PROGRAM FOR CALCULATION OF TDS-CORRECTIONS OF INTEGRATED INTENSITIES FOR SINGLE CRYSTALS

VERSION OF FEBRUARY 1996
INSTITUT LAUE-LANDEVIN

PROGRAM NAME: TDS
PURPOSE: CORRECTION OF BRAGG INTENSITIES FOR THE EFFECT OF ANISOTROPIC THERMAL DIFFUSE SCATTERING (OMEGA-AND OMEGA-"THETA SCANS, CIRCULAR AND RECTANGULAR APERTURE, ALL CRYSTAL SYSTEMS EXCEPT TRICLINIC). THE PRESENT VERSION FORMS PART OF THE COLL5SYSTEM.
AUTHORS: J.KURITTU& M.MERISALO HELSINKI, FINLAND.
WITH CONTRIBUTIONS FROM S.WILKINS, J.TIBBBALLS AND W.F.KUHS.
LOCAL CONTACT: W.F.KUHS ILL19
HOW TO USE: PREPARE INPUT FILE ?????.DAT ACCORDING TO THE MANUAL(FOUND AS TDS. MAN ON (10,25). HAVE YOUR DATAP OUTPUT FILE READY AND DO RUN TDS (10,25)GIVE FILENAMES AND THEN WAIT OR BETTER SUBMIT THE JOB IN BATCH!
MANUAL: AS I SAID IS ON (10,25) AS TDS.MAN.

ABSTRACT

THE PROGRAM CALCULATES THE CORRECTION FACTORS ALPHA FOR ANISOTROPIC THERMAL DIFFUSE SCATERING IN THE LONG WAVELENGTH, CONTIUUM ELASTICITY APPROXIMATION AND APPLIES THESE CORRECTIONS TO THE INTEGRATED INTENSITIES FOR SINGLE CRYSTALS OF CUBIC , TETRAGONAL, ORTHORHOMBIC, MONOCLINIC, HEXAGONAL,AND TRIGONAL SYMMETRIES. THE PROGRAM IS RESTRICTED TO OMEGA OR OMEGA-2THETA SCANS AND DEALS WITH RECTANGULAR AND SPHERICAL RECEIVING SLITS. THE PROGRAM USES THE FACT THAT THE THREEDIMENSIONAL SUMMATION OVER THE WAVEVECTORS CAN BE REDUCED TO A TWODIMENSIONAL NUMERICAL INTEGRATION OVER THE WAVE-VECTORS ENDING AT THE FACES OF THE ACTIVE VOLUME. FOR A MORE DETAILED DESCRIPTION SEE J.KURITTU& M.MERISALO J.APPL.CRYST. 11,179 (1978). A CORRECTION FOR TDS CONTRIBUTIONS FROM TWO-PHONON PROCESSES MAY BE INCLUDED OPTIONALLY, THE SECOND ORDER TDS CORRECTION FOLLOWS E.D.STEVENS, ACTA CRYST.A30,184 (1974).THE EXTENSIONS TO THE ORGINAL VERSION WERE PROGRAMMED BY J.TIBBALLS (2-PHONON TDS) AND W.F.KUHS (2-PHONON TDS AND CIRCULAR APERTURE). S.WILKENS ADAPTED THE PROGRAM TO THE COLL5-SYSTEM.

THE ESTIMATED CPU-TIME FOR ONE REFLECTION WITH A GRID $10 \times 10 \times 10$ IN THE ONE-PHONON APPROXIMATION IS 1.2 SEC.

INPUT

THE INPUT OF THE RUN CONTROL FILE IS IN FREE FORMAT. THIS FILE CONTAIN YOUR CHOICE OF OPTIONS AND PARAMETERS. THE REFLECTION DATA ARE ASSUMED TO BE ON A SECOND FILE. NORMALLY THIS FILE WILL BE A FILE CREATED BY THE PROGRAM DATAP CONTAINING THE UNIT VECTORS WHICH DEFINE THE DIRECTION OF THE PRIMARY AND REFLECTED BEAM. BOTH, THE CONTROL AND THE REFLECTION DATA FILE MUST HAVE THE EXTENSION DAT.

