N64-22419

CODE-1 CAT. 25

NASA CR-56479

96 p.

[illegible] DATA

UNIVERSITY OF MARYLAND
COMPUTER SCIENCE CENTER

COLLEGE PARK, MARYLAND

OTS PRICE

XEROX $ 8.60 ph

MICROFILM $ none

RC#3

Technical Report TR-64-6
NsG-398 April 1964

Crystal Structure Calculations System

X-Ray - 63

for the IBM 709/7090/7094

Computer Science Center
University of Maryland
Research Computer Center
University of Washington

The work on this system has been carried out by a number of people at various laboratories throughout the United States. The project was initiated at the Research Computer Center of the University of Washington and then continued and brought to its present form at the Computer Science Center of the University of Maryland. The major part of the computer time for this project was supported by the National Aeronautics and Space Administration grant NsG-398. The list of principal contributors is included as an appendix.

ABSTRACT

23419

This report is designed to serve as an introduction to a set of programs for doing the calculations necessary to solve crystal structures by diffraction techniques. It briefly describes the structure of the "system", lists the current "links" in the system, and shows an example of the use of some of the programs of the system. The detailed users manual is maintained as an expandable file of card images on magnetic tape to be distributed with the current version of the system tape. The system is designed to be run in conjunction with or exclusive of any monitor. This report is specific for the IBM 709/7090/7094. Author

AUTHOR:

I N D E X

	Page
Abstract	
General Description of the X-Ray 63 System	1-13
Appendix	
List of Contributors	14
Listing of Program to Call X-Ray System from B5	15-16
Listing of Program to Use X-Ray System under the IBSYS Monitor	17-20
Listing of Program to Generate a Card for "Cold-Starting" the X-Ray Monitor	21
Detailed Example with Explanation	22 to end

Purpose of the system

X-Ray 63 is designed to bring together the nucleus of a system to carry out the computations required for the solution of crystal structures by X-Ray diffraction techniques. The authors are building a library of crystallographic programs, gathered from many sources, all stored in a single magnetic tape file. These programs are merged in such a manner that they are executable without modification at any 709, 7090, 7094 installation. In addition they may be used in conjunction with nearly all monitors by the preparation of a simple calling program. A concerted effort has been made to make the system user oriented. Thus there are provided many aids, checks, and conveniences for the crystallographer. Each program in the system (link) is designed to maintain the data which is obtained by diffraction measurements as an expandable file on magnetic tape. Thus for each crystalline substance under study, information is accrued during the course of the calculations in such a way that the results of one serve as the input to others. This approach means that fewer and fewer data cards are required as the crystal structure analysis proceeds.

Scope of the system

This report represents a preliminary and general description of X-Ray 63. The system is designed to be enlarged upon and in fact contains programs within itself to accomplish this objective. In order to maintain correctness and currency the details of all the current links in the system are given in a "users" manual which is maintained and supplied, upon request, as a file of card images on magnetic tape. (A program has been prepared to make possible printing the users manual through the use of an IBM 1401.)

The present operational links of the system are given below.

SYSTEM LINK LABELS AND

CALLING CARDS FOR PROGRAM SYSTEM

as of April 1964

This list is the table of library programs in the X-Ray 63 crystallography program system. The latest is furnished with the users manual printed by the 1401. The list will change as additional programs are added to the system.

LINK LABEL	CALLING CARD	PROGRAM
100	LOADER	BEGINNING PROGRAM (BSS LOADER AND TAPE GENERATOR)

1000	FC	PARAMETER LOADER FOR STRUCTURE FACTOR CALC
1001	(CALLED BY FC)	STRUCTURE FACTOR AND STATISTICS PROGRAM (FCTWO)
2100	DFSYNA	DIFFERENTIAL SYNTHESIS
3600	ORFLS	BUSING-MARTIN-LEVY FULL-MATRIX LEAST-SQUARE
4000	FOURR	FOURIER SYNTHESIS
5000	FOUREF	FOURIER REFINEMENT (SHIFTS ATOMS TO FOURIER PEAK)
5500	SHLPAT	SHELL PATTERSON (MERCATOR PROJ. OF SPHERES IN PATTERSON SPACE)
6000	BONDLA	BOND LENGTHS AND ANGLES AND HYDROGEN COORDINATES
6100	ORFFE	BUSING-MARTIN-LEVY FUNCTION AND ERROR
6300	PROJCT	PROJECTION OF A MOLECULE ON A PLANE
6500	LSQPL	LEAST SQUARES PLANE AND LINE
8000	DELSIG	DELTA F VS FO PLOT FOR SIGMA FOR DATA REDUCTION
10000	DATRDN	DATA REDUCTION (1/LP, ABSORBTION, SCALING FORM FACTOR INTERP., SYMMETRY GENERATION, ETC.)
10300	DATCOR	DATA CORRELATION FOR FILMS
10500	DATFIX	CALCULATION OF SCALED UNITARY STRUCTURE FACTORS (E)
10600	MODIFY	SEARCH AND MODIFY REFLECTION TAPE
10700	WEIGHT	PREPARE WEIGHTS FOR LEAST-SQUARES
10800	ESORT	SORT FOR KARLE-HAUPTMAN PHASE DETERMINATION

11000	LISTFC	FINAL STRUCTURE FACTOR LISTING
11100	CRYSET	DONNAY-TAKEDA CRYSTAL TRANSFORMATIONS
12000	RPLANE	CALC. R OVER A PROJECTION FOR MOVED MOLECULE
12200	RLIST	CALC. R FOR SPECIAL CLASSES OF REFLECTION
12500	PARAM	LEAST-SQUARES REFINEMENT OF LATTICE PARAMETERS
15000	TFINFO	CALCULATES TEMPERATURE FACTOR STATISTICS
20000	GESET	GENERAT. OF REFLECT. AND CRYSTAL SET FOR GE XRD-5
30000	PATCON	PATTERSON CONVOLUTION PROGRAM
30600	PEKPIK	SEARCH FOURIER MAP FOR PEAKS
30900	STUJOB	STUDENT PROBLEM GENERATOR
31000	BYEBYE	CONVERT SYSTEM REFLECT. TAPE TO NON-SYSTEM FORMATS
31100	NRLA	SPARE ENTRY -A- FOR EXPERIMENTAL PURPOSES OR ADDITIONAL LINKS
31200	NRLB	SPARE ENTRY -B- FOR EXPERIMENTAL PURPOSES OR ADDITIONAL LINKS
313		
32700	(CALLED BY EXEMW)	EXECUTION ERROR DIAGNOSTICS

Outline of the approach to Crystallographic Computing under the system

1. Each program has a "calling" card which causes X-Ray 63 to load the appropriate program (link) into the memory and begin execution.
2. Each program has a set of required and optional cards the presence or absence of which supply the data and keying for any requested calculation.
3. All the programs communicate information about each structure problem by means of binary magnetic tapes (reflection tapes) as well as card input. These tapes accumulate the information from the cards supplied by the user and calculations done by the programs. As a result, the binary output tapes are designed to serve as input tapes to subsequent calculations. Each program which generates a new reflection tape is designed to preserve and transcribe all data which it does not require and update data which it is designed to process.
4. A series of various calculations using any of the programs of the system may be executed sequentially by stacking program requests and data.
5. Tape switching, or saving, list titling, and other usual system services are provided by the programs.
6. With few exceptions the programs are automatic for all space groups, settings and special positions.

Some details of the structure of the "system"

The solution of crystal structures by means of X-Ray or neutron diffraction requires the treatment of large quantities of data with lengthy calculations. Many of the calculations required in this process are similar from one crystalline substance to another. However, two main approaches have evolved in writing programs for crystallography. One may write crystal and computer laboratory specific programs thus avoiding the difficulties which arise from the attempt to be general; or one may write general programs and attempt to make these programs as independent and adaptable as possible to computer laboratory procedures. The plan of this "system" is to assemble a set of general and interdependent programs as crystallographically oriented as practicable which may be executed, with little or no modification, at any IBM 709, 7090, or 7094 installation. The system consists of a set of absolute programs stored on binary tape. The method of storage mimics the FORTRAN II chain tape structure. Each program is stored in two records. The first is a label, a data channel command which serves to load the second record and the location of the entry point to the program. The absolute program is stored in the second record. The sequential execution of any number of programs of the system is controlled by the system monitor program CALLER. This program communicates with

the laboratory monitor and with the links of the system through low common (high absolute) storage. The initialization of the system is accomplished by the first link on the tape (LOADER). Execution may therefore be initiated by means of a monitor "start" card (1B5CARD or 1A5CARD). A more usual procedure, however, is to write a calling program assembled and operated under the "house" monitor which initiates common storage for the X-Ray system, calls it, and leaves information necessary to the proper restoration of the "house" system. Examples of programs for accomplishing this function are given below.

In order to make possible the expansion of the system, LOADER not only serves to initiate execution but also has the ability to insert or supersede links and thus to generate a new system tape.

Any FORTRAN II - FAP program may be adapted to the system by suitable changes. Details of the requirements are given in the users manual but may be summarized here as follows:

1) The first executable step of each link should be CALL CALLER (4HNRLA) where NRLA (or NRLB) is the mnemonic of the link being prepared. (Other mnemonics require reassembly of CALLER)
2) All cards must be read through the subroutine IFFI (If Friend or Foe Input) by CALL IFFI (KZZ, 5HFIRST, 6HSECOND, ..., 3HNTH) GO TO

(1, 2, 3, ... M, EXIT), KZZ. Then after screening by IFFI, may be read by 1 READ 101, LIST which serves to reread the card under the specified format.

3) The first 112 words of low common must be protected and used to serve for link and system communication.

4) Before each line of output is written on the print tape (NTØUT) CALL LINES(N) must be called. (Where N is the number of lines)

5) For any failure, especially the detection of an unknown card, EXIT must be called.

6) A successful execution returns to the CALL CALLER ( ) statement.

7) The binary deck of the link, along with <u>all</u> of its subroutines, may then be placed on an updated system tape by means of the LOADER link.

<u>Details of the treatment of Crystallographic Data</u>

The first essential data treatment program (DATRDN) of the system generates a binary tape whose format is such that it serves as input to the other system programs.

Programs such as DATFIX, FC, ORFLS, or DIFSYN in turn update the binary reflection tape as necessary. Thus the

output of many programs serve as input to many other programs. A history of the treatment of the data is automatically formed as the data is copied and updated. One advantage of this method of handling data is the fact that programs of the system often require only control cards as the treatment of the data progresses.

The list of the input cards of a simple run is shown below. The sequence of events in the example show cards for titling the pages of the output, setting the binary tape designations, instructing the operator, and placing remarks on the print tape, as well as calculations pertinant to solving a crystal structure.

In each link of the system which carries out the lengthy calculations of crystallography considerable effort has been expended to find algorithms which give good speed while maintaining flexibility and convenience for the user.

Generalizations on the use of the system

The course of a desired calculation, which may involve any number of the links in the system, is controlled by the sequence of cards in the input data. These control functions are exercised by a subroutine called CALLER through which all input passes. Input data cards are identified by the punching in the first six of the card columns usually a mnemonic of the

card function.

A data deck consists of the following kinds of cards.

(a) Operational cards (which are acceptable at any time) perform immediate operations such as assigning tapes, printing remarks and instructions, and supplying a title.

(b) A calling card serves to call the specific program link and initiate the program.

(c) Other data cards are read under the control of the program link to supply, for example, parameters, intensity data, and control information.

(d) The last card of the data deck must be an END card.

A sequence of interdependent calculations may be performed by stacking up an appropriate set of data decks (for example - FC followed by a Fourier synthesis, or, several cycles of automatic refinement). This set of data decks must be preceded by a *DATA card. Another independent sequence of calculations may be initiated by following the first sequence by a *DATA card and one or more data decks - et continuum. Execution terminates and control is returned to the calling monitor when a FINISH card or an end-of-file is read on the monitor input tape.

The sequence of events during the course of a calculation is as follows:

A *DATA card causes immediate initialization of tape assignments, page numbers, titles, etc. A calling card causes the indicated program to be loaded (if it is not already in core) and control is transferred to the program. Data cards are read by CALLER at the request of the program. The types of cards and their formats are discussed in detail in the program specific write-up. Normally, the program reads and processes data cards until the END card is reached; whereupon the program finishes the calculation, writes summary data, and returns control to CALLER. Another calling card can then initiate a new calculation with this or any other program on the system tape.

If for any reason there is a calculation failure, control is returned to CALLER which skips all subsequent cards until another *DATA card is read, whereupon the calculation is resumed. Because of this procedure, the calculations that run independently should be separated by *DATA cards. A dependent sequence of calculations is not separated by *DATA cards so that failure of one link will cause deletion of the remaining parts. The end of all calculations is indicated by a FINISH card. When this card or an end-of-file is encountered on the BCD input tape, control is returned to the calling monitor.

A current operation manual has been prepared by punching instructions, card formats, and examples in cards. The "system" is then distributed as a binary file of programs and a BCD file suitable for printing a manual on the IBM 1401. The library of symbolic programs and the binary decks are also available upon request.

For convenience in use, the manual which is printed on the IBM 1401 is divided into three parts. The first part is a "users guide" giving an outline of the method and plan of each calculation. The second part gives directions for use of the programs in terms of card formats and card order. The third part is a series of appendices to aid in adapting the system to various monitors and installations. All programs, subprograms, and subroutines in the X-Ray crystallography program system depend upon the FORTRAN II - FAP programming system. Therefore, it is helpful to be aware of the card format, conventions and limitations of this system. The directions attempt to be explicit wherever confusion might arise, but let the user beware of computer laboratory specific procedures.

The system is designed to be run independently of any monitor. The considerations which have gone into the design have tried to be made general whenever possible. There is one area, however, which any potential user in any shop must consider carefully, and that is the use of magnetic tape. It is

always wise to make a careful study of tape handling procedures in order to save the embarrassment that may attend injudicious tape assignments (e.g. rewinding the laboratory BCD output tape and using it for scratch, or trying to write on the shop monitor). The X-Ray system has its own set of logical (illogical?) tape designations which must be followed. If these are used carefully no serious inconvenience will result either to the user or to the shop.

APPENDIX

LIST OF CONTRIBUTORS TO THE SYSTEM

BROWN, DR. BRUCE W.
DEPARTMENT OF CHEMISTRY
PORTLAND STATE COLLEGE
PORTLAND 1, OREGON
PHONE= 503-226-7271

CHASTAIN, MR. ROGER V.
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF WASHINGTON
SEATTLE 5, WASHINGTON
PHONE= 206-543-1686

DAYHOFF, DR. MARGARET
NATIONAL BIOMEDICAL RESEARCH FOUNDATION INCORPORATED
8600 16TH STREET
SILVER SPRING MARYLAND
PHONE 301-JU 7-7014

DICKINSON, MR. CHARLES
U.S. NAVAL ORDNANCE LABORATORY
WHITE OAK
SILVER SPRING, MARYLAND
PHONE= 301-495-8478, HYATTSVILLE, SILVER SPRING

HIGH, DR. DARRELL F.
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF CALIFORNIA AT SAN DIEGO
LA JOLLA, CALIFORNIA
PHONE= 714-459-2388, EXT 529

HOLDEN, DR. JAMES R.
U.S. NAVAL ORDNANCE LABORATORY
WHITE OAK
SILVER SPRING, MARYLAND
PHONE= 301-495-8478, HYATTSVILLE, SILVER SPRING

JARSKI, MRS. MARY ANN
38 EAST 24TH STREET
RIVIERA BEACH, FLORIDA

JENSEN, PROF. LYLE H.
DEPARTMENT OF ANATOMY
UNIVERSITY OF WASHINGTON
SEATTLE 5, WASHINGTON
PHONE= 206-543-1861

LINGAFELTER, PROF. EDWARD C.
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF WASHINGTON
SEATTLE 5, WASHINGTON
PHONE= 206-543-1686 (CHEM DEPT)
206-543-5900 (GRADUATE SCHOOL)

MOROSIN, DR. BRUNO
PHYSICAL SCIENCE RESEARCH (5152)
SANDIA CORPORATION
ALBUQUERQUE, NEW MEXICO
PHONE= 505-256-4411-56169

STEWART, PROF. JAMES M.
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF MARYLAND
COLLEGE PARK, MARYLAND
PHONE= 301-864-8275

