTURE OF RECORD 6-CELL CONTENTS AND FORM FACTORS

WORD 5 F(0,0,0)

WORD 6 E(0,0,0)
WORD 7 NSCAT THE NUMBER OF DIFFERENT ATOM TYPES

FOR EACH ATOM TYPE THERE IS A LIST OF VARIABLE LENGTH WHICH CONTAINS THE FOLLOWING ITEMS IN ORDER, STARTING AT WORD 8 AND REPEATING AS NEEDED.

1 ATOM NAME (A4)
2 BLANKS FOR POSSIBLE EXPANSION OF ATOM NAME ID
3 NUMBER OF ENTRIES (N) IN S.F. TABLES.
4 NUMBER OF ATOMS OF THIS TYPE IN WHOLE UNIT CELL
5 ATOMIC WEIGHT OF THIS SPECIES (SCALE C=12)
6 FLAG THAT NEXT TWO WORDS ARE VALID DISPERSION INFORMATION
0 = NONE 1 = VALID INFORMATION
7 REAL PART OF DISPERSION CORRECTION FOR THIS ATOM TYPE
8 IMAGINARY PART
9 TO 8 + N SINE THETA OVER LAMBDA ENTRIES
9 + N TO 8 +2*N FORM FACTOR ENTRIES AS SUPPLIED

THE WHOLE REPEATED FOR EACH ATOM TYPE.

THERE MAY BE MORE THAN ONE PHYSICAL RECORD IN THIS LOGICAL RECORD.

STRUCTURE OF RECORD 7-SCALE FACTORS

WORD 5 B
WORD 6 NSCALE, THE NUMBER OF SCALE FACTORS GROUPS
WORD 7 TO 6+NSCALE ARE THE F-RELATIVE SCALE FACTORS

STRUCTURE OF RECORD 9-MISCELLANEOUS INFORMATION FOR KEYING
IMPORTANT PROGRAMS

WORD 5 UNUSED
WORDS 6,7, AND 8 NUMBER OF GRID POSITIONS IN X,Y, AND Z DIRECTIONS
WORDS 9,10, AND 11 MAXIMUM MAGNITUDE OF H,K, AND L
WORD 12 UNUSED
WORD 13 TO 29 ARE THE CALCULATION CODES CALCOS(1) TO CALCOS(17)
WORD 30 NUMBER OF POINTS IN X DIRECTION
WORD 31 ORIGIN VALUE IN X DIRECTION
WORD 32 INCREMENT ALONG X DIRECTION
WORDS 33,34,35, FOR Y
WORDS 36,37,38 FOR Z
WORDS 39,40,41 SCANNING INDEX FOR X,Y, AND Z
1 = FIRST, 2 = SECOND, 3 = THIRD
WORD 42 NUMBER OF POINTS ON ONE PAGE LINE
WORD 43 SPACE CONTROL
WORD 44 NUMBER OF TYPE COLUMNS PER GRID COLUMN
WORD 45 INCH PER ANGSTROM SCALE
WORDS 46-47 FOURIER MAPPING LIMITS
WORDS 48-50 SORTING ORDER H,K,L, (1) MINOR, (2) INTERMEDIATE,
AND (3) MAJOR.
WORD 51 MINIMUM VALUE OF SIN(THETA)/LAMBDA
WORD 52 MAXIMUM VALUE OF SIN(THETA)/LAMBDA

STRUCTURE OF RECORDS 10, 11, AND 12, ATOM PARAMETERS, STANDARD
DEVIATIONS OF ATOM PARAMETERS, AND REFINEMENT SIGNALS FOR ATOM
PARAMETERS - THESE LOGICAL RECORDS ARE ALL SUBSTANTIALLY THE
SAME IN STRUCTURE - THEREFORE THEY ARE ALL DESCRIBED TOGETHER.
THESE ATOMS CONSTITUTE AN ASYMMETRIC SET OF THE ATOMS IN THE CELL.