CONTROL DATA

THE FILE CONTROLLING THE PROGRAM CONTAINS ALWAYS THE
FOLLOWING 13 CARDS:

1

FORMAT(16A5)

TITLE: FEEL FREE TO TYPE ANYTHING YOU WANT

2

FORMAT(A5)

CUBIC FOR THE CUBIC SYSTEM
TETRA FOR THE TETRAGONAL SYSTEM
HEXAG FOR THE HEXAGONAL SYSTEM
TRIGO FOR THE TRIGONAL SYSTEM
ORTHO FOR THE ORTHORHOMBIC SYSTEM
MONOC FOR THE MONOCLINIC SYSTEM

THIS PARAMETER HAS TO BE TYPED IN UPPER CASE!

3

FORMAT(6I)

CONTROL PARAMETERS CALLED ICN(I), I=1,6

FIRST: SCAN MODE PARAMETER
= 1 FOR OMEGA-2THETA SCANS
= 2 FOR OMEGA SCANS

SECOND: APERTURE PARAMETER
= 0 FOR CIRCULAR APERTURE
= 1 FOR RECTANGULAR APERTURE

THIRD: SCAN WITH PARAMETER
= 1 SCAN WITH CALCULATED FROM EXPRESSION
A1*TAN(THETA)+A2 (S.CARD 4)
= 2 TAKEN FROMTHE REFLECTION INPUT FILE

FOURTH: = 0 NORMALLY
= 1 RHUMBOHEDRAL SYSTEM WITH HEXAGONAL SETTING

FIFTH: VECTOR DEFINITION PARAMETER
= 0 KEEP DATAP VECTORS (XN PERP. SCATT. PLANE, XNSO,
DIFRACTED BEAM)
= 1 USE TDS VECTORS (XN AS ABOVE, XNSO PERP. PRIMARY
BEAM IN THE SCATTERING PLANE)
FOR THE OUTPUT COLL-5FILE.

SIXTH: = 0 ONE-PHONON TDS CORRECTION ONLY
= 1 TWO-PHONON TDS CORRECTION INCLUDED.

4

FORMAT(7F)

FIRST: A LATTICE CONSTANT

SECOND: B LATTICE CONSTANT

THIRD: C LATTICE CONSTANT; A B C IN ANGSTROM UNITS

FOURTH: MONOCLINIC ANGLE BETA (GIVE 90.0 FOR ALL OTHER SYSTEMS!)

FIFTH: WAVELENGTH IN ANGSTROM

SIXTH: DENSITY IN G/CM^3

SEVENTH: ABSOLUTE TEMPERATURE IN K

NOTE: THE HEXAGONAL SETTING HAS TO BE USED FOR ALL
RHOMBOHEDRAL SYMMETRIES (EVEN IN THE CASE OF ICN(4) =0!).
NOTE: THE PROGRAM TRANSFORM THE MONOCLINIC CELL
INTO AN ORTHOGONAL CELL. IT ASSUMES:
A) THE UNIQUE AXIS IS THE B-AXIS.
B) THE COORDINATE SYSREM OF YOUR ELASTIC
CONSTANTS IS DEFINED AS E(1)//A,

E(2)//B AND E(3) = E(1)×E(2).
IF THIS DOES NOT APPLY TO YOUR DATA, RE-
ARRANGE YOUR HKLS AND YOUR LATTICE CONSTANTS.

5

FORMAT(4F OR 3F)

FIRST: FULL WIDTH OF RECEIVING SLIT IN RADIAN

SECOND: FULL HEIGHT OF RECEIVING SLIT(RECTANGULAR CASE ONLY!); OMIT IN CASE OF CIRCULAR APERTURE.

THIRD: A1 FOR DETERMINING THE

FOURTH: A2 RESOLUTION FUNCTION (S.ICN(3))
FIFTH: A3

6

FORMAT(4I)

FIRST: LMAX FOR DEFINING THE

SECOND: MMAX DENSITY OF THE MASH

THIRD: NMAX FOR NUMERICAL INTEGRATION.

NOTE: MMAX×NMAX, LMAX×MMAX AND LMAX×NMAX IS THE NUMBER OF SURFACE ELEMENTS OF EACH SIDE OF THE ACTIVE VOLUME. NORMALLY 10×10×10 GIVES A SUFFICIENT PRECISION OF THE NUMERICAL INTEGRATION. IF YOU ARE NOT SURE, TRY TO ESTABLISH A BETTER GRID BY TESTING A SMALL DATA SET(USE HIGH ANGLE REFLECTIONS FOR THIS CHECK)

FOURTH: = 0 THE BACKGROUND HAS BEEN SUBSTRACTED FROM THE INTEGRATED INTENSITIES (NORMAL CASE).