TAKEDA, DR. HIROSHI
DEPARTMENT OF CHEMISTRY
JOHNS HOPKINS UNIVERSITY
BALTIMORE, MARYLAND

WAX, MR. SAMUEL
COMPUTOR SCIENCE CENTER
UNIVERSITY OF MARYLAND

SYMBOLIC LISTING OF =B5FORT=

```
*       LABEL
*       FAP
*B5FOR     PROGRAM TO CALL X-RAY SYSTEM FROM B5
        COUNT   100
        TTL VERSION OF 1 JAN 63
*
P       TAPENO  B5
        CLA     =10B17              SET PROGRAM TAPE NUMBER
        STO     NTPROG
*
        AXT     NX,2                MOVE LOADER TO UPPER MEMORY
        CLA     XLA+NX,2
        STO     .XLA+NX,2
        TIX     *-2,2,1
*
        TEFP    *+1
        REWP
 CHC    AXT     5,1
        RTBP                        READ AND CHECK LINK LABEL
        RCHP    CHSEL1
        TCOP    *
        TRCP    CHD
        TEFP    CHD
        AXT     5,1                 GO TO LOADER
        TRA     .XLC
CHD     BSRP                        REDUNDANCY - TRY AGAIN
        TIX     CHC+1,1,1
        TRA     .XXA
CHSEL1  IORT    .XLZ,,4             READ IN LABEL
*
* LINK  LOADER (EXECUTED FROM UPPER MEMORY)     ENTER AT .XLC
XLA     BSRP                        REDUNDANCY - TRY AGAIN
        IOT
        NOP
        TIX     .XLC,1,1
XXA     WPDA                        COMMENT BAD TAPE
        AXT     12,1
        RCHA    .XCIL
        TRA     .XXA1
        LCHA    .XCIL
 XXA1   LCHA    .XCIL+1
        LXA     .XCIL,2
        TXI     .XXA2,2,1
 XXA2   SXA     .XCIL,2
        TIX     .XXA1-1,1,1
 XXA3   HTR     .XXA3
XLC     RTBP                        READ IN LINK
        RCHP    .XLZ+1
XLD     TCOP    .XLD                DELAY
        TRCP    .XLA
        TEFP    .XXA
        TRA     .XLZ+2              OK, GO TO THE LINK (SEE NOTE BELOW)
        REM
XCI     OCT     041100020000   9L X-RAY PROGRAM TAPE UNREADABLE
        OCT     010000000000   8L
        OCT     202201000000   7L
```

```
        OCT     000400000000  6L
        OCT     000000450100  5L
        OCT     000020102000  4L
        OCT     000004000200  3L
        OCT     000000000400  2L
        OCT     020042005000  1L
        OCT     210004100000  0L
        OCT     143521060200 11L
        OCT     020242417500 12L
        REM
 XCIL   IOCT    .XCI,,1
        IOCT    .XL(0),,1
XLZ             ,,**                LABEL
        IOCP    **,,**              IO COMMAND FOR FIRST SEGMENT
        IORT    **,,**              IO COMMAND FOR SECOND SEGMENT OF LINK
        TRA     **                  STARTING INSTRUCTION
        REM IF THE TAPE WAS PREPARED BY MONITOR CHAIN, THERE WILL BE
        REM A SINGLE IORT AT .XLZ+1 AND THE TRA AT .XLZ+2.  TO RETAIN
        REM COMPATIBILITY, WE TRANSFER TO .XLZ+2, WHICH IS EITHER A TRA
        REM OR AN IORT, WHICH IS THE SAME THING AS A (TAGLESS) TXH WHICH
        REM IS THE SAME AS A NOP FOR PRESENT PURPOSES.
 XL(0)  PZE
NX      EQU     *-XLA
        REM
 .X     COMMON  0
 .XLA   EQU     .X+2
 .XXA   EQU     .XLA+4
 .XXA1  EQU     .XXA+5
 .XXA2  EQU     .XXA1+3
 .XXA3  EQU     .XXA2+2
 .XLC   EQU     .XXA3+1
 .XLD   EQU     .XLC+2
 .XCI   EQU     .XLD+4
 .XCIL  EQU     .XCI+12
 .XLZ   EQU     .XCIL+2
.XL(0)  EQU     .XLZ+4
        COMMON  24
NTPROG  COMMON  1
        END
```

SYMBOLIC LISTING OF =B5IBSY=

```
*       LABEL
*       FAP
*B5IBSY     PROGRAM TO USE X-RAY SYSTEM UNDER THE IBSYS MONITOR....
        COUNT   150
        SST                         LETS HAVE A LOOK AT IBSYS SYMBOL TBL
        LTM
        LFTM                        GIVE UP FLOATING TRAP
        STZ     KILL                SHUT OFF TRAPPING MODE
        ENB     KILL                KILL ALL DATA CHANNEL TRAPS
        LSNM                        GIVE UP BEING A 704(IF ANY)
TRICKY  TCOA    *                   MAKE SHURE CHAN A QUIET
        TCOB    *                   DITTO B
        TRCA    *+1                 SHUT OFF ALL IO CHECKS
        TRCB    *+1
        TEFA    *+1
        TEFB    *+1
        DCT                         FORGET ABOUT DIVIDE OVERFLOWS
        NOP
        BTT     1000                SHUT OFF THOSE POSITION INDICATORS
        NOP
        BTT     2000
        NOP
        ETT     1000
        NOP
        ETT     2000
        NOP
        SLF                         TO H  L WITH SENSE LIGHTS
        TOV     *+1                 WHO CARES IF THERE WAS AN OVERFLOW
BURP    AXT     5,1                 GET SET TO MAKE 5 TRIES
        REWB    5                   REWIND THE X-RAY SYSTEM TAPE
        RTBB    5                   SKIP DOWN THE X-RAY TAPE
        TCOB    *
        TEFB    *+2                 TILL AN END OF FILE IS FOUND
        TRA     *-3                 KEEP TRYING
        WTBB    5                   PUT IBSYSES GOODIES ON THE TAIL END OF B
        RCHB    DUMPY               FIVE
        LCHB    DUMPY+1
        TCOB    *                   WAIT
        TRCB    CHDDR               AND HOPE THERE ARE NO REDUNDANCIES...
        TRA     MADEIT              WHEW....
CHDDR   TIX     BURP+1,1,1          TRY FIVE TIMES BEFORE QUITTING
        WPDA                        THEN GIVE UP WITH A BAD TAPE COMMENT
        AXT     12,1
        RCHA    STUFF
        TRA     PRINT
        LCHA    STUFF
PRINT   LCHA    STUFF+1
        LXA     STUFF,2
        TXI     *+1,2,1
        SXA     STUFF,2
        TIX     PRINT-1,1,1
        TCOA    *
        TTR*    SYSRET              AS LONG AS WE CANT GET ON LETS GET OFF..
```

```
DUMPY   IOCT    0,,5
        IOCD    6,,1996
STUFF   IOCT    XCI,,1
        IOCT    XL(0),,1
*  THE FOLLOWING STEPS CLEAR THE MEMORY TO ZERO IN A FAIR IMITATION OF
*  THE STANDARD FORTRAN MONITOR AND ASSURE THAT SYSCOM WILL BE HAPPY....
        AXC     NNEND,4          INITIALIZE CORE TO ZERO
        TXI     *+1,4,32767
        STZ     32767,4
        TIX     *-1,4,1
*  THE FOLLOWING STEPS JAM A WAY OF RESTORING IBSYS INTO QUIT WHICH IS
*       WHERE FINAL, TERMINAL, DONE FOR, I GIVE UP, TYPE TRANSFERS GO TO
MADEIT  CLA     SYSIDR           GET LOC OF IBSYS CLOCK OUT
        STA     HIBSYS           STORE IT IN EXIT ROUTINE
        CLA     SYSRET           GET THE ADDRESS ON SYSTEM RETURN
        ALS     18               DECREMENTIZE IT
        STD     HIBSYS+1         FIX UP CLOCK OUT CALLING SEQUENCE
        REWB    5                REWIND X-RAY SYSTEM TAPE
        AXT     MXL,4
        CLA     MONEX+MXL,4      PICK UP EXIT COMMANDS
        STO     QUIT+MXL,4       AND STUFF THEM IN QUIT
        TIX     *-2,4,1          REGION IN COMMON STORAGE
        TRA     LINFIX
MONEX   AXT     5,1              GIVE FIVE TRIES AT RESTORING IBSYS
        BSRB    5                BACK OFF
        TEFB    QUIT+3           AND LOOK FOR  END OF FILE
        RTBB    5                READ UNTIL EOF DETECTED
        TCOB    QUIT+4           WAIT FOR QUIET CHANNEL
        TEFB    QUIT+7           IS EOF REACHED...
        TRA     QUIT+3           NO    TRY AGAIN
        TRCB    QUIT+7           DONT WORRY ABOUT REDUNDANCIES HERE.
        RTBB    5                LETS TRY TO GET IBSYS BACK ON THE AIR
        RCHB    QUIT+21          BRING BACK IBNUC ET. AL. ......
        LCHB    QUIT+22
        TCOB    QUIT+11          LET IT GET IN ----STEADY NOW-----
        TRCB    QUIT+18          REDUNDANCY HERE COULD REALLY SHOOT US UP
        RUNB    5                REWIND AND UNLOAD X-RAY SYSTEM
        WEFB    2                END OFF THE IBSYS PUNCH TAPE SO THAT
        WEFB    2                  THE NEXT MANS JOB WILL RUN*******
HIBSYS  TSX     **,4             CALL CLOCKOUT
        FIVE    ,,**             CALLING SEQUENCE OF CLOCKING OPERATION
        BSRB    5                NUTS****** $ = * . ( . )//
        TIX     QUIT+8,1,1       TRY IT FOUR MORE TIMES FOR KICKS
        TRA     QUIT+13          HAVING FAILED THAT ...PRAY THAT ENOUGH
        IOCT    0,,5             IS RESTORED TO COMPLETELY BAFFEL THE
        IOCD    6,,1996          OPERATOR.... (DONT CRY THINGS CANT GET
        REM                      MUCH WORSE..... CAN THEY.......
MXL     EQU     *-MONEX
KILL    PZE     0,0,0
*  INITIALIZE OUR SYSTEM TAPES TO AGREE WITH THE USUAL U. MD. SET UP
*  THE FOLLOWING STEPS DEFINE TAPES DIFFERENTLY THAN U.W. STANDARD
*  AS SET BY SYSTEM INITIALIZING SUBROUTINE SYSCOM
*  FINAL VERSION OF B5IBSYS WILL HAVE TO BE MUCH SMARTER....
LINFIX  CLA     =10B17           DEFINE PROGRAM TAPE TO BE B5
        STO     NTPROG
        CLA     =8B17            SET PRINT TAPE TO B1
        STO     NTPROG-2            STD INPUT IS STILL ON A2
        STO     NTPROG-6         FOURIER OUTPUT IS ALSO ON B1
        CLA     =2B17            SET OFFLINE PUNCH TAPE TO BE B2
        STO     NTPROG-5
        CLA     =6B17            SET  SET NTAPEE
        STO     NTPROG-7
*
        AXT     NX,2             MOVE LOADER TO UPPER MEMORY
        CLA     XLA+NX,2
        STO     .XLA+NX,2
        TIX     *-2,2,1
*
        TEFB    *+1
        REWB    5
```

```
 CHC    AXT     5,1
        RTBB    5                       READ AND CHECK LINK LABEL
        RCHB    CHSEL1
        TCOB    *
        TRCB    CHD
        TEFB    CHD
        AXT     5,1                     GO TO LOADER
        TRA     .XLC
CHD     BSRB    5                       REDUNDANCY TRY AGAIN
        TIX     CHC+1,1,1
        TRA     .XXA
CHSEL1  IORT    .XLZ,,4                 READ IN LABEL
*
* LINK  LOADER (EXECUTED FROM UPPER MEMORY)      ENTER AT .XLC
XLA     BSRB    5                       REDUNDANCY TRY AGAIN
        IOT
        NOP
        TIX     .XLC,1,1
XXA     WPDA                            COMMENT BAD TAPE
        AXT     12,1
        RCHA    .XCIL
        TRA     .XXA1
        LCHA    .XCIL
 XXA1   LCHA    .XCIL+1
        LXA     .XCIL,2
        TXI     .XXA2,2,1
 XXA2   SXA     .XCIL,2
        TIX     .XXA1-1,1,1
        TCOA    .XXA2+2
        WPDA
        RCHA    .FUDGE
        AXT     100,1
        LCHA    .FUDGE
        TIX     .XXA3-2,1,1
 XXA3   TRA     QUIT                    AS LONG AS WE CANT GET ON THE AIR LETS
        REM                               TRY TO PUT MAMA B. BACK ON AND LET
        REM                               SOMEONE ELSE PAY THE TAB.....  $$$$$
XLC     RTBB    5                       READ IN LINK
        RCHB    .XLZ+1
XLD     TCOB    .XLD                    DELAY
        TRCB    .XLA
        TEFB    .XXA
        TRA     .XLZ+2                  OK, GO TO THE LINK (SEE NOTE BELOW)
        REM
XCI     OCT     041100020000   9L  X-RAY PROGRAM TAPE UNREADABLE
        OCT     010000000000   8L
        OCT     202201000000   7L
        OCT     000400000000   6L
        OCT     000000450100   5L
        OCT     000020102000   4L
        OCT     000004000200   3L
        OCT     000000000400   2L
        OCT     020042005000   1L
        OCT     210004100000   0L
        OCT     143521060200  11L
        OCT     020242417500  12L
FUDGE   IOCT    NTIN,,1                 FUDGE A FEW EXTRA LINES SO OPERATOR WILL
        REM                               SEE COMMENTS
        REM
 XCIL   IOCT    .XCI,,1
        IOCT    .XL(0),,1
XLZ             ,,**                    LABEL
        IOCP    **,,**                  IO COMMAND FOR FIRST SEGMENT
```

```
        IORT     **,,**            IO COMMAND FOR SECOND SEGMENT OF LINK
        TRA      **                STARTING INSTRUCTION
        REM IF THE TAPE WAS PREPARED BY MONITOR CHAIN, THERE WILL BE
        REM A SINGLE IORT AT .XLZ+1 AND THE TRA AT .XLZ+2.  TO RETAIN
        REM COMPATIBILITY, WE TRANSFER TO .XLZ+2, WHICH IS EITHER A TRA
        REM OR AN IORT, WHICH IS THE SAME THING AS A (TAGLESS) TXH WHICH
        REM IS THE SAME AS A NOP FOR PRESENT PURPOSES.
 XL(0)  PZE
NX      EQU      *-XLA
NNEND   EQU      *                 TO DEFINE LAST LOCATION OF PROGRAM
        REM
.X      EQU      32561
 .XLA   EQU      .X+2
 .XXA   EQU      .XLA+4
 .XXA1  EQU      .XXA+5
 .XXA2  EQU      .XXA1+3
 .XXA3  EQU      .XXA2+8
 .XLC   EQU      .XXA3+1
 .XLD   EQU      .XLC+2
 .XCI   EQU      .XLD+4
.FUDGE  EQU      .XCI+12
.XCIL   EQU      .FUDGE+1
 .XLZ   EQU      .XCIL+2
.XL(0)  EQU      .XLZ+4
NTIN    EQU      32549
NTPROG  EQU      32537
QUIT    EQU      32475
LINMX   EQU      32451
        END
```

SYMBOLIC LISTING OF =1B5CARD=

```
*       LABEL
*        ROW
*        FAP
*1B5CARD - ON-LINE START CARD FOR X-RAY SYSTEM ON B5))
         COUNT    30
         TTL VERSION OF 2 JAN 63
* THIS CARD WILL INITIATE THE XRAY SYSTEM ON B5.  PUT CARD IN ON-LINE
* CARD READER, PUT PROGRAM TAPE ON B5, CLEAR, LOAD CARDS.
* PROVISION IS MADE FOR REDEFINING NTINM AND NTOUTM AT STUFF+2 AND
* STUFF+1, RESPECTIVELY.
         FUL
         ORG      0
P        TAPENO   B5
*
         IOCT     3,,STUFF-3
         LCHA     LDS
         TCOA     *
*
ST       AXT      5,4
         TRA      RD
         TRA      RD
RD       REWP
         RTBP
         RCHP     IO
         TCOP     *
         RTBP
         RCHP     1
         TCOP     *
         TRCP     NG
         TRA      2
NG       TIX      RD,4,1
         HTR      ST
IO       IORT     0,,4
*
LDS      IOCP     QUIT,,1
         IOCD     NTPROG-2,,3
*
STUFF    HTR      QUIT                PROGRAM EXIT
         PZE      ,,                  NTOUTM
         PZE      ,,                  NTINM
         PZE      ,,1C                NTPROG
*
NTPROG   BOOL     77431
QUIT     BOOL     77333
         END
*ENDIN
```

Explanation of the Example

The following concluding pages of this report consist of reproductions of lists of input cards and of printed output. (These lists have been shortened by omitting large quantities of reflection data.) This example of the use of X-Ray 63 (under IBSYS) is intended to show some of the features of the system; it is not exhaustive. Even though this example of the solution of a structure and its partial refinement is shown in these listings as a single 53 minute IBM 7090 run, there were 3 "hand" operations carried out* upon the output in the actual structure determination. The sequence of events was as follows:

1. Data Reduction
2. Calculation of the E's (scaled unitary structure factors).
3. Sorting of the E's into groups of hkl in decending order of E.
4. The hand "$\sum_2$" calculation of probable phases (two sets were found - only the correct solution is shown).
5. Application of the determined phases to the appropriate reflections.

*Programming and check-out is currently being carried out to further automate these operations.