WORD CONTENTS IN LOGICAL RECORD 10 IN 11 IN 12

4	19	19	19
5	FIRST PART OF ATOM ID (A4)	SAME AS IN 10	SAME
6	LAST PART OF ATOM ID (A2)	SAME AS IN 10	SAME
7	FRACTIONAL X PARAMETER	STAND. DEV. IN X	SIGNAL
8	FRACTIONAL Y PARAMETER	STAND. DEV. IN Y	SIGNAL
9	FRACTIONAL Z PARAMETER	STAND. DEV. IN Z	SIGNAL
10	SCATTERING FACTOR POINTER. INTEGER GIVES POSITION OF S.F. IN REFLECTION RECORD.	SAME AS IN 10	SAME
11	TEMPERATURE FACTOR TYPE 0 OVERALL 1 INDIVIDUAL ISOTROPIC 2 INDIVIDUAL ANISOTROPIC	SAME AS IN 10	NOT USED
12	B ISOTROPIC TEMPERATURE FACTOR.	STANDARD DEVIATION IN B.	SIGNAL
13	BETA 11	S. D. IN BETA 11	SIGNAL
14	BETA 22	S. D. IN BETA 22	SIGNAL
15	BETA 33	S. D. IN BETA 33	SIGNAL
16	BETA 12	S. D. IN BETA 12	SIGNAL
17	BETA 13	S. D. IN BETA 13	SIGNAL
18	BETA 23	S. D. IN BETA 23	SIGNAL
19	INDIVIDUAL ATOM SCALE FACTOR(POPULATION PARAMETER)	S. D. IN POPULATION PARAMETER.	SIGNAL
20	DISPERSION CORRECTION SIGNAL	NOT USED	NOT USED
21	SPARE	NOT USED	NOT USED
22	SPARE	NOT USED	NOT USED
23	SPARE	NOT USED	NOT USED

THE 19 WORDS ARE REPEATED AS NEEDED TO FORM THE LOGICAL RECORDS WITH UP TO 13 ATOMS PER PHYSICAL RECORD.

THE REFINEMENT SIGNALS ARE AS FOLLOWS
SIGNAL MEANING (BELOW N IS 1 TO 9 RESPECTIVELY FOR X,Y,Z,BETA11, BETA22,BETA33,BETA12,BETA13,BETA23

0 NO REFINEMENT PARAMETER IS FIXED

1 STANDARD REFINEMENT SHIFT PARAMETER NORMALLY

1N SET PARAMETER EQUAL TO NEW PARAMETER N

2N SET PARAMETER EQUAL TO MINUS THE NEW PARAMETER N

3N SET PARAMETER EQUAL TO HALF N

4N SET TO -1/2 N

STRUCTURE OF RECORD 15 REFLECTION INFORMATION..

THERE ARE AS MANY REFLECTIONS PER PHYSICAL RECORD AS THE BUFFER SIZE WILL PERMIT. MORE FOR LOW SYMMETRY FEW SCATTERING FACTORS FEWER FOR HIGH SYMMETRY MANY S. F. TYPES.
WORD 4 IS USED TO SUPPLY THE NUMBER OF ENTRIES PER REFLECTION
36 + NSCAT + JGEN
WHERE NSCAT IS THE NUMBER OF DIFFERENT SCATTERING FACTOR TYPES
AND JGEN THE NUMBER OF WORDS OF SYMMETRY INFORMATION PER REFLECTIO
WORD 5 - H
WORD 6 - K
WORD 7 - L
WORD 8 - INTENSITY
WORD 9 - BACKGROUND INTENSITY
WORD 10 - SCALE FACTOR GROUP
WORD 11 - NUMBER OF TIMES REFLECTION OBSERVED
WORD 12 - ABSORPTION CORRECTION (1/TRANSMISSION COEFFICIENT)
WORD 13 - JCODE
1 - - OBSERVED
2 - - LESS THAN
3 - - EXTINCT
4 - - IGNORE REFLECTION
5 - - SPACE GROUP EXTINCT
WORD 14 - SIN(THETA) /LAMBDA
WORD 15 - 1/LP
WORD 16 - MAGNITUDE OF F(RELATIVE)
WORD 17 - THRESHOLD F(RELATIVE)
WORD 18 - WEIGHT FOR LEAST SQUARES
WORD 19 - MAGNITUDE OF F(CALCULATED)
WORD 20 - A
WORD 21 - B
WORD 22 - NORMALIZED STRUCTURE FACTOR (E)
WORD 23 - EPSILON
WORD 24 - ESTIMATED PHASE (CYCLES)
WORD 25 - PROBABILITY THAT ESTIMATED PHASE CORRECT
WORD 26 - A CORRECTED FOR DISPERSION
WORD 27 - B CORRECTED FOR DISPERSION
WORD 28 - PARTIAL CONTRIBUTION TO A
WORD 29 - PARTIAL CONTRIBUTION TO B
WORD 30 - PARTIAL CONTRIBUTION TO A WITH DISPERSION
WORD 31 - PARTIAL CONTRIBUTION TO B WITH DISPERSION
WORD 32 - STANDARD DEVIATION OF INTENSITY