= 1 THE BACKGROUND HAS NOT BEEN SUBSTRACTED.

7

FORMAT(1I)

FIRST: = 0 INCLUDE ALL PHONONS (USUALLY X-RAY CASE)
= 1 INCLUDE ONLY PHONONS SLOWER THAN THE NEUTRON VELOCITY(NORMAL NEUTRON CASE)

8-13

EACH FORMAT(6F)

HERE GOES THE MATRIX OF ELASTIC CONSTANTS IN UNITS OF 10^{12} DYNE/CM^2. THE FIRST CARD GIVES THE FIRST ROW(C11,C12,C13,C14,C15,C16)OF THE MATRIX, THE SECOND CARD GIVES THE SECOND ROW AND SO ON.
NOTE: THE FULL MATRIX HAS TO BE GIVEN, BUT ONLY THE UPPER RIGHT CORNER IS USED FOR THE CALCULATION. $\frac{1N}{M^2} = \frac{10DYNE}{CM^2}$

DATAP

Program for calculation of absorption correction and quantities for extinction and TDS corrections.

Version of January 1992

Institut Laue-langevin
Uni Karlsruhe

INTRODUCTION AND HISTORY

The program calculates absorption corrections using a Gaussian grid integration. For further reference see for example P. Coppens: The Evaluation of Absorption and Extinction in Single Crystal Structure Analysis in 'Crystallographic Computing', ed. F.R. Ahmed, Munksgaard, 1970.

In addition the vectors needed in anisotropic extinction corrections and for the TDS calculation can be obtained.

The vectors in question are:

XN(I),I=1,3: Components, in angstroms, of the unit vector normal to the plane containing the incident and diffracted beams, given in the real cell axis A,B and C.

XNSO(I),I=1,3: Components of unit vector parallel to the diffracted beam given in the real cell axis A,B and C.

Other quantity of interest is TBAR , which is the mean path for a reflection , weigthed by absorption.

For more detailed definitions of directions see Coppens, P. and Hamilton , W.C. (1970) Acta Cryst. A26 , 71-83 and Becker, P. and Coppens, P. (1974) Acta Cryst. A30 , 129-153. To learn more about the formalisms see Nelmes, R.

The program has been tested using literature data by Flack, H.D., Vincent, M.G. and Alcock, N.W. Acta Cryst. (1980) A36 , 682-686. The usual disclaimers apply. We can take no resposabilities for any erroneous calculation produced by this program.

The program comes to the ILL from S.U.N.Y., Buffalo (P.Coppens) , via the University of Aarhus (F.Z.S.Pedersen and F.K. Larsen). Modifications were done in Berlin (H. Dietrich), and at the ILL (S.W. Wilkins).

In case of problems contact M.S. Lehmann ,ext. 7382, room 210, ILL 20.

INPUT

Input is in free format (format is indicated for each kind of data).

All numbers must be given.

In principle two input data files are needed. One file controls the running of the program (choice of options, unit cell etc.). The other holds the Bragg reflection data as produced by the program COLL5N (or others in the same format).

CONTROL DATA

The file controlling the program contains:

1

FORMAT(20A5)

Title : anything you might want to write

2

FORMAT(7F)

Cell constants and wavelength. Cell can be real or reciprocal, angles or cosines. If a value is less than 1.0, it is assumed to be a cosine.

3

FORMAT(3(7F/))

Three reflections
h,k,l,theta,omega,chi,phi
exactly as found on COLL5N output or similar. Note NOT 2theta.

4

FORMAT(6I)

Six control parameters called ICN(I),I=1,6

first: =0 no absorption correction
=1 absorption correction: crystal boundary planes described by h,k,l and d in cm. Preferred option.
=2 absorption correction: crystal boundary planes described by observed setting angles nescessary to bring plane into diffraction condition plus d in cm.
=3 absorption correction: crystal boundary planes described by equation of planes in Seattle coordinate system; a,b,c and d in cm.

second: =0 no quantities for extinction correction (only if first number is zero; elsewhere quantities are always calculated)
=1 quantities nescessary for extinction correction as used in LINUS. Likewise used in TDS calculations

=-1 only vector components for extinction, but no
TBAR.

third: =0 normally
=1 calculate distance between pairs of vertices.
vertex cards follow boundary plane cards

fourth: =0 normally, four-circle with observed setting
angles given on data file with reflections
=-1 no angles are given, so four-circle bisecting
geomtry is assumed
=1 normal beam (experimental part of program)
=2 for data from STOE-PICKER: Needs angles on
input data file and STOE-PICKER UB on
card *** 3 *** for orientation . This option works
o.k. also for non-bisecting orientations.
(NB: STOE-PICKER-UB transformed into BUSING&LEVY-UB
by signs changed in line 2 and 3)
fifth: =0 normally. Output of corrected data on a file
=-1 no output of reflection data

sixth: =N for setting angles check. If this (ICN(6)) is N
then below must follow N cards with h,k,l.
The program will give the angles assuming
bisecting geometry.