6. Calculation of an "E" map.

7. Search of the "E map" for peaks.

8. Hand examination by plotting of the configuration of peaks.

9. Calculation of structure factors based on the strongest, best appearing arrangement of peaks.

10. Fourier refinement of the coordinates of these peaks.

11. Calculation of a difference map in the region of the missing oxygen atoms.

12. Further Fourier refinement of all the "heavy" atoms of the asymmetric unit.

13. Full matrix least squares refinement of the "isotropic" structure.

```
$EXECUTE        FORTRAN
$ID     STEWART*001/63/006  $DICKINSON, C.
*      ESTIMATED RUNNING TIME 60 MIN.
*       REEL 0267 ON B5 RING IN..
*      SCRATCH TAPES ON A5,A6,B6
*      PAUSE
*       XEQ
*
*****************************************************************************
*
                      BINARY DECK OMITTED FROM LIST  (10 CARDS)
*
*****************************************************************************
*
*      DATA
OPRATR $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
OPRATR
OPRATR  THIS IS A RUN OF X-RAY 63 UNDER IBSYS.  DURING EXECUTION
OPRATR  IBSYS IS SAVED BUT NOT IN CONTROL.
OPRATR  IF IT IS NECESSARY TO RESTORE IBSYS BEFORE THE NORMAL END OF
OPRATR THE RUN TRA EITHER TO OCTAL 400 OR 77333.
OPRATR
OPRATR SENSE SWITCH 1 MUST BE OFF OR ELSE ALL PRINT WILL BE ON LINE.
OPRATR YOU MAY THEREFORE SAMPLE THE BCD OUTPUT AT ANY TIME.
OPRATR
OPRATR $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
OPRATR
OPRATR
OPRATR
REMARK $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
REMARK
REMARK      THE FOLLOWING RUN ON X-RAY 63 IS INTENDED TO ILLUSTRATE SOME
REMARK OF THE FEATURES OF THE SYSTEM.  THE EXAMPLE CHOSEN IS THAT OF
REMARK THE STRUCTURE DETERMINATION AND PARTIAL REFINEMENT OF
REMARK 2,3,4,6 - TETRANITROANILINE (TENA).  AT THE TIME THE ACTUAL
REMARK DETERMINATION WAS CARRIED OUT IT WAS NECESSARY TO BREAK IT INTO
REMARK SEVERAL SEPARATE EXECUTIONS.
REMARK
REMARK $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
TITLE   2,3,4,6 - TETRANITROANILINE  PREPARE DATA (DATA REDUCTION)
DATRDN TENA
LABEL  CELL PARAMETERS  3/25/64  INTENSITIES 12/18/63
CELL   TENA      7.271  11.056  12.271          -0.15261            552.
FORMFX C         0.00    6.00  I.U.CR., INTERNATIONAL TABLES FOR X-RAY
FORMFX C         0.10    5.14  CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNOCH
FORMFX C         0.20    3.61  PRESS.  VOL 3, PHYSICAL AND CHEMICAL
FORMFX C         0.30    2.54  TABLES (1960).
FORMFX C         0.40    1.98
FORMFX C         0.50    1.71
FORMFX C         0.60    1.55
FORMFX C         0.70    1.42
FORMFX C         0.80    1.31
FORMFX C         0.90    1.20
FORMFX C         1.00    1.10
FORMFX C         1.10    1.00
FORMFX C         1.20    0.90
FORMFX C         1.30    0.80
FORMFX C         1.40    0.73
FORMFX C         1.50    0.65
FORMFX C         1.60    0.57
FORMFX C         1.70    0.50
FORMFX N         0.00    7.00  I.U.CR., INTERNATIONAL TABLES FOR X-RAY
FORMFX N         0.10    6.20  CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNOCH
FORMFX N         0.20    4.60  PRESS.  VOL 3, PHYSICAL AND CHEMICAL
FORMFX N         0.30    3.24  TABLES (1960).
FORMFX N         0.40    2.40
FORMFX N         0.50    1.94
FORMFX N         0.60    1.70
FORMFX N         0.70    1.55
FORMFX N         0.80    1.44
FORMFX N         0.90    1.35
FORMFX N         1.00    1.26
FORMFX N         1.10    1.17
FORMFX N         1.20    1.08
FORMFX N         1.30    1.01
FORMFX N         1.40    0.93
FORMFX N         1.50    0.85
FORMFX N         1.60    0.77
FORMFX N         1.70    0.70
FORMFX O         0.00    8.00  I.U.CR., INTERNATIONAL TABLES FOR X-RAY
FORMFX O         0.10    7.25  CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNOCH
FORMFX O         0.20    5.63  PRESS.  VOL 3, PHYSICAL AND CHEMICAL
```

```
FORMFX O          0.30     4.09  TABLES (1960).
FORMFX O          0.40     3.01
FORMFX O          0.50     2.34
FORMFX O          0.60     1.94
FORMFX O          0.70     1.71
FORMFX O          0.80     1.57
FORMFX O          0.90     1.46
FORMFX O          1.00     1.37
FORMFX O          1.10     1.30
FORMFX O          1.20     1.22
FORMFX O          1.30     1.15
FORMFX O          1.40     1.08
FORMFX O          1.50     1.01
FORMFX O          1.60     0.95
FORMFX O          1.70     0.89
FORMFX H          0.00     1.00  I.U.CR., INTERNATIONAL TABLES FOR X-RAY
FORMFX H          0.10     0.82  CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNOCH
FORMFX H          0.20     0.47  PRESS.  VOL 3, PHYSICAL AND CHEMICAL
FORMFX H          0.30     0.25  TABLES (1960).
FORMFX H          0.40     0.13
FORMFX H          0.50     0.08
FORMFX H          0.60     0.04
FORMFX H          0.70     0.02
FORMFX H          0.80     0.01
FORMFX H          0.90     0.00
FORMFX H          1.00     0.00
FORMFX H          1.10     0.00
FORMFX H          1.20     0.00
FORMFX H          1.30     0.00
LATICE  C  P
SYMTRY   X,        Y,        Z
SYMTRY  -X,      1/2+Y,     1/2-Z
CONDIT TENA    1.5418   .98870  0.07     1  3  1  1  1  2
SCALE 1.00000       1        7.0 2 10.  1.0  0.0  0.0  10.
                1   0   0   2   2173.28                                    041 0001
                1   0   0   4    330.95                                    041 0002
                1   0   0   6      9.00                                    041 0003
                1   0   0   8     57.96                                    041 0004
                1   0   0  10     29.00                                    041 0005
                1   0   0  12     53.54                                    041 0006
REMARK
REMARK*************************************************************************
REMARK
REMARK                    MOST REFLECTION CARDS OMITTED FROM LIST
REMARK
REMARK*************************************************************************
REMARK
                2   7   9  -2      7.00                                     041 1691
                1   7   9  -3     54.00                                     041 1692
                1   7   9  -4     54.00                                     041 1693
ENDOBS
                1   1   0   1
                1   1   0 - 1
                1   1   0   3
                1   1   0 - 3
REMARK
REMARK*************************************************************************
REMARK
REMARK                    MOST REFLECTION CARDS OMITTED FROM LIST
REMARK
REMARK*************************************************************************
REMARK
END
TITLE  CALCULATE SCALED UNITARY STRUCTURE FACTORS (KARLE - HAUPTMAN E'S)
DATFIX TENA
EPSILON  1  1  1  1  2  1
CELCON  24C
CELCON  20N
CELCON  32O
CELCON  12H
END
TITLE   SORT E'S INTO ORDER FOR =HAND= PHASE DETERMINATION
ESORT  TENA  1
END
TITLE  APPLY SET OF CALCULATED PHASES TO APPROPRIATE REFLECTIONS
TAPES        12 11        6
MODIFY TENA    2 10  1
MODREF            1   0 -12        +1
MODREF            2       6        -1
MODREF            5      -4        +1
MODREF            6                -1
MODREF                1  12        +1
```

```
REMARK
REMARK*************************************************************************
REMARK
REMARK                MOST MODREF CARDS OMITTED FROM LIST
REMARK
REMARK*************************************************************************
REMARK
END
TITLE    2,3,4,6 - TETRANITROANILINE
FOURR   TENA              13     1000.
GRID    TENA     24  37  40
MAP     TENA      3 15  -99
LAYOUT  TENA     13   0   1  37   0   1  21   0   1 123  21 1
END
TITLE   GENERATE NEW SYSTEM TAPE WITH PEAK SEARCHING ROUTINE INCLUDED
LOADER  PIKTES  9
LINK    30600
REMARK
REMARK*************************************************************************
REMARK
REMARK                 BINARY DECK OMITTED FROM LIST
REMARK
REMARK*************************************************************************
REMARK
END
TITLE   SEARCH MAP FOR HIGHEST PEAKS (19 ATOMS IN ASSYMETRIC UNIT)
PEKPIK  TENA                                  1
END
TITLE  CALCULATE STRUCTURE FACTORS FROM SET OF PEAKS IN E MAP
TAPES          11 12
FC      TENA                                     2
REMARK   SCALE AND TEMPERATURE FACTOR FROM DATFIX
REMARK   THE PEAK PICKING LINK LOCATED ALL BUT O41 AND O42
SCALE   .87
B       TENA    4.321
ATOM    C1       0.2517  0.8320  0.2847
ATOM    C2       0.4286  0.9009  0.2923
ATOM    C3       0.4464  0.3837  0.1216
ATOM    C4       0.4500  0.2864  0.0488
ATOM    C5       0.3980  0.7065  0.4310
ATOM    C6       0.2512  0.7376  0.3521
ATOM    N1       0.1169  0.8469  0.1993
ATOM    N2       0.4321  0.      0.2275
ATOM    N3       0.2746  0.4597  0.1031
ATOM    N4       0.3091  0.2458  0.4636
ATOM    N6       0.0943  0.6628  0.3511
ATOM    O21      0.3332  0.0175  0.1306
ATOM    O22      0.4651  0.1169  0.2791
ATOM    O31      0.1943  0.4731  0.1899
ATOM    O32      0.2650  0.5162  0.0194
ATOM    O61      0.0846  0.5708  0.4156
ATOM    O62      0.0393  0.1703  0.2342
END
TITLE    REFINE ROUGH COORDINATES OF THE MOLECULE BY BLOCK FOURIERS
TAPES          12 11
FOUREF  TENA    321 2 1
REMARK  SCALE FACTORS FROM FC
CYCLES   5 .5    .02     .2 .02      .01      .008
END
TITLE   SEARCH IN REGION OF MISSING OXYGENS
FOURR   TENA              8  1            .2
GRID    TENA     48  74  80
LAYOUT  TENA     24   2   2  18  12   1  15  26   1 123      2
END
TITLE    REFINE ALL HEAVY ATOMS
TAPES          11 12
FOUREF  TENA    321 2 1
REMARK    ADD OXYGEN ATOMS FROM DIFFERENCE FOURIER
GRID    TENA     48  74  80
ATOMG   O41        15.0     24.0     33.0
ATOMG   O42         7.0     16.0     39.0
CYCLES   5 .5    .02     .2 .02      .01      .008
END
TITLE    REFINE WITH ISOTROPIC CYCLES OF FULL-MATRIX LEAST SQUARES
TAPES          12 11
ORFLS   TENA     2  1      1
END
SAVE    11 12
FINISH
```

```
$ID    STEWART*OO1/63/006  $DICKINSON, C.                      12500  04/25/64 ON 13-16-03

 *      ESTIMATED RUNNING TIME 60 MIN.
 *       REEL 0267 CN B5 RING IN..
 *      SCRATCH TAPES ON A5,A6,B6
 *      PAUSE
 *       XEQ
  NAME  ENTRY       NAME  ENTRY       NAME  ENTRY       NAME  ENTRY       NAME  ENTRY       NAME  ENTRY

 *MAIN* 03734      *FREE* 04205      **TU** 77777
BEGIN EXECUTION  13-16-58    FOR II/FAP
X-RAY PROGRAM TAPE 240364 CPERATING FROM LOGICAL UNIT 10
                                                                                            PAGE    1

OPRATR $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

         THIS IS A RUN CF X-RAY 63 UNDER IBSYS.  DURING EXECUTION
         IBSYS IS SAVED BUT NOT IN CONTROL.
         IF IT IS NECESSARY TO RESTORE IBSYS BEFORE THE NORMAL END CF
        THE RUN TRA EITHER TO OCTAL 400 OR 77333.

        SENSE SWITCH 1 MUST BE OFF CR ELSE ALL PRINT WILL BE ON LINE.
        YOU MAY THEREFORE SAMPLE THE BCD OUTPUT AT ANY TIME.

        $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$


REMARK $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

            THE FOLLOWING RUN ON X-RAY 63 IS INTENDED TO ILLUSTRATE SOME
        OF THE FEATURES CF THE SYSTEM.  THE EXAMPLE CHOSEN IS THAT OF
        THE STRUCTURE DETERMINATION AND PARTIAL REFINEMENT OF
        2,3,4,6 - TETRANITRCANILINE (TENA).  AT THE TIME THE ACTUAL
        DETERMINATICN WAS CARRIED OUT IT WAS NECESSARY TO BREAK IT INTO
        SEVERAL SEPARATE EXECUTIONS.

        $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
```

TAPE LABEL CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63

```
F(0,0,0) =    552.0
VCLUME =      974.888573

                DIRECT CELL CONSTANTS AND FACTORS
     A =   7.271                                    COSA = -0.
     B =  11.056                                    COSB = -0.15261
     C =  12.271                                    COSG = -0.

  A**2 =     52.867440                          A*B*COSG =    -0.
  B**2 =    122.235135                          A*C*COSB =   -13.6162363
  C**2 =    150.577438                          B*C*COSA =    -0.

                RECIPROCAL CELL CONSTANTS AND FACTORS
  ASTAR = 0.139163                                  COSAS =  0.
  BSTAR = 0.090449                                  COSBS =  0.15261
  CSTAR = 0.082459                                  COSGS =  0.

ASTAR**2/4 = 0.004841566                  ASTAR*BSTAR*COSGS/2 = 0.
BSTAR**2/4 = 0.002045237                  ASTAR*CSTAR*COSBS/2 = 0.000875615
CSTAR**2/4 = 0.001699857                  BSTAR*CSTAR*COSAS/2 = 0.
```

ATOM TYPE	SINT/LAMBDA	F(J)	SOURCE REFERENCE
C	0.	6.000	I.U.CR., INTERNATIONAL TABLES FOR X-RA CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNO PRESS. VOL 3, PHYSICAL AND CHEMICAL TABLES (1960).
C	0.10000	5.140	
C	0.20000	3.610	
C	0.30000	2.540	
C	0.40000	1.980	
C	0.50000	1.710	
C	0.60000	1.550	
C	0.70000	1.420	
C	0.80000	1.310	
C	0.90000	1.200	
C	1.00000	1.100	
C	1.10000	1.000	
C	1.20000	0.900	
C	1.30000	0.800	
C	1.40000	0.730	
C	1.50000	0.650	
C	1.60000	0.570	
C	1.70000	0.500	
N	0.	7.000	I.U.CR., INTERNATIONAL TABLES FOR X-RA CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNO PRESS. VOL 3, PHYSICAL AND CHEMICAL TABLES (1960).
N	0.10000	6.200	
N	0.20000	4.600	
N	0.30000	3.240	
N	0.40000	2.400	
N	0.50000	1.940	
N	0.60000	1.700	
N	0.70000	1.550	
N	0.80000	1.440	
N	0.90000	1.350	
N	1.00000	1.260	
N	1.10000	1.170	
N	1.20000	1.080	
N	1.30000	1.010	
N	1.40000	0.930	
N	1.50000	0.850	
N	1.60000	0.770	
N	1.70000	0.700	

ATOM TYPE	SINT/LAMBDA	F(J)	SOURCE REFERENCE
C	0.	8.000	I.U.CR., INTERNATIONAL TABLES FOR X-RA
C	0.10000	7.250	CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNO
C	0.20000	5.630	PRESS. VOL 3, PHYSICAL AND CHEMICAL
C	0.30000	4.090	TABLES (1960).
C	0.40000	3.010	
C	0.50000	2.340	
C	0.60000	1.940	
C	0.70000	1.710	
C	0.80000	1.570	
C	0.90000	1.460	
C	1.00000	1.370	
C	1.10000	1.300	
C	1.20000	1.220	
C	1.30000	1.150	
C	1.40000	1.080	
C	1.50000	1.010	
C	1.60000	0.950	
C	1.70000	0.890	
H	0.	1.000	I.U.CR., INTERNATIONAL TABLES FOR X-RA
H	0.10000	0.820	CRYSTALLOGRAPHY, BIRMINGHAM - THE KYNO
H	0.20000	0.470	PRESS. VOL 3, PHYSICAL AND CHEMICAL
H	0.30000	0.250	TABLES (1960).
H	0.40000	0.130	
H	0.50000	0.080	
H	0.60000	0.040	
H	0.70000	0.020	
H	0.80000	0.010	
H	0.90000	0.	
H	1.00000	0.	
H	1.10000	0.	
H	1.20000	0.	
H	1.30000	0.	

TABLE OF SYMMETRY OPERATIONS

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

CENTRIC CELL OF LATTICE TYPE P.
SYMMETRY OPERATION CHECKING COMPLETE.

	ROTATION MATRIX			TRANSLATION VECTOR (IN TWELFTHS)
1	1	0	0	0
	0	1	0	0
	0	0	1	0
2	-1	0	0	0
	0	1	0	6
	0	0	-1	6

USUAL FC MULTIPLICITY IS 2.

APPLY LORENTZ AND/OR POLARIZATION CORRECTION.

DATA SOURCE WEISSENBERG METHOD.

LAMBDA = 1.54180 MAXIMUM SIN THETA = 0.989 RADIATION = X-RAY

TREAT DATA BY TAKING SQUARE ROOT OF INTENSITY INPUT.

B IS THE AXIS OF ROTATION.

STANDARD REFLECTION CARDS REQUIRED.