WORD 33 - RATIO OF FC WITHOUT DISPERSION CORRCTION TO FC WITH
DISPERSION CORRECTION
WORD 34 - UNUSED
WORD 35 - UNUSED
WORD 36 - UNUSED
WORD 37 - UNUSED
WORD 38 - UNUSED
WORD 39 - UNUSED
WORD 40 - UNUSED
WORD 41 - INTERPOLATED SCATTERING FACTOR ENTRIES FOR EACH ATOM
TYPE - STORED IN ORDER SCATTERING FACTS ENTERED IN
RECORD 6
WORD 40 + NSCAT LAST OF THE SCATTERING FACTOR ENTRIES
WORD 41 + NSCAT FIRST ENTRY IN THE SYMMETRY DIRECTOR LIST(JGENER)
WORD 40 + NSCAT + JGEN LAST OF THE SYM. DIR.(REFLECTION MULTIPL.)
WORD 41 + NSCAT + JGEN IS THE H OF THE NEXT UNIQUE REFLECTION
THE WHOLE IS REPEATED UNTIL BUFFER IS FULL OR REFLECTION LIST IS
COMPLETED. ALL REFLECTIONS ARE IN ONE LOGICAL RECORD.
-THE FORMAT OF THE SYMMETRY DIRECTORS IS AS FOLLOWS.....
THE BAND OF S.D. HAS BEEN CALLED THE JGENER(J) BAND FROM TIME
IMMEMORIAL. SO BE IT NOW. JGENER(1) IS PACKED WITH THE NO. OF
SYMMETRY OPERATIONS FOR A VALUE OF H,K,L ALONG WITH THE MAGNITUDES OF
H,K, AND L. PACKING IS ACCOMPLISHED BY .... (IN FORTRAN)
JGENER(J) = ICOUNT + IH*128 + IK*16384 + IL*2097152
MULTIPLIES SERVE AS SHIFTS FOR PACKING PURPOSES ALL QUANTITIES
ARE MAGNITUDES SO NO - SIGNS ARE INVOLVED.
JGENER(2) ET. SEQ. CONTAIN THE ICOUNT PAIRS OF SIGN AND PHASE
SHIFT INFORMATION PACKED AS 4 PAIRS PER WORD(SEE RDGN (XRY134)
FOR DETAILS OF PACKING PROCESS)
WHEN THE ICOUNT IS SATISFIED THERE MAY BE ANOTHER ICOUNT MAG(H), M
MAG(K), AND MAG(L) DEPENDING UPON THE SPACE GROUP BEING TREATED
THE LAST JGENER (JGENER(JGEN)) IS THE REFLECTION MULTIPLICITY,
THAT IS THE NUMBER OF SYMMETRICALLY EQUIVALENT UNIQUELY OBSERVABLE
REFLECTIONS.

STRUCTURE OF RECORD 16 RESCALE INFORMATION
WORD 5 B (NEW VALUE)
WORD 6 NSCALE, THE NUMBER OF SCALE FACTORS GROUPS
WORD 7 TO 6+NSCALE ARE THE F-RELATIVE RESCALE FACTORS
***THE STRUCTURE OF RECORDS 17 AND 19 ARE NOT DEFINED. RECORD 18 IS
STRUCTURED LIKE RECORD 10, 11 AND 12.***