5 OPTIONAL

FORMAT(3F)

ICN(6) cards for angles check. Each card holds h,k,l.

6

FORMAT(2I,2F)

first: first reflection number to be treated

second: last reflection number

third: theta minimum to be considered

fourth: theta maximum to be considered

7 OPTIONAL

FORMAT(4I)

Supply only if ICN(1) > 0, or ICN(2) > 0

Specifications for grid for absorption or extinction correction. A Gaussian integration formula is used. The first three numbers define the number of grid points along the three axial directions. The product of the three numbers must be less than 4097, and they must all be even. The fourth number is number of bounding planes. As a rule of thumb use N = 15 * mu * T, where mu is absorption coefficient and T is thickness in the direction in question. If you do not believe this try various grids.

first: grid along A

second: grid along B

third: grid along C

fourth: number of planes

8 OPTIONAL

FORMAT(4F)

Supply only if 7 is supplied

One card for each boundary plane, option depending upon the value of ICN(1) (card 4, first number). The number of cards is given in card 7.

ICN(1)=1: The boundary planes are given in terms of crystallgraphic planes and the perpendicular distances in cm. of these planes from an arbitrary origin within the crystal.
' h,k,l,d ' is input

ICN(1)=2: The unique observed setting angles omega -teta, chi and phi nescessary to bring the bounding plane normal into the diffracting condition are used, with distance d in cm.
' omega-teta,chi,phi,d ' is input

ICN(1)=3: The coefficients of the equation of plane: a*x + b*y + c*z = d are used
' a,b,c,d ' is input

9 OPTIONAL

FORMAT(2I)

Supply only if ICN(3) > 0

Vertex numbers for two vertices. The program will calculate the distance between the two vertices. Can only be done in second run of program. Is intended as check. Two numbers per line. If the are the same, stop reading 9.

10

FORMAT(2F)

first: absorption coefficient. Unit is reciprocal cm.

second: scale factor to apply to F squared. Usually 1 will do.

11 OPTIONAL

FORMAT(3(3F/))

Transformation Tij of indices and vectors on output data, given in three lines. If the vector (or indices) is x1,x2,x3 then output is

```
x'1        T11  T12  T13     x1
x'2   =    T21  T22  T23  *  x2
x'3        T31  T32  T33     x3
```

REFLECTION DATA

The file containing structure factors is assumed to come from the COLL5N program. If you have other sources, conform with the format

This data file might contain several card images per reflection. The various types are:

Type1: h,k,l,Fsquared,sigma, angles, etc.

Type2: other experimental information.

Type3: absorption and TDS corrections.

Type4: the counts, and other junk.

All cards have the reflection number in the first 6 columns.
The DATAP program finds out which kind of cards are available. It then adds a card of type 3 if none is there.

OUTPUT

Output is on lineprinter and a file with card images.
The program copies all reflection information, and adds one line with the absorption correction.

This line has FORMAT(I6,F9.5,F8.4,F9.5,6F7.4,'ABTDS')
and contains:

Reflection number
Absorption correction factor
TBAR
Alpha, the TDS correction (none=-99.0)
XN(I),I=1,3 see page 2
XNO(I),I=1,3 see page 2

NOTE: if a card with 'ABTDS' is present, then the program will stop if the absorption correction found is between 0 and 1.

G E N E R A L

THE DIFFERENT PROGRAMS OF THE PROMETHEUS SYSTEM ARE CALLED BY A MONITORING PROGRAM. TO TELL THIS MONITOR WHICH PROGRAM HAS TO BE CALLED EACH RUN MUST START WITH A -PROGRAM CALLING CARD- . THE CARDS DESCRIBED IN THE CARD ORDER OF THE CALLED PROGRAM MUST FOLLOW IMMEDIATELY BEHIND THIS CALLING CARD.