SCALE FACTOR	GROUP	I MINIMUM	WEIGHT SCHEME	Q1	Q2	Q3	Q4	Q5
1.0000	1	7.0000	2	10.0000	1.0000	0.	0.	10.0000

H	K	L	FREL	CODE	WEIGHT	1/LP	SINT/LAM	MULT	FORM FACTORS			
0	0	2	23.793	1	0.4203	0.260491	0.08246	1	5.371	6.428	7.471	0.872
0	0	4	13.608	1	0.7349	0.559495	0.16492	1	4.097	5.148	6.209	0.576
0	0	6	2.906	1	1.0000	0.938466	0.24738	1	3.026	3.882	4.840	0.351
0	0	8	9.073	1	1.0000	1.420430	0.32984	1	2.332	2.940	3.717	0.203
0	0	10	7.410	1	1.0000	1.893185	0.41229	1	1.938	2.327	2.910	0.124
0	0	12	10.143	1	0.9859	1.921473	0.49475	1	1.721	1.958	2.368	0.082
0	0	14	4.537	1	1.0000	1.210608	0.57721	1	1.583	1.745	2.013	0.047
1	0	0	56.732	1	0.1763	0.218290	0.06958	1	5.524	6.576	7.614	0.907
1	0	2	1.618	2	1.0000	0.374190	0.11572	1	4.871	5.944	7.005	0.755
1	0	-2	12.158	1	0.8225	0.317683	0.09945	1	5.148	6.208	7.257	0.822
1	0	4	41.805	1	0.2392	0.658035	0.18853	1	3.763	4.777	5.819	0.503
1	0	-4	47.892	1	0.2088	0.575744	0.16893	1	4.038	5.085	6.143	0.563
1	0	6	42.703	1	0.2342	1.044295	0.26700	1	2.826	3.624	4.545	0.310
1	0	-6	18.235	1	0.5484	0.934107	0.24654	1	3.035	3.893	4.853	0.353
1	0	8	8.800	1	1.0000	1.530653	0.34733	1	2.227	2.785	3.519	0.181
1	0	-8	7.099	1	1.0000	1.399711	0.32654	1	2.353	2.971	3.756	0.208
1	0	10	5.228	1	1.0000	1.952178	0.42847	1	1.887	2.239	2.786	0.115
1	0	-10	3.620	2	1.0000	1.872293	0.40752	1	1.954	2.355	2.948	0.126
1	0	12	4.499	1	1.0000	1.840031	0.51003	1	1.692	1.910	2.290	0.075
1	0	-12	20.012	1	0.4997	1.944785	0.48899	1	1.733	1.977	2.399	0.085
1	0	14	5.932	1	1.0000	1.035016	0.59184	1	1.562	1.716	1.965	0.042
1	0	-14	2.999	2	1.0000	1.285036	0.57075	1	1.593	1.759	2.036	0.049

H	K	L	FREL	CODE	WEIGHT	1/LP	SINT/LAM	MULT	FORM FACTORS			
7	0	5	-0.	1	1.0000	1.434707	0.55712	1	1.614	1.789	2.086	0.054
7	0	-5	-0.	1	1.0000	1.901234	0.49909	1	1.712	1.943	2.345	0.080
7	0	-7	-0.	1	1.0000	1.718970	0.52690	1	1.663	1.864	2.211	0.067
7	0	-9	-0.	1	1.0000	1.344219	0.56548	1	1.601	1.770	2.055	0.051
8	0	1	-0.	1	1.0000	1.355919	0.56442	1	1.603	1.772	2.059	0.051
8	0	-1	-0.	1	1.0000	1.489289	0.55187	1	1.623	1.801	2.106	0.056
8	0	-3	-0.	1	1.0000	1.493086	0.55149	1	1.623	1.802	2.108	0.056
8	0	5	-0.	1	1.0000	0.632021	0.62240	1	1.518	1.662	1.878	0.034
8	0	-5	-0.	1	1.0000	1.367924	0.56332	1	1.605	1.775	2.063	0.052

```
                    CONSTANTS REFERRING TO CARD COUNTS AND RUNS.

                        FORM FACTOR COUNTS
                        TOTAL TYPES OF ATOMS =   4
                       TOTAL FORM FACTORS OF C    = 18
                       TOTAL FORM FACTORS OF N    = 18
                       TOTAL FORM FACTORS OF O    = 18
                       TOTAL FORM FACTORS OF H    = 14

                        SYMMETRY CARD COUNT =   2

                        REFLECTION CARD COUNTS
NO. REFL. CARDS (OR RECORDS) = 1779   REJECTED CARDS =  3   OBSERVED CARDS = 1074   LESS-THAN CARDS = 616   SYSTEM EXT. =  86

                        TOTAL REFLECTIONS ON BINARY TAPE =  1776

              CONSTANTS AND CALCULATED VALUES AT END OF CALCULATION.
                       MINIMUM INTENSITY =    7.0000
                       MAXIMUM SIN THETA =    0.9887
                                  LAMBDA =    1.5418
                                   SCALE =    1.0000
                                  WEIGHT =    1.0000
                                   LEVEL =    10
                                   ERROR =    0.
                                    ZETA =    0.0049
                                  J AXIS =     2
                                  K AXIS =    -0

MAXIMUM VALUES OF....

                       H   5
                       K   5
                       L  15
            MULTIPLICITY   2
               SINTH/LAM  0.640882
             F RELTIV  140.708401
                   1/LP  1.999772
                 WEIGHT  1.000000
                  LEVEL  10
    SCATTERING FACTORS  5.52  6.58  7.61  0.91

MINIMUM VALUES OF....
             F RELATIVE -0.
                   1/LP  0.218290
                 WEIGHT  0.071069
    SCATTERING FACTORS  1.49  1.63  1.83  0.03
```

UNIT CELL CONTAINS
24 C ATOMS, ATOMIC NUMBER = 6.00
20 N ATOMS, ATOMIC NUMBER = 7.00
32 O ATOMS, ATOMIC NUMBER = 8.00
12 H ATOMS, ATOMIC NUMBER = 1.00

B REFINEMENT, X = 2.00000

		CYCLE 1	CYCLE 2	CYCLE 3	CYCLE 4	CYCLE 5	CYCLE 6	CYCLE 7
TEMP. FACTORS		3.00000	4.00000	5.00000	4.33737	4.43737	4.23737	4.32058
F RELATIVE SCALE FACTORS								
	REFLNS.**							
OVERALL	3365	1.14800	0.93391	0.74574	0.86742	0.84830	0.88682	0.87066
SUGGESTED LEVEL SCALE FACTORS, OVERALL SCALE FACTOR APPLIED								
LEVEL 1	101	0.90149	0.76083	0.68141	0.71581	0.70272	0.72901	0.71802
LEVEL 2	438	1.11959	0.92165	0.74170	0.85864	0.84039	0.87709	0.86172
LEVEL 3	420	1.14242	0.95170	0.77481	0.89017	0.87227	0.90823	0.89319
LEVEL 4	384	1.39600	1.19003	0.99234	1.12206	1.10214	1.14209	1.12542
LEVEL 5	390	1.10735	0.91508	0.74302	0.85465	0.83720	0.87231	0.85760
LEVEL 6	326	1.07307	0.90117	0.74608	0.84692	0.83122	0.86280	0.84958
LEVEL 7	332	1.24185	0.99827	0.79213	0.92470	0.90369	0.94607	0.92826
LEVEL 8	324	1.39004	1.09059	0.84314	1.00157	0.97628	1.02735	1.00586
LEVEL 9	300	0.97449	0.75602	0.57877	0.69190	0.67376	0.71043	0.69498
LEVEL 10	264	1.00624	0.77859	0.59767	0.71280	0.69426	0.73177	0.71595
SUM (E**2-1)**2		12192.3	11450.3	11594.4	11406.9	11412.4	11409.6	11406.7

** NUMBER OF REFLECTIONS IN ENTIRE HEMISPHERE

FINAL VALUES AND STATISTICS

	APPLIED TO E VALUES	STORED ON OUTPUT TAPE
TEMPERATURE FACTOR	4.32058	4.32058
(SINE THETA)/LAMBDA EXPONENT	2.00000	(2.00000)
F RELATIVE SCALE FACTORS		
LEVEL 1	0.87066	0.87066
LEVEL 2	0.87066	0.87066
LEVEL 3	0.87066	0.87066
LEVEL 4	0.87066	0.87066
LEVEL 5	0.87066	0.87066
LEVEL 6	0.87066	0.87066
LEVEL 7	0.87066	0.87066
LEVEL 8	0.87066	0.87066
LEVEL 9	0.87066	0.87066
LEVEL 10	0.87066	0.87066

E(0,0,0) = 8.8345, F(0,0,0) = 552.00

AVERAGE VALUES - /E/ = 0.7360, E**2 = 1.0000, /E**2-1/ = 1.1028

(SINE THETA)/LAMBDA RANGE	REFLTNS.	AVERAGE E**2
0. TO 0.30	445	0.9443
0.30 TO 0.38	461	0.8364
0.38 TO 0.43	426	1.0196
0.43 TO 0.48	450	1.3991
0.48 TO 0.52	427	1.2160
0.52 TO 0.56	444	0.9151
0.56 TO 0.60	418	0.8080
0.60 TO 0.64	208	0.9257

FRACTION OF E VALUES GREATER THAN 1.0 =0.2743
2.0 =0.0597
3.0 =0.0125

DATFIX COMPLETED

GGG

68 REFLECTIONS

H	K	L	E
2	4	0	3.250
6	0	0	3.224
4	4	6	3.157
2	8	6	2.799
8	4	-4	2.503
6	2	-10	2.464
0	4	2	2.411
8	2	-4	2.226
2	6	-10	2.223
2	0	6	2.202
4	6	-4	2.129
8	2	4	2.086
6	2	-4	2.072
6	8	6	1.933
6	2	-12	1.865
6	6	-4	1.845
0	8	6	1.744
2	8	10	1.739
2	4	-6	1.726
0	4	10	1.710
2	8	-2	1.703
0	8	8	1.647
4	2	-10	1.620
4	2	-2	1.613
8	2	-2	1.613
2	4	8	1.605
4	2	-4	1.580
2	0	12	1.562
2	2	-8	1.551
2	4	-10	1.538
0	8	12	1.538
6	2	2	1.488
6	2	8	1.479
0	6	2	1.476
4	4	-2	1.437
6	6	4	1.430
0	0	12	1.406
6	4	-4	1.387
8	6	0	1.384
2	6	8	1.382
4	6	-10	1.369
2	0	-2	1.366
4	4	-6	1.342
4	8	6	1.337
4	0	4	1.317
2	0	-8	1.310
4	4	4	1.286
2	0	-10	1.280
2	2	-2	1.256
4	2	-12	1.229

GGL

59 REFLECTIONS

H	K	L	E
0	8	9	3.346
8	2	-3	3.066
6	4	5	3.020
4	4	7	2.919
2	8	-1	2.771
2	2	-1	2.539
4	8	-7	2.370
4	8	1	2.329
6	2	3	2.303
2	6	7	2.267
4	6	-9	2.228
8	4	-3	2.215
4	8	5	2.047
8	4	-5	2.016
4	6	-1	1.961
6	2	-11	1.926
2	8	-3	1.916
6	2	-9	1.876
4	8	-3	1.785
0	2	11	1.740
6	8	-3	1.683
4	6	-5	1.622
2	6	9	1.601
6	8	-5	1.474
2	2	-3	1.450
6	6	3	1.436
2	8	3	1.426
2	8	9	1.401
8	2	-5	1.349
2	8	-11	1.341
2	2	11	1.327
8	4	1	1.315
2	4	7	1.305
8	4	-1	1.299
2	8	1	1.295
6	6	-1	1.270
4	4	-1	1.259
2	4	-7	1.257
2	4	-11	1.254
6	8	-1	1.227
2	8	11	1.192
4	2	-11	1.189
4	2	-9	1.182
6	2	9	1.176
4	4	5	1.172
8	4	-7	1.141
8	4	3	1.136
8	2	-1	1.119
6	6	1	1.112
0	2	9	1.111

GUG

59 REFLECTIONS

H	K	L	E
6	1	2	3.926
4	9	2	3.774
0	9	6	3.572
0	1	12	3.208
2	9	-2	3.140
2	5	6	2.835
2	9	0	2.672
2	1	4	2.234
4	7	-6	2.172
4	7	-8	2.152
4	5	-6	2.113
6	1	0	1.895
0	5	10	1.847
2	5	10	1.802
4	9	-8	1.734
4	1	10	1.696
6	3	-8	1.691
2	9	-8	1.679
0	5	2	1.630
6	7	0	1.628
2	3	-6	1.586
2	7	12	1.531
4	9	4	1.509
4	5	8	1.498
8	3	-6	1.489
0	7	4	1.488
4	9	-2	1.485
8	3	-2	1.437
6	1	-10	1.401
8	7	-2	1.393
0	3	12	1.379
0	5	8	1.328
4	7	8	1.327
2	9	-4	1.314
6	9	-6	1.313
2	5	2	1.300
6	9	-2	1.279
4	9	8	1.278
2	7	-4	1.248
6	5	4	1.244
8	3	2	1.225
4	7	-12	1.216
2	9	-6	1.208
0	9	4	1.177
4	7	-10	1.160
0	1	2	1.158
2	5	-6	1.118
8	7	0	1.107
0	7	6	1.100
2	1	12	1.096

GUU

58 REFLECTIONS

H	K	L	E
2	9	-3	3.920
2	5	-5	3.391
4	9	3	3.127
2	5	9	2.831
8	1	-3	2.659
2	3	1	2.620
0	5	3	2.336
8	3	-3	2.332
4	9	-3	2.164
6	1	7	2.070
4	1	-1	2.063
2	7	11	2.036
6	9	-7	1.948
2	9	-1	1.900
2	1	1	1.866
6	1	-3	1.843
2	9	-7	1.826
4	7	-9	1.824
6	9	-5	1.818
2	7	9	1.814
4	3	7	1.688
4	5	11	1.658
4	7	-5	1.649
2	5	3	1.570
0	3	11	1.534
4	5	9	1.514
6	1	-9	1.490
0	5	11	1.487
4	7	5	1.478
2	7	-9	1.466
2	9	9	1.456
8	1	5	1.426
4	7	-11	1.403
0	1	13	1.383
4	5	-7	1.367
2	1	-15	1.319
2	1	-11	1.288
4	1	1	1.278
4	1	9	1.269
2	7	5	1.222
0	1	5	1.186
4	5	1	1.175
2	3	13	1.170
4	5	7	1.160
4	5	-9	1.149
4	9	7	1.148
4	7	-3	1.108
2	3	11	1.104
4	7	9	1.089
6	7	-3	1.051

GGG

H	K	L	E
6	C	-4	1.215
2	C	4	1.2C5
4	8	-1C	1.189
2	4	-4	1.181
6	6	-2	1.175
C	4	8	1.159
4	2	2	1.154
8	4	-2	1.143
6	4	-10	1.123
2	6	-12	1.113
4	0	8	1.106
0	6	8	1.060
6	C	2	1.059
0	4	6	1.C55
4	0	-2	1.052
0	0	14	1.052
8	4	2	1.043
0	2	2	1.C27

GGL

H	K	L	E
2	8	-9	1.C90
2	8	7	1.C71
4	8	-5	1.C71
6	2	1	1.C62
6	2	5	1.C59
C	4	5	1.C56
4	2	-3	1.C33
4	4	1	1.C22
4	4	-9	1.C18
0	0	0	0.
C	0	C	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	C	0.
0	0	C	0.

GUG

H	K	L	E
4	5	-4	1.C95
6	5	C	1.C86
0	1	14	1.C84
4	7	4	1.C33
0	7	1C	1.C33
8	1	4	1.C32
0	5	14	1.C22
0	7	12	1.C06
2	5	-4	1.C01
0	0	C	0.
0	0	0	0.
0	C	0	0.
C	0	0	0.
0	C	0	0.
0	C	0	0.
0	C	0	0.
0	C	0	0.

GUU

H	K	L	E
8	3	-5	1.C41
6	5	3	1.C35
6	9	3	1.C16
2	9	-11	1.C16
4	3	5	1.C12
4	9	-5	1.C07
4	1	-7	1.C05
2	5	7	1.C03
0	0	0	0.
C	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.

LGG

66 REFLECTICNS

H	K	L	E
3	6	8	3.911
7	8	-6	3.209
3	8	-2	2.954
3	4	-12	2.789
5	4	6	2.699
1	2	-2	2.607
1	2	8	2.577
1	8	-8	2.444
1	6	2	2.356
5	4	-6	2.317
7	2	-2	2.267
1	8	0	2.194
3	6	6	2.120
5	0	-4	2.032
7	6	6	2.004
7	0	-2	1.996
1	2	10	1.960
3	2	-12	1.951
1	0	-12	1.893
7	4	4	1.882
5	0	10	1.798
5	4	-2	1.692
5	8	4	1.681
1	2	14	1.672
3	8	6	1.665
1	4	-10	1.645
3	2	2	1.629
1	6	12	1.612
3	6	-8	1.609
1	4	10	1.576
1	6	8	1.565
3	8	10	1.530
7	8	-4	1.530
5	2	6	1.484
1	8	-2	1.463
7	2	-6	1.455
3	0	10	1.443
7	0	4	1.431
3	0	-4	1.383
5	0	4	1.333
1	6	-6	1.308
1	2	-10	1.292
5	2	4	1.288
5	4	0	1.243
3	2	6	1.226
1	8	-10	1.208
3	0	-10	1.205
5	8	-6	1.179
5	0	-2	1.175
3	4	-8	1.165

LGL

52 REFLECTICNS

H	K	L	E
5	8	7	3.604
3	8	-3	2.685
1	8	11	2.557
1	4	9	2.485
5	2	5	2.449
3	6	3	2.428
3	8	5	2.421
5	4	-9	2.418
7	8	-5	2.239
3	8	1	2.186
3	8	-7	2.171
1	8	-1	2.057
5	8	5	2.046
7	8	3	2.010
5	8	1	1.835
5	8	-9	1.826
5	6	9	1.819
7	2	-1	1.711
5	4	-7	1.649
3	6	-3	1.483
1	2	3	1.425
1	6	-11	1.411
3	2	-1	1.398
3	8	-5	1.392
7	4	-3	1.380
3	4	-3	1.365
3	6	-9	1.360
5	2	-5	1.359
1	8	-3	1.356
3	6	11	1.317
3	4	-5	1.297
5	4	5	1.274
7	2	-5	1.238
1	2	-3	1.234
3	6	9	1.231
7	6	5	1.231
5	6	5	1.222
7	2	1	1.216
1	4	3	1.184
1	8	7	1.089
1	6	-9	1.083
1	6	5	1.077
1	2	7	1.074
7	2	-9	1.068
7	8	-1	1.061
7	2	-11	1.056
5	2	7	1.032
7	2	-3	1.013
1	4	-7	1.010
5	8	-3	1.006

UUG

55 REFLECTICNS

H	K	L	E
7	1	0	3.761
1	1	-14	3.492
3	5	-6	3.095
7	1	8	2.711
5	9	-6	2.658
3	7	4	2.546
5	1	-6	2.227
7	7	4	2.194
5	5	-8	2.137
3	7	-4	1.919
1	3	-4	1.883
5	3	4	1.829
1	7	4	1.819
3	5	-10	1.737
7	5	2	1.736
3	9	6	1.703
3	5	10	1.653
3	9	0	1.631
3	1	12	1.501
5	5	-6	1.497
1	9	-8	1.482
1	5	-12	1.478
7	5	-2	1.441
5	5	8	1.422
3	1	-8	1.417
7	9	-4	1.392
5	3	-8	1.389
7	3	-2	1.379
7	1	2	1.372
1	7	-4	1.366
1	5	0	1.333
3	5	-4	1.307
1	9	-6	1.299
1	3	10	1.255
7	1	6	1.228
1	5	2	1.227
5	3	-4	1.219
1	1	-2	1.201
7	5	4	1.185
1	7	-2	1.167
1	3	-2	1.149
5	1	8	1.142
5	1	-2	1.135
1	5	12	1.124
1	1	-4	1.101
1	9	0	1.098
3	5	-8	1.096
1	1	10	1.059
1	1	-8	1.051
5	1	-12	1.047

UUU

53 REFLECTICNS

H	K	L	E
1	3	-3	3.199
3	9	-1	2.965
5	1	3	2.736
5	9	1	2.596
7	1	-1	2.531
1	3	11	2.345
3	5	-1	2.297
1	1	-13	2.263
1	1	-3	2.260
3	9	3	2.150
3	1	-1	2.012
5	1	9	1.995
3	3	9	1.923
3	1	-3	1.886
3	1	11	1.885
7	1	-5	1.785
1	5	-1	1.717
3	7	5	1.702
1	5	9	1.610
5	5	-7	1.593
5	9	-3	1.525
5	1	-11	1.499
7	9	-3	1.476
5	9	-9	1.436
3	5	9	1.435
3	3	1	1.429
7	7	1	1.403
7	7	-5	1.388
1	5	1	1.373
5	7	5	1.365
3	9	5	1.364
3	3	3	1.353
1	1	-15	1.323
1	9	-7	1.321
3	5	7	1.304
1	3	-5	1.279
3	9	-3	1.263
5	1	5	1.234
5	3	1	1.204
3	7	3	1.172
1	1	-7	1.159
7	1	-3	1.141
1	5	7	1.140
3	7	9	1.135
1	5	3	1.126
5	3	-11	1.114
3	5	-7	1.062
5	5	9	1.056
5	5	-1	1.036
3	3	7	1.031

LGG

H	K	L	E
5	2	0	1.141
7	4	-4	1.134
5	4	-8	1.128
5	2	-2	1.114
7	C	0	1.108
3	6	-6	1.104
7	4	-2	1.096
7	6	2	1.C93
5	4	2	1.C92
3	6	0	1.089
1	C	6	1.C71
1	C	14	1.C69
3	C	12	1.C59
1	4	8	1.C5C
3	6	-4	1.C17
5	6	-4	1.C07

LGU

H	K	L	E
3	2	1	1.006
1	2	9	1.C02
0	0	C	0.
C	0	C	0.
0	0	C	C.
C	0	C	C.
0	0	0	0.
0	C	C	0.
C	C	C	C.
0	C	C	0.
0	0	0	0.
0	C	C	0.
0	0	C	0.
0	0	C	0.
0	0	C	0.
0	0	C	0.
0	0	0	0.

UUG

H	K	L	E
3	7	-8	1.042
3	1	-4	1.C36
1	5	-10	1.C30
3	9	-10	1.C14
5	5	0	1.C01
0	0	0	0.
0	0	0	0.
0	C	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	C	0	0.
0	0	C	0.
0	0	0	0.

UUU

H	K	L	E
1	3	7	1.C15
7	3	-5	1.C04
5	1	-3	1.C03
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.
0	0	0	0.

SUMMARY OF ESORT RESULTS

THE MINIMUM ACCEPTED E VALUE WAS 1.000.

THE TOTAL NUMBER OF REFLECTIONS READ WAS 1690.

THE NUMBER OF OBSERVED REFLECTIONS IS 1074.

THE NUMBER OF REFLECTIONS SORTED WAS 470.

TAPE ASSIGNMENTS - NTIN NTOUT NTAPEA NTAPEB .....
5 8 12 11 2 8 6 4

LIST A SAMPLE OF MODIFIED REFLECTIONS.

MODIFY PHASE OF E IN CENTROSYMMETRIC CASE.

MODIFY THE CONTENTS OF WORD 10 BY REPLACEMENT WITH QUANTITIES SHOWN BELOW.

INPUT TAPE CONTAINS DATA FOR TENA AND HAS BEEN REWRITTEN 1 TIMES.
TAPE LABEL - CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63
THE MOST RECENT WRITINGS WERE BY DATFIX DATRON

H	K	L	NEW CONTENTS OF WORD	10	...REPLACES OLD VALUE
1	0	-12	0.		0.200000E 01
2	0	6	0.500000E 00		0.200000E 01
5	0	-4	0.		0.200000E 01
6	0	0	0.500000E 00		0.200000E 01
0	1	12	0.		0.200000E 01
1	1	-3	0.500000E 00		0.200000E 01
1	1	-14	0.		0.200000E 01
2	1	1	0.		0.200000E 01
2	1	4	0.500000E 00		0.200000E 01
3	1	-3	0.500000E 00		0.200000E 01
3	1	11	0.500000E 00		0.200000E 01
4	1	-1	0.500000E 00		0.200000E 01
5	1	3	0.		0.200000E 01
5	1	-6	0.		0.200000E 01
6	1	0	0.500000E 00		0.200000E 01
6	1	2	0.		0.200000E 01
6	1	-9	0.		0.200000E 01

OF THE 113 CARDS READ 113 ACCEPTED AS VALID REFLECTION CARDS. OF THE 1776
REFLECTIONS ON THE BINARY TAPE 113 WERE MODIFIED.

INPUT TAPE CONTAINS DATA FOR TENA AND HAS BEEN REWRITTEN 2 TIMES.
TAPE LABEL - CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63
THE MOST RECENT WRITINGS WERE BY MODIFY DATFIX DATRON

ELECTRON DENSITY SCALE FACTOR = 1000.00000

SUMMARY OF CONTROL DATA

	H	K	L	
SUMMATION ORDER	1ST	2ND	3RD	SIN THETA/LAMBDA BETWEEN
MAXIMUM VALUES	9	5	15	0.0000 AND 5.0000
	X	Y	Z	
GRID	24	37	40	21 GRID POINTS ACROSS ONE PAGE
NUMBER OF POINTS	13	37	21	
ORIGIN	0	0	0	1 SPACES PER LINE
INCREMENT	1	1	1	

PROGRAM KEYED TO CALCULATE E MAP PHASES FROM STATISTICS

NUMBER OF PASSES REQUIRED-- 1

TENA E PAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 40THS X = 0 24THS

	C	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0																					
1																					
2																					
3																					
4																					
5																					
6										202	186										
7										162											
8																					
9											-122										
10																					
11																					
12																					
13																					
14																					
15																					
16																					
17																					
18																					
19																					
20																					
21																					
22																					
23																					
24											156	166									
25											176	200									
26																					
27																					
28											-105										
29																					
30																					
31																					
32																					
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 1 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	2C
C																					
1																					
2																					
3																					
4																					
5																					
6										327	292										
7										278	223										
8																					
9																					
1C																					
11												158	2C9	174							
12													164								
13				223	177																
14				161																	
15																					
16																					
17																					
18																					
19																					
2C																		157			
21																					
22																					
23															172						
24															164						
25																					
26																					
27											-11C										
28											-1C6										
29																					
3C																					
31																		-1C2			
32																					
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 2 24THS

	0	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	20
C																					
1																					
2																					
3																					
4																					
5																					
6																					
7											172										
8																					
9											-100										
1C											-101			-113							
11																					
12																					
13			164																		
14																					
15																					
16																					
17																					
18																					
19																					
2C																					
21																169	160				
22																248	272				
23																	203				
24																					
25													188	366							
26													175	371	206						
27														155							
28																					
29																					
30							-99														
31																					
32							156	218													
33							17C	222									-116				
34			-102																		
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 40THS X = 3 24THS

	C	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
C																					
1																					
2																					
3																					
4																					
5																		-105			
6																					
7																					
8														-115							
9																					
10																					
11																					
12																					
13																					
14																					
15																					
16		191																			
17																					
18																					
19																					
20																					
21																	158				
22																					
23																					
24															302						
25															306	188					
26																					
27																					
28																					
29																					
30																					
31								201	335	185											
32								179	292												
33																					
34																					
35																					
36					154									-111							

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 40THS X = 4 24THS

	C	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0																					
1																					
2																					
3																					
4																				-118	
5																				-108	
6																					
7																					
8																					
9																					
10																156					
11																					
12																					
13																					
14	-134																				
15																					
16																					
17																					
18							162														
19																					
20																					
21																					
22																					
23																					
24																					
25																					
26																					
27																					
28																					
29																					
30																					
31																					
32																-106					
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 40THS X = 5 24THS

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0																					
1																					
2																					
3																					
4																					
5																					
6																					
7																					
8																					
9																					
10																					
11																					
12																					
13																		-125			
14	-99																	-114			
15							-106														
16																					
17									170												
18								159	170											-117	
19																					
20																					187
21																					
22																					
23																					
24															-112	-122					
25															-119	-144					
26	153																				
27	165														218						
28															177						
29																					176
30																					
31										-120		168									
32																					
33																	-103				
34																					
35	177																				
36	157																				

TEMA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 6 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	2C
C																					19C
1																					
2																					
3																					
4		-103																			
5																					
6																					
7																					
8																					
9																					
1C																					
11																					
12														-134							
13																					
14																	-127				
15							-112														
16					2C4	156															
17					222																
18	159	153																			
19	184	243																			
2C		183																			
21																					
22																					
23																					
24																					
25																					
26	173														165						
27	163													202	383	255					
28														158	325	211					
29																					185
30											220	156			-113						
31											277	248									
32												156									
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 7 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	2C
C																					151
1						152			-128												
2																					
3						-119															
4		-104																			
5																					
6																					
7																					
8																					
9																			205	21C	
1C																					
11																					
12														-1C0							
13																					
14																					
15																					
16																					
17				256	172																
18				151																	
19		2C3																			
2C		151																			
21																					
22																					
23																					
24																					
25																					
26																					
27															24C						
28															197						
29																					
3C																					
31												175	179								
32			-104																		
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 8 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	2C
C						175															
1						2CC															
2																					
3		-103																			
4																					
5																					
6																					
7																					
8																					
9																			176	187	
1C																					
11																					
12																					
13																					
14				-122																	
15				-141																	
16																					
17																					
18																					
19																					
2C																					
21																					
22		-101																			
23																					
24																					
25																					
26																					
27																					
28																					
29																					
3C																					
31																				-104	
32																					
33																					
34																					
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 9 24THS

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0						151															
1						165															
2															-102						
3																					
4																					
5																					
6																					
7																					
8																					
9																					
10																					
11																					
12																					
13																					
14																					
15																					
16					-113																
17					-101																
18																					
19																					
20																					
21																					
22																					
23																					
24																				168	
25																					
26																					
27																	222	160			
28																	185	195			
29																					
30																					
31																					
32																					
33	160																				
34																					
35																					
36											-101										

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 1C 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	20
C										2CC											
1										182											
2																					
3																					
4												155									
5																					
6																					
7																					
8																					
9																					
1C			165																		
11			187																		
12																					
13																					
14					175	262															
15						2C3															
16																					
17						-99															
18																					
19																					
2C																					
21																					
22																					
23																					
24																					
25																					
26																		237	183		
27																		169	184		
28																					
29																		-105			
3C																175					
31																					
32												157	153								
33												288	335								
34												251	299								
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 4CTHS X = 11 24THS

	C	1	2	3	4	5	6	7	8	9	1C	11	12	13	14	15	16	17	18	19	2C
C																					
1										154											
2																					
3										-122											
4												186									
5												161									
6																					
7																					
8																					
9																					
1C			221	161																	
11			234																		
12																					
13																					
14					2C1	31C															
15						239															
16																					
17						-1C8															
18																					
19																					
2C																					
21																					
22																					
23																					
24																					
25																					
26																					
27																					
28																					
29																					
3C																					
31																					
32																					
33							-1C5					228	238								
34												162	198								
35																					
36																					

TENA E MAP PHASES FROM STATISTICS 2,3,4,6 - TETRANITROANILINE

Y IN 37THS Z IN 40THS X = 12 24THS

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0																					
1																					
2																					
3																			-111	-101	
4												160	165								
5																					
6																					
7																					
8																					
9																					
10																					
11																					
12																					
13																					
14																					
15																					
16																					
17																					
18																					
19																					
20																					
21																					
22		-99	-103																		
23									151	162											
24																					
25																					
26																					
27																					
28																					
29																					
30																					
31																					
32																					
33																					
34																					
35																					
36																					

FCURR 2,3,4,6 - TETRANITROANILINE TENA PAGE 65

FOURIER SYNTHESIS COMPLETED IN 1.4303 MIN. R = 1.00000

OF THE 1690 REFLECTIONS READ, 113 CONTRIBUTED TO SUMS
0 WERE OUT OF SIN-THETA RANGE
1577 WERE REJECTED

```
GENERATE X-RAY PROGRAM TAPE PIKTES ON LOGICAL UNIT  9
UPDATE CURRENT TAPE - 240364

. . . LINK   100 . . .   COPIED

. . . LINK  1000 . . .   COPIED

. . . LINK  1001 . . .   COPIED

. . . LINK  3600 . . .   COPIED

. . . LINK  4000 . . .   COPIED

. . . LINK  5000 . . .   COPIED

. . . LINK  5500 . . .   COPIED

. . . LINK  6100 . . .   COPIED

. . . LINK  6500 . . .   COPIED

. . . LINK 10000 . . .   COPIED

. . . LINK 10300 . . .   COPIED

. . . LINK 10500 . . .   COPIED

. . . LINK 10600 . . .   COPIED

. . . LINK 10800 . . .   COPIED

. . . LINK 11100 . . .   COPIED

. . . LINK 12000 . . .   COPIED

. . . LINK 30300 . . .   COPIED

. . . LINK 30600 . . .
```

```
PROGRAM 000000 (MAIN)      RELOCATION INCREMENT = 05503
ENTRY POINTS--   000000 05520

PROGRAM AP                 RELOCATION INCREMENT = 06371
ENTRY POINTS--   AP     06375

PROGRAM LINAP2             RELOCATION INCREMENT = 06506
ENTRY POINTS--   LINAP2 06514

PROGRAM PICOUT             RELOCATION INCREMENT = 06775
ENTRY POINTS--   PICOUT 07004

PROGRAM PEAKPK             RELOCATION INCREMENT = 07356
ENTRY POINTS--   PEAKPK 07370

PROGRAM (SLI)              RELOCATION INCREMENT = 10562
ENTRY POINTS--   (SLI)  10562

PROGRAM SQRT               RELOCATION INCREMENT = 10577
ENTRY POINTS--   SQRT   10577

10653 IS PROGRAM BREAK      75354 IS COMMON BREAK
THE STORAGE BETWEEN THESE INCLUSIVE LIMITS IS UNUSED.


. . . LINK 31000 . . .   COPIED


. . . LINK 32700 . . .   COPIED

X-RAY PROGRAM TAPE PIKTES OPERATING FROM LOGICAL UNIT  9
```

PEKPIK SEARCH MAP FOR HIGHEST PEAKS (19 ATOMS IN ASSYMETRIC UNIT) TENA PAGE 68

FRACTIONAL COORDINATES IN TERMS OF XTAL AXIS				COORDINATES IN TERMS OF POINTS IN THE ARRAY PRINTED BY FOURIER		
X	Y	Z	VALUE OF FUNCTION AT POINT	ACROSS PAGE	DOWN PAGE	PAGE TO PAGE
0.	0.6691	0.2658	216.1937	10.6310	24.7561	0.
0.0393	0.1703	0.2342	355.7105	9.3684	6.3007	0.9425
0.0550	0.3543	0.0812	243.0225	3.2473	13.1098	1.3207
0.0473	0.3010	0.3023	213.8145	12.0908	11.1371	1.1346
0.0846	0.5708	0.4156	287.6963	16.6245	21.1182	2.0302
0.0943	0.6628	0.3511	405.6874	14.0432	24.5219	2.2635
0.1169	0.8469	0.1993	355.5265	7.9711	31.3363	2.8049
0.1250	0.4321	0.0260	190.9356	1.0388	15.9859	3.0000
0.1325	0.9730	0.0948	162.1697	3.7927	36.0000	3.1791
0.1667	0.2785	0.3718	162.8362	14.8735	10.3062	4.0000
0.1943	0.4731	0.1899	202.9160	7.5970	17.5048	4.6629
0.0917	0.5444	0.5000	292.9294	20.0000	20.1443	2.2015
0.2083	0.9546	0.	183.2514	0.	35.3219	5.0000
0.2640	0.	0.5000	202.9299	20.0000	0.	6.3372
0.2650	0.5162	0.0194	267.7259	0.7741	19.0981	6.3597
0.2512	0.7376	0.3521	395.6443	14.0850	27.2902	6.0280
0.2517	0.8320	0.2847	301.5995	11.3884	30.7854	6.0406
0.2313	0.7135	0.	190.9168	0.	26.3978	5.5503
0.2322	0.7863	0.5000	197.0270	20.0000	29.0938	5.5717
0.3091	0.2458	0.4636	243.4836	18.5447	9.0931	7.4195
0.2746	0.4597	0.1031	274.3317	4.1255	17.0078	6.5898
0.3332	0.0175	0.1306	213.8988	5.2232	0.6490	7.9968
0.3890	0.6196	0.5000	179.3474	20.0000	22.9242	9.3364
0.3852	0.8815	0.	173.2977	0.	32.6137	9.2445
0.4321	0.	0.2275	217.3153	9.0992	0.	10.3698
0.4286	0.9009	0.2923	377.0873	11.6932	33.3327	10.2874
0.3980	0.7065	0.4310	264.1099	17.2401	26.1399	9.5525
0.4254	0.8065	0.3715	183.7281	14.8586	29.8415	10.2094
0.4651	0.1169	0.2751	197.2154	11.1625	4.3264	11.1623
0.4500	0.2864	0.0488	248.4769	1.9535	10.5968	10.7995
0.4464	0.3837	0.1216	325.2758	4.8643	14.1960	10.7141
0.5000	0.6164	0.2145	173.0918	8.5968	22.8084	12.0000

32 PEAKS LOCATED AMONG THE 1010 POINTS SUPPLIED

CALCULATE STRUCTURE FACTORS FROM SET OF PEAKS IN E MAP TENA PAGE 69

TAPE ASSIGNMENTS - NTIN NTOUT NTAPEA NTAPEB .....
5 8 11 12 2 8 6 4

FC CALCULATE STRUCTURE FACTORS FROM SET OF PEAKS IN E MAP

INPUT TAPE CONTAINS DATA FOR TENA AND HAS BEEN REWRITTEN 2 TIMES.
TAPE LABEL - CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63
THE MOST RECENT WRITINGS WERE BY MODIFY CATFIX CATRON
REMARK SCALE AND TEMPERATURE FACTOR FROM CATFIX
THE PEAK PICKING LINK LOCATED ALL BUT C41 AND C42

OVERALL F-RELATIVE SCALE FACTOR OF 0.87000 APPLIED.