AFTER THE LAST CARD DEMANDED BY THE CARD ORDER, THERE CAN FOLLOW A SECOND PROGRAM CALLING CARD IN ORDER TO RUN ANOTHER (OR AGAIN THE SAME) PROGRAM.

THE END OF A RUN MUST BE INDICATED BY A -FINISH CARD- TO TELL THE MONITORING PROGRAM THAT NO FURTHER PROGRAM CALL IS WHISHED.

REMARK

THE PLOT FILE (OUTPUT OF PROGRAM PLOTTE) IS ONLY FINISHED BY AN ***END OF FILE*** MARK IF THE MONITORING PROGRAM READS THE FINISH CARD. SO IF SEVERAL CALLS OF THE PROGRAM PLOTTE ARE EXECUTED DURING ONE RUN THESE PLOTS ARE WRITTEN BEHIND EACH OTHER ON THE SAME PLOT FILE. (E.G. IT IS LIKE ONE BIG PLOT JOB).

PROGRAM CALLING CARDS

FORMAT (A4,A2)

THE FOLLOWING PROGRAM CALLING CARDS CAN BE RECOGNICED BY THE PROMETHEUS SYSTEM VERSION OF DECEMBER 1982

ARBSEC

AVERAG

BONVIB

FOURIE

LISTFC

PDFMAP

PLOTTE

POTCAL

PREDES

REFINE

SPHERE

TDSCOR

THE LABELS MUST BE WRITTEN IN COLUMNS l-6.

THE PROGRAMS AND THEIR INPUT CARDS ARE DESCRIBED UNDER THESE LABELS IN THE DESCRIPTION AND THE CARD ORDER PART.

FINISH CARD

FORMAT (A4,A2)

THE FINISH CARD CONTAINING THE WORD FINISH IN COLUMNS 1-6

INDICATES THE END OF A RUN OF THE PROMETHEUS SYSTEM.

A R B S E C

CARD ORDER SUMMARY OF THE PROGRAM ARBSEC

TITLE	CARD

CONTROL CARD
INPUT-OUTPUT CARD
SECTION CARD
* CELL CARD

* THIS CARD IS OPTIONAL

FORMAT (18A4)

COLUMN	NAME	FUNCTION
1-72	TITEL	ANY SEQUENCE OF SYMBOLS USED AS TITLE OF THE PROGRAM.

CONTROL CARD

FORMAT (4Il,7I3)

COLUMN NAME FUNCTION ANO P055IBLE VALUE5

1 IO SWITCH FOR SAVE THE CALCULATED MAP FOR LATER PLOTTING
(WITH THE PROGRAM PLOTTE).

0 DO NOT SAVE THE MAP.
NOT 0 SAVE THE MAP.

2 NP SWITCH FOR NO PRINTING OF THE CALCULATED POINT ARRAY

0 PRINT THE POINT ARRAY.
1 DO NOT PRINT THE POINT ARRAY.

3 I5PC SWITCH FOR SINGLE- OR DOUBLE SPACED PRINTED OUTPUT.

0 DOUBLE SPACED LINES.
1 SINGLE SPACED LINES.

4 MRK SWITCH FOR READ NEW LIMITS FOR THE AXIS OF THE MAP
TO BE CALCULATED.

0 THE LIMITS OF THE AXIS PRINTED DOWN THE PAGE IN
THE INPUT SECTIONS WILL BE THE LIMITS OF THE
AXIS PRINTED ACROSS THE PAGE (TRANSFORMED X)
IN THE SELECTED ARBITRARY SECTION.
THE LIMITS OF THE AXIS GOING FROM SECTION TO
SECTION OF THE INPUT SECTIONS WILL BE THE
LIMITS OF THE AXIS PRINTED DOWN THE PAGE
TRANSFORMED Y) IN THE SELECTED ARBITRARY
SECTION.
NOT 0 READ NEW LIMITS FOR TRANSFORMED X AND
TRANSFORMED Y FROM THIS CARD.
(SEE THE FOLLOWING VARIABLES IYI,IYF,IZI,IZF).

5 - 7 IZO NUMBER OF THE SECTION

(NEEDED TO RECOGNIZE THE SECTION WHEN A CONTOUR MAP
IS PLOTTED (PROGRAM PLOTTE).

THE FOLLOWING FOUR VALUES ARE ONLY READ IF MRK IS NOT 0

8-10	IYI	INITIAL VALUE OF TRANSFORMED X .
11-13	IYF	FINAL VALUE OF TRANSFORMED X .
14-16	IZI	INITIAL VALUE OF TRANSFORMED Y .
17-19	IZF	FINAL VALUE OF TRANSFORMED Y .