CHANGE APPLIED TO OVERALL E.

ATOM	X	Y	Z	B OR B11	B22	B33	B12	B13	B23
				OVERALL TEMPERATURE FACTOR.					
C1	0.25170	0.83200	0.28470	4.321					
C2	0.42860	0.90090	0.29230						
C3	0.44640	0.38370	0.12160						
C4	0.45000	0.28640	0.04880						
C5	0.39800	0.70650	0.43100						
C6	0.25120	0.73760	0.35210						
N1	0.11690	0.84690	0.19930						
N2	0.43210	0.	0.22750						
N3	0.27460	0.45970	0.10310						
N4	0.30910	0.24580	0.46360						
N6	0.09430	0.66280	0.35110						
O21	0.33320	0.01750	0.13060						
O22	0.46510	0.11690	0.27910						
O31	0.19430	0.47310	0.18990						
O32	0.26500	0.51620	0.01940						
O61	0.08460	0.57080	0.41560						
O62	0.03930	0.17030	0.23420						

USE F RELATIVE SCALE FACTORS
THERE ARE 2 EQUIVALENT POSITIONS FOR ATOMS IN GENERAL POSITIONS.

17 ATOMS IN THE ASYMMETRIC SET. CALCULATION IS OVER 34 ATOMS TOTAL.

REFLECTION STATISTICS**

GROUP	REFLECTIONS	FREL SCALE	FREL RESCALE	R
1	101	0.8700	0.7936	0.49310
2	219	0.8700	0.8635	0.39261
3	210	0.8700	0.8194	0.42772
4	192	0.8700	1.0007	0.46587
5	195	0.8700	0.7971	0.39711
6	163	0.8700	0.7395	0.45206
7	166	0.8700	0.9063	0.37585
8	162	0.8700	0.9122	0.42617
9	150	0.8700	0.6202	0.44274
10	132	0.8700	0.6421	0.45883
OVERALL	1690 TOTAL			0.43083
	1074 OBS.			
	616 UNOBS.			
	0 EXT.			

586 WHERE FO/FC LIES OUTSIDE 2/3 TO 3/2

OVERALL LINEAR SCALING RATIO 0.9437

SUGGESTED CHANGE IN THE OVERALL ISOTROPIC T.F. = -0.076

1.09 MIN TO CALCULATE FC. 0.001 MIN PER REFLECTION.

TAPE ASSIGNMENTS - NTIN NTOUT NTAPEA NTAPEB .....

NTIN	NTOUT	NTAPEA	NTAPEB				
5	8	12	11	2	8	6	4

INPUT FROM REFLECTION TAPE (CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63)
REWRITTEN 3 TIMES
MOST RECENT WRITINGS BY FC MODIFY DATFIX DATRON
REMARK SCALE FACTORS FROM FC

MULTIPLICITY OF GENERAL POSITION - 2

17 ATOMS IN ASSYMETRIC UNIT, SUMMATION IS OVER 34 ATOMS

TEMPERATURE FACTOR 4.3210

SCALE FACTORS
LEVEL 1 0.7936
LEVEL 2 0.8635
LEVEL 3 0.8154
LEVEL 4 1.0007
LEVEL 5 0.7971
LEVEL 6 0.7395
LEVEL 7 0.9063
LEVEL 8 0.9122
LEVEL 9 0.6202
LEVEL 10 0.6421

CYCLE 1, R = 0.430 FROM INPUT PARAMETERS CYCLE CALCULATION TIME 2.3228 MIN.
FC/FO LESS THAN 0.20 FOR 112 REFLECTIONS

	INPUT PARAMETERS			OUTPUT PARAMETERS			CHANGE			
ATOM	X	Y	Z	X	Y	Z	DX	DY	DZ	
C1	2517	8320	2847	2504	8358	2810	-13	38	-37	
C2	4286	9009	2923	4086	9109	3003	-200	100	80	NO PEAK
C3	4464	3837	1218	4452	3832	1206	-12	-5	-10	
C4	4500	2864	488	4509	2834	495	9	-30	7	
C5	3980	7065	4310	3980	7165	4390	0	100	80	NO PEAK
C6	2512	7376	3521	2448	7382	3536	-64	6	15	
N1	1169	8469	1993	1169	8569	1993	0	100	0	NO PEAK
N2	4321	0	2275	4121	100	2275	-200	100	0	NO PEAK
N3	2746	4597	1031	2787	4620	1035	41	23	4	
N4	3091	2458	4636	3091	2558	4716	0	100	80	NO PEAK
N6	943	6628	3511	881	6598	3514	-62	-30	3	
O21	3332	175	1306	3532	175	1386	200	0	80	NO PEAK
O22	4651	1169	2791	4651	1169	2871	0	0	80	NO PEAK
O31	1943	4731	1899	1943	4731	1819	0	0	-80	NO PEAK
O32	2650	5162	194	2610	5206	201	-40	44	7	
O61	846	5708	4156	846	5808	4156	0	100	0	NO PEAK
O62	393	1703	2342	393	1703	2262	0	0	-80	NO PEAK

CYCLE 2, R = 0.361 FROM INPUT PARAMETERS CYCLE CALCULATION TIME 2.3750 MIN.
FC/FO LESS THAN 0.20 FOR 79 REFLECTIONS

	INPUT PARAMETERS			OUTPUT PARAMETERS			CHANGE			
ATOM	X	Y	Z	X	Y	Z	DX	DY	DZ	
C1	2504	8358	2810	2493	8362	2816	-11	4	6	
C2	4086	5109	3003	4082	5088	3000	-4	-21	-3	
C3	4452	3832	1206	4461	3825	1212	5	-7	6	
C4	4505	2834	495	4521	2838	501	12	4	6	
C5	3980	7165	4390	3902	7161	4372	-78	-4	-18	
C6	2448	7382	3536	2416	7384	3540	-32	2	4	
N1	1165	6569	1593	1150	8575	1994	-15	6	1	
N2	4121	100	2275	4121	200	2355	0	100	80	NO PEAK
N3	2787	4620	1035	2814	4639	1040	27	19	5	
N4	3091	2558	4716	2891	2558	4716	-200	0	0	NO PEAK
N6	881	6598	3514	846	6584	3509	-35	-14	-5	
O21	3532	175	1386	3606	164	1369	74	-11	-17	
O22	4651	1169	2871	4735	1148	2866	84	-21	-5	
O31	1943	4731	1819	1925	4694	1795	-18	-37	-24	
O32	2610	5206	201	2566	5217	191	-44	11	-10	
O61	846	5808	4156	848	5818	4196	2	10	40	
O62	393	1703	2262	393	1703	2182	0	0	-80	NO PEAK

CYCLE 3, R = 0.341 FROM INPUT PARAMETERS CYCLE CALCULATION TIME 2.3958 MIN.
FC/FO LESS THAN 0.20 FOR 62 REFLECTIONS

	INPUT PARAMETERS			OUTPUT PARAMETERS			CHANGE		
ATOM	X	Y	Z	X	Y	Z	DX	DY	DZ
C1	2493	8362	2816	2475	8363	2810	-18	1	-6
C2	4082	5088	3000	4095	5080	2998	17	-8	-2
C3	4461	3825	1212	4449	3820	1200	-12	-5	-12
C4	4521	2838	501	4526	2832	504	5	-6	3
C5	3902	7161	4372	3879	7144	4367	-23	-17	-5
C6	2416	7384	3540	2404	7390	3547	-12	6	7
N1	1150	8575	1994	1145	8568	1986	-5	-7	-8
N2	4121	200	2355	4149	207	2344	28	7	-11
N3	2814	4639	1040	2827	4645	1043	13	6	3
N4	2891	2558	4716	2939	2577	4744	48	19	28
N6	846	6584	3509	834	6579	3507	-12	-5	-2
O21	3606	164	1369	3622	159	1360	16	-5	-9
O22	4735	1148	2866	4760	1140	2866	25	-8	-0
O31	1925	4694	1795	1907	4677	1782	-18	-17	-13
O32	2566	5217	191	2561	5223	190	-5	6	-1
O61	848	5818	4196	836	5825	4194	-12	7	-2
O62	393	1703	2182	466	1738	2194	73	35	12

CYCLE 4, R = 0.335 FROM INPUT PARAMETERS CYCLE CALCULATION TIME 2.4094 MIN.
FC/FO LESS THAN 0.20 FOR 58 REFLECTIONS

	INPUT PARAMETERS			OUTPUT PARAMETERS			CHANGE		
ATOM	X	Y	Z	X	Y	Z	DX	DY	DZ
C1	2475	8363	2810	2482	8361	2815	7	-2	5
C2	4099	5080	2998	4091	9079	2998	-8	-1	0
C3	4449	3820	1200	4462	3820	1208	13	-0	8
C4	4526	2832	504	4526	2828	508	0	-4	4
C5	3879	7144	4367	3865	7140	4355	-14	-4	-12
C6	2404	7390	3547	2407	7394	3548	3	4	1
N1	1145	8568	1986	1142	8564	1987	-3	-4	1
N2	4149	207	2344	4158	208	2341	9	1	-3
N3	2827	4645	1043	2828	4647	1047	1	2	4
N4	2939	2577	4744	2963	2582	4755	24	5	11
N6	834	6579	3507	826	6579	3503	-8	-0	-4
C21	3622	159	1360	3630	166	1365	8	7	5
C22	4760	1140	2866	4772	1137	2865	12	-3	-1
C31	1907	4677	1782	1917	4680	1797	10	3	15
C32	2561	5223	190	2549	5218	180	-12	-5	-10
C61	836	5825	4194	848	5811	4198	12	-14	4
C62	466	1738	2194	500	1749	2195	34	11	1

FINAL R = 0.333

INPUT TAPE CONTAINS DATA FOR TENA AND HAS BEEN REWRITTEN 4 TIMES.
TAPE LABEL - CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63
THE MOST RECENT WRITINGS WERE BY FOUREF FC MODIFY DATFIX DATRON

ELECTRON DENSITY SCALE FACTOR = 10.00000

SUMMARY OF CONTROL DATA

	H	K	L	
SUMMATION ORDER	1ST	2ND	3RD	SIN THETA/LAMBDA BETWEEN
MAXIMUM VALUES	9	5	15	0.0000 AND 5.0000

	X	Y	Z	
GRID	48	74	80	14 GRID POINTS ACROSS ONE PAGE
NUMBER OF POINTS	24	16	15	
ORIGIN	2	12	26	2 SPACES PER LINE
INCREMENT	2	1	1	

REJECT OBS. REF. WHERE (FC * 0.200 - FO) ZERO OR GREATER. ALL REJECTED REFL. MARKED R.

PROGRAM KEYED TO CALCULATE DATF REJT ON R TEST

NUMBER OF PASSES REQUIRED-- 1

TENA CATF REJT CN R TEST SEARCH IN REGICN OF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 2 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	3	6	8	9	1C	9	8	6	6	6	7	9	1C	9
13	3	6	8	1C	1C	1C	9	7	6	5	6	8	9	9
14	3	6	8	1C	11	11	1C	8	6	5	5	6	7	8
15	4	6	8	9	1C	11	1C	8	6	4	4	4	5	6
16	6	7	8	8	9	1C	9	8	6	4	3	3	4	5
17	7	7	7	7	7	8	8	6	5	3	2	2	2	3
18	8	8	7	6	5	5	5	4	3	2	1	1	2	2
19	8	8	6	4	4	3	3	2	1	-C	-1	-C	1	1
2C	9	7	5	3	2	1	1	-1	-2	-3	-2	-2	-1	0
21	9	7	5	3	2	C	-1	-3	-4	-5	-4	-3	-2	-1
22	8	7	5	3	1	-C	-2	-4	-6	-7	-6	-5	-4	-3
23	8	7	5	3	1	-C	-2	-5	-7	-8	-7	-6	-5	-5
24	8	7	5	3	1	-C	-2	-4	-6	-7	-7	-7	-6	-6
25	8	6	5	3	2	C	-2	-4	-5	-6	-6	-6	-6	-6
26	7	6	5	3	2	C	-1	-3	-4	-5	-4	-4	-4	-5
27	6	6	5	4	2	1	-1	-2	-3	-3	-2	-2	-2	-3
28	6	6	5	4	3	1	0	-1	-1	-1	-C	-0	-1	-2
29	6	6	5	5	4	2	1	0	-C	C	1	1	1	-0

TENA CATF REJT CN R TEST SEARCH IN REGICN OF MISSING OXYGENS

Y IN 74THS Z IN 8CTHS X = 4 48THS

	26	27	28	29	30	31	32	33	34	35	36	37	38	39
12	-C	3	5	7	8	7	7	6	6	7	9	12	13	13
13	-C	3	5	7	8	8	8	7	7	8	1C	14	16	17
14	C	3	5	7	8	9	9	8	8	9	12	15	18	19
15	1	3	5	6	8	9	9	9	9	1C	12	16	19	20
16	1	3	4	5	7	8	9	9	9	1C	12	15	18	19
17	2	3	3	4	6	7	8	8	8	9	11	14	16	17
18	2	3	3	3	4	6	6	7	7	7	9	11	13	14
19	3	3	3	3	3	4	5	5	4	5	6	7	9	10
20	3	3	2	2	3	3	3	3	2	1	2	3	4	5
21	3	3	2	1	2	2	2	1	-1	-1	-1	-1	0	1
22	3	2	1	1	1	1	C	-1	-2	-3	-4	-3	-3	-3
23	3	2	1	C	C	-C	-1	-2	-3	-4	-5	-5	-5	-5
24	2	1	1	C	-C	-1	-1	-3	-4	-5	-5	-5	-6	-6
25	2	1	1	C	-C	-1	-2	-3	-4	-4	-5	-5	-5	-6
26	1	1	1	1	1	-C	-1	-2	-3	-3	-4	-4	-4	-5
27	1	2	2	2	2	1	C	-1	-2	-2	-3	-3	-3	-4
28	1	2	3	4	4	3	1	0	-1	-2	-2	-2	-3	-3
29	2	3	4	5	5	4	3	1	-C	-1	-1	-2	-2	-3

TENA DATF REJT CN R TEST SEARCH IN REGICN OF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 6 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	-2	-1	1	2	3	3	3	3	4	7	1C	14	17	18
13	-3	-1	-0	1	3	3	4	5	6	1C	14	2C	24	25
14	-3	-2	-1	1	2	4	5	6	8	12	18	25	3C	32
15	-4	-3	-2	-C	2	3	5	7	1C	15	21	29	34	37
16	-5	-4	-3	-1	1	3	5	7	1C	15	22	3C	36	38
17	-5	-4	-3	-1	1	3	5	7	1C	15	21	28	34	36
18	-5	-4	-3	-1	1	3	5	7	9	13	18	24	29	31
19	-4	-4	-3	-1	1	3	5	6	8	1C	14	18	21	23
2C	-4	-3	-2	-1	1	3	5	6	6	8	1C	12	14	15
21	-3	-2	-2	-1	1	3	4	5	5	5	6	7	7	7
22	-2	-2	-2	-1	1	2	3	3	3	3	3	3	2	2
23	-1	-1	-1	-C	1	2	2	2	2	1	1	C	-1	-2
24	-1	-1	-1	-C	1	1	1	1	C	-C	-1	-1	-2	-3
25	-1	-1	-0	1	1	1	C	-0	-1	-1	-2	-2	-3	-4
26	-1	-C	1	1	2	1	C	-1	-2	-2	-3	-3	-4	-4
27	-1	C	2	3	3	2	1	-1	-2	-3	-3	-4	-4	-5
28	-1	1	2	3	4	3	2	C	-1	-3	-4	-4	-5	-5
29	-1	1	2	4	5	4	3	1	-1	-2	-3	-4	-5	-6

TENA DATE REJT CN R TEST SEARCH IN REGICN CF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 8 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	-3	-3	-3	-3	-2	-1	-C	1	2	4	7	1C	13	15
13	-3	-4	-4	-3	-2	-1	1	2	4	7	12	17	21	22
14	-4	-5	-4	-3	-2	C	2	3	6	10	16	22	27	29
15	-5	-5	-5	-3	-1	1	2	4	7	12	19	26	32	35
16	-6	-6	-5	-3	-1	1	3	5	8	13	2C	28	34	37
17	-6	-6	-5	-3	-C	2	4	6	8	13	19	26	33	36
18	-6	-5	-4	-2	C	3	5	6	8	12	17	23	28	31
19	-5	-5	-3	-1	1	4	5	7	8	10	14	18	22	24
2C	-4	-4	-3	-1	2	4	6	7	8	9	11	13	15	16
21	-3	-3	-2	-C	2	4	6	7	7	7	8	9	9	9
22	-2	-2	-1	C	2	4	5	6	6	6	5	5	5	4
23	-1	-1	-1	C	2	3	4	4	4	4	4	3	2	1
24	-1	-0	-0	1	2	2	2	2	2	2	2	1	0	-1
25	-1	-0	0	1	2	2	1	1	C	-0	-C	-C	-1	-2
26	-1	-0	1	1	2	1	1	-C	-1	-2	-2	-2	-2	-2
27	-2	-1	1	1	2	2	1	-1	-2	-2	-3	-3	-3	-3
28	-2	-1	0	1	2	2	1	-C	-2	-3	-3	-4	-4	-4
29	-3	-2	-1	1	2	2	1	-C	-1	-3	-4	-4	-5	-5