20-22 MINI IN THE PRINTED POINT ARRAY ALL VALUES BETWEEN MINI
23-25 MAXI AND MAXI ARE SUPPRESSED.

INPUT-OUTPUT CARD

FORMAT (4I3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
l - 3	IALP	SHEER ANGLE OF THE PRINTED POINT ARRAY. 0 DO NOT SHEER THE OUTPUT l THE REAL ANGLE BETWEEN THE AXIS CALCULATED BY THE PROGRAMME WILL BE APPROXIMATED BY THE SHEER ANGLE. GREATER THAN 30 THE VALUE OF IALP WILL BE THE APPROXIMATED BY THE SHEER ANGLE. (THE VALUE MUST BE LESS THAN 151).
4 - 6	LESE	SWITCH FOR READ THE CELL CARD. (READING NEW CELL PARAMETERS CAN BE NECESSARY IF IN THE PROGRAMME REFINE NOT THE EXACT CELL CONSTANTS HAVE BEEN USED). 0 TAKE THE DATA OF THE UNIT CELL FROM THE DATA FILE. 1 READ THE DATA OF THE UNIT CELL FROM THE CELL CARD.
7 - 9	IEIN	LOGICAL NUMBER OF THE INPUT FILE. 0 THE DEFAULT VALUE ll WILL BE USED. NOT 0 IEIN IS THE LOGICAL NUMBER OF THE INPUT FILE.
10 -12	IAUS	LOGICAL NUMBER OF THE OUTPUT FILE. 0 THE DEFAULT VALUE 12 WILL BE USED. NOT 0 IAUS IS THE LOGICAL NUMBER OF THE OUTPUT FILE.

SECTION CARD

FORMAT (9F7.0I5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-63	POINTS	COORDINATES OF THE POINTS DEFINING THE SECTION TO BE CALCULATED.
1-7		X
8-14		Y FOR THE FIRST POINT.
15-21		Z
22-28		X
29-35		Y FOR THE SECOND POINT.
36-42		Z
43-49		X
50-56		Y FOR THE THIRD POINT.
57-63		Z
64-68		INDICATOR FR FRACTIONAL COORDINATES 0 THE COORDINATES OF THE THREE POINTS ARE GIVEN IN THE GRID COORDINATES DEFINED IN THE PROGRAMME WHICH HAS WRITTEN IN THE INPUT FILE. NOT 0 THE COORDINATES ARE GIVEN IN FRACTIONAL COORDINATES OF THE UNIT CELL.

CELL CARD

(ONLY NEEDED IF THE PARAMETER LESE ON THE INPUT-OUTPUT CARD IS 1 . IT MAY BE NECESSARY TO READ THE CELL CARDS HERE, IF INACCURATE VALUES HAVE BEEN GIVEN TO THE PROGRAM REFINE , BECAUSE ACCURATE VALUES WERE NOT NEEDED.)

FORMAT (6F7.0)

COLUMN	NAME	FUNCTION
1- 7	A	LENGTH OF THE A-AXIS OF THE UNIT CELL IN ANGSTROMS.
8-14	B	LENGTH OF THE B-AXIS OF THE UNIT CELL IN ANGSTROMS.
15-21	C	LENTH OF THE C-AXIS OF THE UNIT CELL IN ANGSTROMS.

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22-28  ALPHA ANGLE BETWEEN  THE  B-  AND  THE  C-AXIS IN DEGREES.
29-35  BETA  ANGLE BETWEEN  THE  A-  AND  THE  C-AXIS IN DEGREES.
36-42  GAMMA ANGLE BETWEEN  THE  A-  AND  THE  B-AXIS IN DEGREES.
```

CARD ORDER SUMMARY OF THE PROGRAMME AVERAG

```
    LABEL           CARD
    TITLE           CARD
    CONTROL         CARD  ++
  * PARAMETER       CARD  ++
  * INPUT FORMAT    CARD  ++
  * OUTPUT FORMAT   CARD  ++
  * SCALE FACTOR    CARD  ++
  * MATRIX          CARD  ++
  * CELL            CARD  ++
  * HKL             CARDS
    END             CARD


  *   THESE CARDS ARE OPTIONAL
  ++  THE SEQUENCE OF THESE CARDS IS ARBITRARY
```

LABEL CARD

```
FORMAT (A4,A2,1X,I1)