TENA DATF REJT CN R TEST SEARCH IN REGICN CF MISSING OXYGENS

Y IN 74THS Z IN 8CTHS X = 1C 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	-3	-4	-5	-5	-5	-4	-3	-2	-1	C	2	3	5	7
13	-3	-4	-5	-5	-4	-3	-1	C	1	3	5	7	9	1C
14	-3	-4	-5	-4	-3	-1	C	2	3	5	7	11	13	14
15	-3	-4	-4	-3	-2	C	2	3	4	6	9	13	16	17
16	-3	-3	-3	-2	-C	2	3	4	5	7	1C	14	17	19
17	-2	-2	-1	-C	1	3	4	4	5	6	9	13	16	18
18	-1	-1	C	1	3	4	5	5	5	6	8	11	14	16
19	-C	1	1	2	3	5	6	6	5	5	6	8	11	13
2C	1	2	2	3	4	5	6	6	5	5	5	6	7	9
21	2	2	3	3	4	6	6	6	5	4	3	4	4	5
22	2	2	2	3	4	5	6	6	5	3	2	2	2	2
23	2	2	2	2	3	4	5	4	3	2	1	1	C	-C
24	2	1	1	1	2	3	3	3	2	1	C	-C	-C	-1
25	1	1	0	C	1	2	2	1	C	-1	-1	-1	-1	-1
26	C	-C	-C	-C	C	1	1	C	-1	-2	-2	-2	-2	-2
27	-1	-1	-1	-1	-1	-C	-C	-C	-1	-2	-3	-3	-2	-2
28	-2	-2	-2	-2	-1	-1	-C	-1	-1	-2	-3	-3	-3	-2
29	-3	-3	-3	-2	-2	-1	-C	-1	-1	-2	-3	-3	-3	-3

TENA DATE REJT CN R TEST SEARCH IN REGICN CF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 12 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	-2	-3	-5	-6	-6	-5	-4	-3	-3	-3	-2	-1	-C	1
13	-2	-4	-5	-6	-5	-4	-3	-2	-1	-1	-1	C	1	2
14	-3	-4	-5	-5	-4	-3	-2	-1	-C	C	1	2	2	3
15	-3	-3	-4	-4	-3	-2	-1	C	1	1	2	3	3	4
16	-2	-2	-3	-3	-2	-1	C	1	1	2	2	3	4	5
17	-1	-1	-1	-1	-C	1	1	2	2	2	2	3	4	5
18	C	1	1	1	2	3	3	3	3	2	2	3	4	6
19	2	3	3	4	4	5	6	5	4	3	2	2	4	5
2C	3	4	5	6	7	8	9	8	6	4	2	2	3	4
21	4	5	6	7	9	11	12	11	8	5	2	1	2	3
22	3	4	5	7	1C	13	14	13	9	6	3	1	1	1
23	3	3	4	7	1C	13	15	13	1C	6	2	C	-C	-C
24	2	2	3	5	9	12	14	13	1C	5	2	-C	-1	-1
25	2	1	2	4	7	11	12	11	8	4	1	-1	-1	-1
26	2	1	1	2	5	8	10	9	7	3	C	-1	-2	-1
27	1	1	0	1	3	5	7	7	5	2	-C	-1	-2	-1
28	1	1	0	C	1	3	5	5	4	2	-C	-1	-2	-1
29	1	C	-C	-C	1	2	3	4	3	2	0	-1	-2	-1

TENA CATF REJT CN R TEST SEARCH IN REGICN OF MISSING OXYGENS

Y IN 74THS Z IN 8CTHS X = 14 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	-C	-2	-4	-5	-5	-4	-3	-3	-4	-5	-5	-5	-3	-2
13	-1	-2	-4	-5	-5	-4	-3	-3	-3	-4	-5	-4	-3	-2
14	-2	-3	-4	-5	-5	-4	-3	-3	-3	-4	-4	-4	-3	-2
15	-2	-3	-4	-5	-5	-5	-4	-3	-3	-3	-4	-3	-3	-2
16	-2	-3	-4	-5	-5	-5	-4	-3	-3	-3	-3	-3	-2	-1
17	-2	-2	-3	-3	-4	-4	-3	-2	-2	-2	-2	-2	-1	-C
18	-1	-1	-1	-1	-1	-1	C	1	1	1	-C	-C	0	1
19	C	1	1	2	3	4	5	6	5	4	2	2	2	3
2C	1	2	3	5	8	1C	12	12	1C	7	5	3	3	3
21	1	2	5	8	13	17	19	19	16	11	7	5	4	4
22	1	2	6	11	17	23	26	25	20	14	9	5	4	3
23	C	2	6	12	19	26	3C	29	24	16	1C	5	3	2
24	-C	1	5	11	19	27	31	3C	24	17	9	5	2	2
25	-C	1	4	1C	17	25	29	28	23	16	9	4	2	1
26	C	1	3	8	14	21	25	25	2C	14	8	3	1	1
27	1	1	3	6	11	16	2C	2C	17	12	7	3	1	1
28	2	2	3	4	7	11	14	15	14	1C	6	3	2	2
29	3	3	3	3	5	8	1C	11	11	9	6	4	2	2

TENA DATE REJT ON R TEST SEARCH IN REGION OF MISSING OXYGENS

Y IN 74THS Z IN 80THS X = 16 48THS

	26	27	28	29	30	31	32	33	34	35	36	37	38	39
12	-0	-2	-3	-4	-5	-4	-3	-3	-4	-5	-6	-6	-5	-4
13	-1	-2	-4	-5	-5	-5	-4	-4	-4	-5	-6	-6	-5	-4
14	-1	-2	-4	-5	-6	-6	-5	-5	-5	-6	-6	-6	-5	-4
15	-1	-2	-4	-6	-7	-7	-7	-6	-6	-6	-6	-6	-5	-5
16	-1	-2	-3	-5	-7	-8	-8	-7	-7	-6	-6	-5	-5	-4
17	-1	-1	-3	-5	-6	-7	-7	-6	-5	-5	-4	-4	-4	-3
18	-0	-0	-1	-3	-4	-4	-4	-3	-2	-2	-2	-2	-2	-2
19	1	1	0	0	0	1	2	3	3	3	2	1	1	0
20	1	2	2	4	6	8	10	10	10	8	6	4	3	2
21	1	2	4	8	12	16	19	19	17	13	9	7	5	4
22	1	2	6	11	17	23	27	26	23	17	12	8	6	5
23	-0	2	6	13	21	28	32	32	27	20	14	9	6	5
24	-1	1	6	13	22	30	35	34	29	21	14	9	6	5
25	-1	1	5	12	20	29	34	34	29	21	13	8	6	5
26	-1	1	4	9	17	25	30	30	26	19	12	8	5	5
27	-0	1	3	7	13	19	24	25	22	17	11	7	5	5
28	1	2	3	5	9	14	18	19	18	14	10	7	5	4
29	3	3	3	4	6	10	13	14	14	12	9	6	4	3

TENA CATF REJT CN R TEST SEARCH IN REGICN OF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 18 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	C	-2	-4	-5	-6	-6	-5	-5	-5	-6	-6	-5	-5	-4
13	-C	-2	-4	-7	-8	-8	-7	-7	-6	-6	-6	-5	-5	-4
14	-1	-3	-5	-7	-9	-9	-9	-8	-8	-7	-6	-5	-4	-4
15	-2	-3	-5	-7	-9	-1C	-1C	-1C	-9	-8	-7	-5	-4	-3
16	-2	-2	-4	-7	-9	-11	-11	-11	-9	-8	-6	-4	-3	-3
17	-1	-2	-3	-6	-8	-1C	-1C	-10	-9	-7	-5	-3	-2	-2
18	-C	-1	-2	-4	-6	-8	-8	-7	-6	-4	-2	-1	-1	-1
19	1	1	-C	-2	-3	-4	-4	-3	-2	-C	1	1	1	0
2C	1	2	2	1	1	1	2	3	4	4	4	4	3	2
21	2	3	4	5	6	8	9	10	9	8	7	6	5	4
22	1	3	5	7	1C	13	15	16	14	12	9	7	6	6
23	C	2	5	9	14	18	21	21	18	14	11	9	8	7
24	-C	2	5	9	15	2C	23	23	20	16	12	9	8	8
25	-1	1	4	9	15	2C	24	24	20	16	12	9	8	8
26	-1	C	3	7	12	18	21	22	19	15	11	9	8	8
27	-C	C	2	5	1C	14	18	18	16	13	1C	8	7	6
28	1	1	2	4	7	11	14	14	13	1C	8	6	5	4
29	2	2	2	3	5	8	1C	11	1C	8	6	4	3	2

TENA CATF REJT CN R TEST SEARCH IN REGICN CF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 20 48THS

	26	27	28	29	30	31	32	33	34	35	36	37	38	39
12	2	-0	-3	-5	-6	-6	-6	-5	-5	-6	-6	-5	-5	-5
13	1	-1	-4	-7	-8	-8	-8	-7	-7	-7	-7	-6	-5	-5
14	-1	-3	-5	-8	-9	-10	-10	-9	-9	-8	-7	-6	-5	-4
15	-2	-4	-6	-8	-10	-11	-11	-11	-10	-9	-8	-6	-4	-3
16	-3	-4	-6	-8	-10	-12	-12	-12	-11	-9	-7	-5	-3	-2
17	-3	-4	-6	-8	-10	-11	-12	-11	-10	-8	-6	-4	-2	-1
18	-3	-3	-4	-7	-9	-10	-11	-10	-8	-6	-4	-2	-1	-0
19	-2	-2	-3	-5	-7	-8	-8	-7	-6	-3	-1	0	1	1
20	-2	-1	-2	-3	-4	-5	-5	-4	-2	-0	1	2	2	2
21	-2	-1	-1	-1	-2	-2	-1	0	2	3	4	4	4	3
22	-2	-1	-0	0	1	2	3	4	5	6	6	6	6	5
23	-2	-1	-0	1	3	5	7	8	8	8	8	8	7	7
24	-3	-2	-0	2	5	7	10	11	10	9	9	9	9	8
25	-3	-2	-0	2	5	8	11	12	11	10	9	9	9	9
26	-2	-2	-1	2	5	8	11	11	11	9	8	8	9	8
27	-1	-1	-1	1	4	7	9	10	9	8	7	7	7	6
28	-1	-1	-1	0	3	5	8	8	7	6	5	4	4	4
29	0	-0	-1	-0	1	4	6	6	6	4	3	2	1	0

TENA DATE REJT CN R TEST SEARCH IN REGICN CF MISSING CXYGENS

Y IN 74THS Z IN 8CTHS X = 22 48THS

	26	27	28	29	3C	31	32	33	34	35	36	37	38	39
12	1	1	-C	-2	-3	-3	-3	-2	-2	-3	-4	-4	-5	-6
13	1	-C	-2	-4	-5	-5	-4	-4	-4	-4	-5	-6	-7	-7
14	C	-1	-4	-6	-7	-7	-6	-6	-5	-6	-6	-7	-7	-7
15	-1	-3	-5	-7	-8	-8	-8	-7	-7	-7	-7	-7	-7	-7
16	-1	-4	-6	-8	-9	-9	-9	-8	-8	-7	-7	-6	-6	-5
17	-2	-4	-6	-8	-9	-1C	-1C	-9	-8	-7	-6	-5	-5	-4
18	-2	-4	-6	-7	-9	-1C	-1C	-9	-8	-6	-5	-4	-3	-3
19	-3	-3	-5	-7	-8	-9	-9	-8	-7	-5	-3	-2	-1	-1
2C	-3	-3	-4	-6	-7	-8	-8	-7	-5	-3	-1	C	C	-C
21	-3	-3	-4	-5	-6	-6	-6	-4	-2	-C	2	2	2	1
22	-3	-3	-4	-5	-5	-4	-3	-2	0	2	4	5	4	3
23	-3	-3	-4	-4	-4	-2	-1	1	3	4	6	6	6	4
24	-3	-3	-4	-4	-3	-1	1	3	5	6	7	7	7	6
25	-2	-3	-4	-3	-1	1	3	4	5	6	7	8	8	7
26	-2	-3	-4	-3	-1	2	4	5	5	6	6	7	7	7
27	-2	-3	-4	-3	-1	2	4	5	5	5	5	6	6	6
28	-2	-3	-4	-3	-1	2	4	4	4	4	4	4	4	4
29	-2	-4	-4	-4	-2	1	3	4	4	3	2	2	2	2

FCLRR SEARCH IN REGICN CF MISSING CXYGENS TENA PAGE 77

FCURIER SYNTHESIS COMPLETED IN 1.6244 MIN. R = C.33336

CF THE 16SC REFLECTICNS READ, 1288 CONTRIBUTED TC SUMS
C WERE OUT OF SIN-THETA RANGE
4C2 WERE REJECTED

REFINE ALL HEAVY ATCMS TENA PAGE 78

TAPE ASSIGNMENTS - NTIN NTOUT NTAPEA NTAPEB .....
5 8 11 12 2 8 6 4

INPLT FRCM REFLECTION TAPE (CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63)
REWRITTEN 4 TIMES
MCST RECENT WRITINGS BY FCLREF FC MCDIFY DATFIX DATRDN
REMARK ADD OXYGEN ATCMS FRCM DIFFERENCE FOURIER

MULTIPLICITY CF GENERAL PCSITICN - 2

19 ATCMS IN ASSYMETRIC UNIT, SUMMATICN IS OVER 38 ATCMS

TEMPERATURE FACTOR 4.3210

SCALE FACTCRS
LEVEL 1 C.7936
LEVEL 2 C.8635
LEVEL 3 C.8194
LEVEL 4 1.0007
LEVEL 5 0.7971
LEVEL 6 0.7355
LEVEL 7 C.9063
LEVEL 8 0.9122
LEVEL 9 C.62C2
LEVEL 1C 0.6421

CYCLE 1, R = C.212 FRCM INPLT PARAMETERS CYCLE CALCULATICN TIME 2.6700 MIN.
FC/FC LESS THAN 0.2C FCR 17 REFLECTIONS

	INPUT PARAMETERS			OUTPLT PARAMETERS			CHANGE			
ATCM	X	Y	Z	X	Y	Z	DX	DY	DZ	
C1	2482	8361	2815	2466	8363	2796	-16	2	-19	
C2	4091	9079	2998	409C	9076	3002	-1	-3	4	
C3	4462	382C	12C8	4449	3824	1193	-13	4	-15	
C4	4526	2828	5C8	4532	2847	514	6	19	6	
C5	3865	7140	4355	3876	7152	4373	11	12	18	
C6	24C7	7394	3548	2423	7405	3566	16	11	18	
N1	1142	8564	1987	1145	8569	1994	3	5	7	
N2	4158	2C8	2341	4159	213	2336	1	5	-5	
N3	2828	4647	1C47	2825	4640	1044	-3	-7	-3	
N4	2963	2582	4755	2937	2575	4743	-26	-7	-12	
N6	826	6579	3503	819	6583	3498	-7	4	-5	
C21	363C	166	1365	3632	163	1360	2	-3	-5	
C22	4772	1137	2865	4751	1131	2857	-21	-6	-8	
C31	1917	468C	1797	19C7	4679	1799	-1C	-1	2	
C32	2549	5218	18C	2558	5225	197	9	7	17	
C61	848	5811	4198	859	5801	4196	11	-1C	-2	
C62	5CC	1749	2195	5C7	1755	2205	7	6	10	
C41	3125	3243	4125	3125	3243	4C45	C	0	-80	NC PEAK
C42	1458	2162	4875	1442	2178	4858	-16	16	-17	

CYCLE 2, R = 0.200 FROM INPUT PARAMETERS CYCLE CALCULATION TIME 3.0075 MIN.
FO/FC LESS THAN 0.20 FOR 20 REFLECTIONS

	INPUT PARAMETERS			OUTPUT PARAMETERS			CHANGE		
ATOM	X	Y	Z	X	Y	Z	DX	DY	DZ
C1	2466	8363	2796	2471	8363	2792	5	-0	-4
C2	4090	9076	3002	4089	9076	3001	-1	-0	-1
C3	4449	3824	1193	4456	3824	1194	7	-0	1
C4	4532	2847	514	4526	2852	514	-6	5	-0
C5	3876	7152	4373	3873	7158	4376	-3	6	3
C6	2423	7405	3566	2414	7406	3558	-9	1	-8
N1	1145	8569	1994	1141	8564	1994	-4	-5	0
N2	4159	213	2336	4159	210	2334	-0	-3	-2
N3	2825	4640	1044	2823	4637	1044	-2	-3	0
N4	2937	2575	4743	2937	2576	4749	0	1	6
N6	819	6583	3498	816	6585	3498	-3	2	0
C21	3632	163	1360	3633	162	1365	1	-1	5
C22	4751	1131	2857	4758	1130	2855	7	-1	-2
C31	1907	4679	1799	1903	4680	1801	-4	1	2
C32	2558	5225	197	2548	5216	182	-10	-9	-15
C61	859	5801	4196	856	5811	4196	-3	10	-0
C62	507	1755	2205	498	1742	2207	-9	-13	2
C41	3125	3243	4045	3193	3265	4032	68	22	-13
O42	1442	2178	4858	1442	2184	4858	-0	6	0

FINAL R = 0.195

TAPE ASSIGNMENTS - NTIN NTOUT NTAPEA NTAPEB .....

5	8	12	11	2	8	6	4

WEIGHTS FROM TAPE

LC-FI TRIG

INPUT TAPE CONTAINS DATA FOR TENA AND HAS BEEN REWRITTEN 5 TIMES.
TAPE LABEL - CELL PARAMETERS 3/25/64 INTENSITIES 12/18/63
THE MOST RECENT WRITINGS WERE BY FOUREF FOUREF FC MODIFY DATFIX DATRDN

NUMBER OF OBSERVATIONS TO BE READ IS 1776

BASED ON F

ISOTROPIC TEMPERATURE FACTORS

PARAMETERS FROM BINARY TAPE.

USE F REL. RESCALE FACTORS.

1	0.79357
2	0.86350
3	0.81939
4	1.00071
5	0.79705
6	0.73952
7	0.90629
8	0.91221
9	0.62022
10	0.64210

THERE ARE 19 ATOMS IN THE ASSYMETRIC UNIT WITH 125 POSSIBLE PARAMETERS. 86 OF THESE ARE TO BE VARIED FOR 2 CYCLES.

10 SCALE FACTORS TO BE VARIED.

ATOM	MULTIPLIER	X	Y	Z	B OR B11	B22	B33	B12	B13	B23	(WITH VARIABLE NUMBERS)
C1	1.0000	0.24710	0.83630	0.27920	4.32100						
		11	12	13	14						
C2	1.0000	0.40890	0.90760	0.30010	4.32100						
		15	16	17	18						
C3	1.0000	0.44560	0.38240	0.11940	4.32100						
		19	20	21	22						
C4	1.0000	0.45260	0.28520	0.05140	4.32100						
		23	24	25	26						
C5	1.0000	0.36730	0.71580	0.43760	4.32100						
		27	28	29	30						
C6	1.0000	0.24140	0.74060	0.35560	4.32100						
		31	32	33	34						
N1	1.0000	0.11410	0.85640	0.19940	4.32100						
		35	36	37	38						

ATOM	MULTIPLIER	X	Y	Z	B OR B11	B22	B33	B12	B13	B23	(WITH VARIABLE NUMBERS)
N2	1.0000	0.41590 35	0.02100 40	0.23340 41	4.32100 42						
N3	1.0000	0.28230 43	0.46370 44	0.10440 45	4.32100 46						
N4	1.0000	0.25370 47	0.25760 48	0.47490 49	4.32100 50						
N6	1.0000	0.06160 51	0.65850 52	0.34980 53	4.32100 54						
C21	1.0000	0.36330 55	0.01620 56	0.13650 57	4.32100 58						
C22	1.0000	0.47580 59	0.11300 60	0.28550 61	4.32100 62						
O31	1.0000	0.19030 63	0.46800 64	0.18010 65	4.32100 66						
O32	1.0000	0.25480 67	0.52160 68	0.01820 69	4.32100 70						
O61	1.0000	0.08560 71	0.58110 72	0.41960 73	4.32100 74						
O62	1.0000	0.04980 75	0.17420 76	0.22070 77	4.32100 78						
O41	1.0000	0.31930 79	0.32650 80	0.40320 81	4.32100 82						
O42	1.0000	0.14420 83	0.21840 84	0.48580 85	4.32100 86						

AGREEMENT FACTORS BEFORE CYCLE 1 FROM TAPE REWRITTEN 5 TIMES.

SUM(W*(C-C)**2) IS 0.6073E 05

SQRTF(SUM(W*(C-C**2)/(1690 - 86)) 6.1530

	NUMERATOR	DENOMINATOR	R
R FACTOR OMITTING LESS-THANS	2317.6	11888.6	0.195
R FACTOR WITH REFLECTION MULTIPLICITY OMIT L-T	4403.7	22603.2	0.195
WEIGHTED R FACTOR OMITTING LESS-THANS	65.5	216.3	0.303
R FACTOR OF LESS-THANS	3306.6	755.3	4.378

OBSERVATIONS READ 1690, 558 OF THE 616 LESS-THANS CALCULATED GREATER THAN THE LESS-THAN THRESHOLD VALUE
OVERALL LINEAR SCALING RATIO 1.3879

PARAMETERS AFTER CYCLE 1

PARAMETER	OLD	CHANGE	NEW	ERROR
FRL SC	0.79357	0.0999625	0.89353	0.1007430
FRL SC	0.86350	0.0965269	0.96003	0.0787583
FRL SC	0.81939	0.0898915	0.90928	0.0812922
FRL SC	1.00071	0.2058121	1.20652	0.0730158
FRL SC	0.79705	0.1057087	0.90276	0.0849044
FRL SC	0.73552	0.1173365	0.85686	0.0994489
FRL SC	0.90629	0.0723059	0.97859	0.0982125
FRL SC	0.91221	0.1064812	1.01870	0.1038663
FRL SC	0.62022	0.0765268	0.69675	0.1357216
FRL SC	0.64210	0.0557579	0.69786	0.1537757
C1				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.24710	-0.0009033	0.24620	0.0027371
Y	0.83630	0.0006643	0.83636	0.0019127
Z	0.27920	-0.0000690	0.27913	0.0016344
ATOM B	4.32100	-0.4358351	3.88516	0.3799433
C2				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.40890	-0.0002060	0.40869	0.0026392
Y	0.90760	0.0003208	0.90792	0.0019772
Z	0.30010	-0.0001391	0.29996	0.0015613
ATOM B	4.32100	-0.4779976	3.84300	0.3799525
C3				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	

PARAMETERS AFTER CYCLE 1

PARAMETER	OLD	CHANGE	NEW	ERROR
X	0.44560	-0.0002778	0.44532	0.0026841
Y	0.38240	0.0006905	0.38309	0.0019859
Z	0.11940	-0.0000404	0.11936	0.0016201
ATOM B	4.32100	-0.4088359	3.91216	0.3768976
C4				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.45260	0.0002744	0.45287	0.0027711
Y	0.28520	-0.0006032	0.28460	0.0019790
Z	0.05140	-0.0004693	0.05093	0.0015920
ATOM B	4.32100	-0.4121349	3.90887	0.3739923
C5				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.38730	-0.0000469	0.38725	0.0027224
Y	0.71580	-0.0003324	0.71547	0.0019327
Z	0.43760	-0.0000969	0.43750	0.0016303
ATOM B	4.32100	-0.2355757	4.08542	0.3774464
C6				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.24140	0.0017128	0.24311	0.0028233
Y	0.74060	-0.0001752	0.74042	0.0018842
Z	0.35580	0.0008172	0.35662	0.0016124
ATOM B	4.32100	-0.4198745	3.90113	0.3782861
N1				
NEUT F	2.00000		2.00000	

PARAMETERS AFTER CYCLE 1

PARAMETER	OLD	CHANGE	NEW	ERROR
MULT	1.00000		1.00000	
X	0.11410	-0.0000411	0.11406	0.0022937
Y	0.85640	0.0011323	0.85753	0.0016128
Z	0.19940	-0.0013425	0.19806	0.0013283
ATOM B	4.32100	-0.0114236	4.30958	0.3383394
N2				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.41590	0.0005874	0.41649	0.0022555
Y	0.02100	-0.0005398	0.02046	0.0015956
Z	0.23340	0.0009085	0.23431	0.0013815
ATOM B	4.32100	-0.2734735	4.04753	0.3304538
N3				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.28230	0.0000889	0.28239	0.0022825
Y	0.46370	0.0005096	0.46421	0.0016084
Z	0.10440	0.0001278	0.10453	0.0013359
ATOM B	4.32100	-0.2585991	4.06240	0.3362289
N4				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.29370	-0.0006042	0.29310	0.0022902
Y	0.25760	-0.0004198	0.25718	0.0015941
Z	0.47490	-0.0004531	0.47445	0.0013753
ATOM B	4.32100	-0.0084488	4.31255	0.3348138
N6				

PARAMETERS AFTER CYCLE 1

PARAMETER	OLD	CHANGE	NEW	ERROR
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.08160	0.0007884	0.08239	0.0023277
Y	0.65850	0.0002246	0.65872	0.0015887
Z	0.34980	0.0002798	0.35008	0.0013417
ATOM B	4.32100	-0.1157513	4.20525	0.3337836
O21				
NEUT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.36330	0.0009386	0.36424	0.0018779
Y	0.01620	0.0006503	0.01685	0.0013019
Z	0.13650	0.0005344	0.13703	0.0010857
ATOM B	4.32100	0.1576183	4.47862	0.2901678
O22				
NEUT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.47580	-0.0010363	0.47476	0.0018282
Y	0.11300	-0.0004152	0.11258	0.0013532
Z	0.28550	-0.0001367	0.28536	0.0010337
ATOM B	4.32100	0.2550645	4.57606	0.2855267
O31				
NEUT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.19030	-0.0003217	0.18998	0.0018078
Y	0.46800	0.0003658	0.46837	0.0012857
Z	0.18010	-0.0005257	0.17957	0.0011027
ATOM B	4.32100	0.3636323	4.68463	0.2849109

C32				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.25480	-0.0000609	0.25474	0.0018870
Y	0.52160	0.0000236	0.52162	0.0012945
Z	0.01820	0.0003757	0.01858	0.0010708
ATOM B	4.32100	0.2780717	4.59907	0.2874373
C61				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.08560	0.0005544	0.08615	0.0017866
Y	0.58110	-0.0004525	0.58065	0.0013188
Z	0.41960	0.0004560	0.42006	0.0010649
ATOM B	4.32100	0.3141293	4.63513	0.2873739
C62				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.04980	0.0004663	0.05027	0.0018962
Y	0.17420	0.0000027	0.17420	0.0012899
Z	0.22070	0.0002280	0.22093	0.0010799
ATOM B	4.32100	0.2753152	4.59632	0.2872763
O41				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.31930	0.0008591	0.32016	0.0018026
Y	0.32650	0.0008165	0.32732	0.0012797
Z	0.40320	-0.0005171	0.40268	0.0011197
ATOM B	4.32100	0.4999950	4.82099	0.2952200

C42

NELT F	3.00000		3.00000	
MLLT	1.00000		1.00000	
X	0.14420	-0.0006595	0.14354	0.0018560
Y	0.21840	0.0001742	0.21857	0.0013137
Z	0.48580	-0.0002717	0.48553	0.0010694
ATOM B	4.32100	0.4640802	4.78508	0.2831377

ESTIMATED AGREEMENT AFTER CYCLE 1

SUM(W*(O-C)**2) IS 0.5829E 05

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 6.0284

AGREEMENT FACTORS BEFORE CYCLE 2 FROM TAPE REWRITTEN 5 TIMES.

SUM(W*(C-O)**2) IS 0.5625E 05

SQRTF(SUM(W*(C-O**2)/(1650 - 86)) 5.9218

	NUMERATOR	DENOMINATOR	R
R FACTOR OMITTING LESS-THANS	2120.8	13431.1	0.158
R FACTOR WITH REFLECTION MULTIPLICITY OMIT L-T	4016.7	25540.2	0.157
WEIGHTED R FACTOR OMITTING LESS-THANS	53.0	244.6	0.217
R FACTOR OF LESS-THANS	3112.7	853.9	3.645

OBSERVATIONS READ 1690, 549 OF THE 616 LESS-THANS CALCULATED GREATER THAN THE LESS-THAN THRESHOLD VALUE
OVERALL LINEAR SCALING RATIO 1.2260

PARAMETERS AFTER CYCLE 2

PARAMETER	OLD	CHANGE	NEW	ERROR
FRL SC	0.89353	-0.0116116	0.88192	0.0998676
FRL SC	0.96003	-0.0103557	0.94967	0.0774457
FRL SC	0.90928	-0.0096331	0.89965	0.0801980
FRL SC	1.20652	-0.0138154	1.19271	0.0719510
FRL SC	0.90276	-0.0117623	0.89100	0.0841911
FRL SC	0.85686	-0.0091336	0.84772	0.0974837
FRL SC	0.97859	-0.0102096	0.96838	0.0971729
FRL SC	1.01870	-0.0111924	1.00750	0.1022117
FRL SC	0.69675	-0.0098370	0.68691	0.1343318
FRL SC	0.69786	-0.0144917	0.68337	0.1541915
C1				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.24620	-0.0000529	0.24614	0.0024688
Y	0.83636	-0.0000946	0.83627	0.0017471
Z	0.27913	0.0000484	0.27918	0.0014822
ATOM B	3.88516	-0.3017333	3.58343	0.3397477
C2				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.40869	0.0006793	0.40937	0.0023574
Y	0.90792	0.0000772	0.90800	0.0017949
Z	0.29996	0.0000724	0.30003	0.0014058
ATOM B	3.84300	-0.2788863	3.56412	0.3380319
C3				
NEUT F	1.00000		1.00000	
MULT	1.00000		1.00000	

PARAMETERS AFTER CYCLE 2

PARAMETER	OLD	CHANGE	NEW	ERROR
X	0.44532	0.0000091	0.44533	0.0024405
Y	0.38309	0.0006278	0.38372	0.0018115
Z	0.11936	0.0000014	0.11936	0.0014765
ATOM B	3.91216	-0.2232716	3.68889	0.3390188
C4				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.45287	0.0003676	0.45324	0.0025090
Y	0.28460	-0.0006506	0.28395	0.0018077
Z	0.05093	-0.0002833	0.05065	0.0014476
ATOM B	3.90887	-0.2430140	3.66545	0.3378508
C5				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.38725	0.0001929	0.38745	0.0025462
Y	0.71547	-0.0009073	0.71456	0.0018199
Z	0.43750	0.0000185	0.43752	0.0015296
ATOM B	4.08502	-0.0851225	4.00030	0.3514826
C6				
NELT F	1.00000		1.00000	
MULT	1.00000		1.00000	
X	0.24311	0.0002606	0.24337	0.0025478
Y	0.74042	0.0001533	0.74058	0.0017168
Z	0.35662	0.0005079	0.35713	0.0014638
ATOM B	3.90113	-0.1650040	3.73612	0.3412631
N1				
NELT F	2.00000		2.00000	

PARAMETERS AFTER CYCLE 2

PARAMETER	OLD	CHANGE	NEW	ERROR
MULT	1.00000		1.00000	
X	0.11406	-0.0001645	0.11389	0.0022243
Y	0.85753	0.0007487	0.85828	0.0015730
Z	0.19806	-0.0009180	0.19714	0.0012934
ATOM B	4.30958	0.0076456	4.31722	0.3288204
N2				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.41649	-0.0001126	0.41637	0.0020982
Y	0.02046	0.0000492	0.02051	0.0014965
Z	0.23431	0.0005294	0.23484	0.0012901
ATOM B	4.04753	-0.1917373	3.85579	0.3071102
N3				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.28239	0.0000332	0.28242	0.0021173
Y	0.46421	0.0003472	0.46456	0.0015095
Z	0.10453	-0.0000065	0.10452	0.0012506
ATOM B	4.06240	-0.1529802	3.90942	0.3144698
N4				
NEUT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.29310	0.0003662	0.29346	0.0022387
Y	0.25718	-0.0002636	0.25692	0.0015566
Z	0.47445	-0.0002007	0.47425	0.0013411
ATOM B	4.31255	-0.0034227	4.30913	0.3258864
N6				

PARAMETERS AFTER CYCLE 2

PARAMETER	OLD	CHANGE	NEW	ERROR
NELT F	2.00000		2.00000	
MULT	1.00000		1.00000	
X	0.08239	0.0004566	0.08284	0.0022252
Y	0.65872	0.0000888	0.65881	0.0015256
Z	0.35008	0.0002912	0.35037	0.0012796
ATOM B	4.20525	-0.0354767	4.16977	0.3186849
C21				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.36424	0.0004860	0.36472	0.0018683
Y	0.01685	0.0006069	0.01746	0.0013005
Z	0.13703	0.0003732	0.13741	0.0010809
ATOM B	4.47862	0.0423110	4.52093	0.2900259
C22				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.47476	-0.0005813	0.47418	0.0018565
Y	0.11258	-0.0001651	0.11242	0.0013698
Z	0.28536	-0.0000780	0.28529	0.0010448
ATOM B	4.57606	0.2420775	4.81814	0.2905625
C31				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.18598	-0.0002349	0.18574	0.0018533
Y	0.46837	0.0001195	0.46849	0.0013210
Z	0.17557	-0.0004091	0.17517	0.0011351
ATOM B	4.68463	0.3706856	5.05532	0.2954677

C32				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.25474	-0.0001039	0.25464	0.0019146
Y	0.52162	-0.0001767	0.52145	0.0013133
Z	0.01858	0.0002156	0.01879	0.0010887
ATOM B	4.59907	0.2090451	4.80812	0.2934985
C61				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.08615	0.0000290	0.08618	0.0018310
Y	0.58065	-0.0005256	0.58012	0.0013454
Z	0.42006	0.0003108	0.42037	0.0010893
ATOM B	4.63513	0.2299094	4.86504	0.2945826
C62				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.05027	0.0001700	0.05044	0.0019267
Y	0.17420	0.0002212	0.17442	0.0013080
Z	0.22093	0.0000459	0.22097	0.0010936
ATOM B	4.59632	0.2469012	4.84322	0.2918510
O41				
NELT F	3.00000		3.00000	
MULT	1.00000		1.00000	
X	0.32016	0.0010718	0.32123	0.0018919
Y	0.32732	0.0005178	0.32783	0.0013382
Z	0.40268	-0.0002934	0.40239	0.0011724
ATOM B	4.82099	0.4451068	5.26610	0.3115313

C42

NELT F	3.00000		3.00000	
MLLT	1.00000		1.00000	
X	0.14354	-0.0000938	0.14345	0.0019398
Y	0.21857	0.0000128	0.21859	0.0013707
Z	0.48553	-0.0002185	0.48531	0.0011114
ATOM B	4.78508	0.4304291	5.21551	0.2967195

ESTIMATED AGREEMENT AFTER CYCLE 2

SUM(W*(O-C)**2) IS 0.5561E 05

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 5.8882

AGREEMENT FACTORS BEFORE CYCLE 3 FROM TAPE REWRITTEN 5 TIMES.

SUM(W*(O-C)**2) IS 0.5491E 05

SQRTF(SUM(W*(O-C**2)/(1650 - 86)) 5.8505

	NUMERATOR	DENOMINATOR	R
R FACTOR OMITTING LESS-THANS	1944.6	13271.7	0.147
R FACTOR WITH REFLECTION MULTIPLICITY OMIT L-T	3684.1	25238.7	0.146
WEIGHTED R FACTOR OMITTING LESS-THANS	47.8	241.7	0.198
R FACTOR OF LESS-THANS	3103.3	843.8	3.678

OBSERVATIONS READ 1690, 569 OF THE 616 LESS-THANS CALCULATED GREATER THAN THE LESS-THAN THRESHOLD VALUE
OVERALL LINEAR SCALING RATIO 1.2334

17.4611 MIN FOR LEAST SQUARES (7.39014 MIN. PER CYCLE.) R = 0.147

$ID STEWART*001/63/006 $DICKINSON, C. 12500 04/25/64 ON 13-16-03 OFF 14-09-10

TYPE OF PROCESS	COMPILER	ASSEMBLER	LOADER	EXECUTION	UTILITY	OTHER	TOTAL TIME
TIME FOR EACH	000.00	000.00	000.01	052.19	000.00	000.93	053.14

END OF JOB