COLUMN NAME    FUNCTION

 1- 6  LABEL   LABEL TO BE WRITTEN ON THE OUTPUT CARDS

    8  ICV     SET TO NON-ZERO IF HKL-CARDS ARE NOT COLL5 TYPE
```

TITLE CARD

```
FORMAT (18A4)

COLUMN NAME    FUNCTION

 1-72  TITEL   ANY SEQUENCE OF SYMBOLS TO BE PRINTED AS TITLE ON
               THE OUTPUT.
```

CONTROL CARD

```
FORMAT (A4,1X,A4,A1,12I3)

COLUMN NAME    FUNCTION AND POSSIBLE VALUES

 1- 4  IBUFF   LABEL FOR IDENTIFYING THE CARD AS TO BE THE CONTROL
               CARD.

               CNTR   LABEL OF THE CONTROL CARD

 6-10  ICHAR   NAME OF THE CRYSTAL CLASS TO BE USED IN THE AVERAGING
```

PROCESS. (LIST OF THE NAMES AT END OF FILE)

11-13 IKART SWITCH FOR HKL-CARDS OR FOUIER-FILE TO BE READ.

0	READ HKL-CARDS
1	READ OBSERVED F-VALUES FROM A FOURIER-FILE
-1	READ CALCULATED F-VALUES FROM A FOURIER-FILE

IF IKART = 1 THE INTENSITIES ARE CORRECTED FOR EXTINCTION USING THE CORRECTION FACTORS READ FROM THE FOURIER FILE.

14-16 IFHKL VERSION NUMBER OF THE HKL-CARDS TO BE READ (SEE TABLE)
NOT USED FOR FOURIER OR COLL5 TYPE HKL-CARD FILES

17-19 IGNO SWITCH FOR CHANGE THE IGNORANCE FACTOR (SEE DESCRIPTION PART).

0	NO CHANGE
NOT 0	CHANGE THE IGNORANCE FACTOR ACCORDING TO THE VALUES OF DIGN1 AND DIGN2 ON THE PARAMETER CARD.

20-22 ISYS SWITCH FOR CALCULATE A SYSTEMATIC ERROR SIGMA(S)

0	NO SYSTEMATIC ERROR TO BE CALCULATED
NOT 0	CACULATE A SYSTEMATIC ERROR USING THE VALUE OF SYSDEV ON THE PARAMETER CARD.

23-25 ISST SWITCH FOR DIFFERENT STANDARD DEVIATIONS TO BE WRITTEN ONTO THE OUTPUT FILE.

0	WRITE SIGMA(T) (DEFINITION OF THE DIFFERENT SIGMA SEE DESCRIPTION PART OF THE PROGRAMME AVERAG) ONTO THE OUTPUT FILE.
-N	IF THERE ARE MORE THAN OR EQUAL TO N SYMMETRICALLY EQUIVALENT REFLECTIONS WRITE SIGMA(D) ONTO THE OUTPUT FILE, IF LESS THAN N REFLECTIONS WRITE SIGMA(T)
+N	LIKE +N BUT TAKE SIGMA(D) ONLY IF IT IS GREATER THAN SIGMA(T).

26-28 MODU SWITCH FOR SELECTION OF PREAVERAGING POSSIBILITIES

0	NO PREAVERAGING
1	AVERAGE FIRST ONLY IDENTICAL REFLECTIONS THEN THE SYMMETRY OF THE CRYSTAL CLASS .
2	AVERAGE FIRST IDENTICAL REFLECTIONS, THEN FRIEDEL-REFLECTIONS AND AT LAST THE SYMMETRY OF THE CRYSTAL CLASS .
3	AVERAGE FIRST IDENTICAL- PLUS FRIEDEL-REFLEC-TIONS AND THEN THE SYMMETRY OF THE CRYSTAL CLASS .

29-31 IREJEC SWITCH FOR DIFFERENT REJECT POSSIBILITIES

0	DO NOT REJECT ANY REFLECTION
+1	A REFLECTION WILL BE REJECTED IF THEIR INTEN-SITY DEVIATES MORE THAN REJE*SIGMA(T) (SEE DESCRIPTION PART) FROM THE MEAN VALUE OF THE GROUP. (REJE MUST BE GIVEN ON THE PARAMETER CARD
-1	A REFLECTIONS WILL BE REJECTED IF THEIR INTEN-SITY IS MORE THAN REJE*SIGMA(C) LESS THAN THE HIGHEST INTENSITY WITHIN THE GROUP. (SIGMA(C) IN THIS CASE IS THE STANDARD DEVIATION OF THE STRONGEST REFLECTION OF THIS GROUP).
+2,-2	LIKE +1 OR -1 RESPECTIVELY BUT REFLECTIONS WILL ONLY BE REJECTED IN THE SELECTED PRE-AVERAGING PROCESSES.
+3,-3	LIKE +1 OR -1 RESPECITVELY BUT REFLECTIONS WILL NOT BE REJECTED IN PREAVERAGING PROCESSES BUT ONLY WHEN AVERAGING THE SYMMETRY OF THE CRYSTAL CLASS .

32-34 NOR SWITCH FOR WHAT TO DO, IF WITHIN A GROUP OF REFLEC-
TIONS ALL BUT ONE ARE REJECTED.

0 THE MEAN VALUE WILL BE REJECTED TOO.
1 IN A SELECTED PREAVERAGING PROCESS THE MEAN VALUE WILL BE REJECTED TOO, BUT WHEN AVERAGING THE SYMMETRY OF THE CRYSTAL CLASS THE REMAINING REFLECTION WILL BE TREATED AS MEAN VALUE.
2 WHEN PREAVERAGING THE REMAINING REFLECTION WILL BE TREATED AS MEAN VALUE, BUT WHEN AVERGING THE SYMMETRY OF THE CRYSTAL CLASS THE MEAN VALUE WILL BE REJECTED .

3 THE REMAINING REFLECTION WILL ALWAYS BE TREATED AS MEAN VALUE.

35-37 NULL SWITCH FOR SET NEGATIVE INTENSITIES TO ZERO

0 AFTER AVERGING NEGATIVE INTENSITIES WILL BE SET TO ZERO.
NOT 0 THEY WILL NOT BE SET TO ZERO.

38-40 IABSO SWITCH FOR CORRECT THE INTENSITIES FOR ABSORPTION

0 NO ABSORPTION CORRECTION
> 0 INTENSITIES AND STANDARD DEVIATIONS WILL BE MULTIPLIED BY THE ABSORPTION FACTORS READ FROM THE HKL-CARDS.
(IF THERE IS NO TBAR ON CARDS SEE MU ON THE PARAMETER CARD).
< 0 PSI-DATA TREATMENT
NO ABSORPTION CORRECTION. PSI-VALUES FOUND ON THE INPUT-FILE ARE USED ON THE HKL-FILE (NOTE. NO SORTING ON SIN(THETA)/LAMBA IS POSSIBLE)

41-43 IPSO SWITCH FOR THE USE OF THE QUICKSORT PROCESS AND FOR AVERAGING OR ONLY SORTING.

(THE USE OF QUICKSORT SAVES CPU-TIME BUT CHANGES THE SEQUENCE OF THE REFLECTIONS. ONLY SORTING MEANS THAT THE REFLECTIONS WILL BE WRITTEN ONTO THE OUPUT FILE WITHOUT AVERAGING BUT IN GROUPS OF SYMMETRICALLY EQUIVALENT REFLECTIONS).
(ABSORPTION OR EXTINCTION CORRECTION IS MADE ALSO WHEN ONLY SORTING IS SELECTED).

IPSO	QUICKSORT USED	ONLY SORTING
0	YES	NO
1	NO	NO
2	YES	YES
3	NO	YES

44-46 ILIST SWITCH FOR DIFFERENT OUPUT VERSIONS.

0 COMPLETE OUTPUT TO BE PRINTED
1 NO LIST OF REFLECTIONS
2 NO LIST OF THE DATA READ BUT LIST OF THE GROUPS OF SYMMETRICALLY EQUIVALENT REFLECTIONS.
3 PRINT ONLY THE AVERAGED REFLECTIONS

PARAMETER CARD

FORMAT (A4,1X,8F8.3)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1 -4 IBUFF LABEL FOR IDENTIFYING THE CARD TO BE THE PARAMETER CARD.

PARA LABEL OF THE PARAMETER CARD.

6-13 DIGN1 IGNORANCE FACTOR INCLUDED IN THE SIGMA(C) READ
(ONLY NEEDED IF THE PARAMETER IGNO ON THE CONTROL
CARD IS NOT 0).
(FOR IGNORANCE FACTOR AND SIGMA(C) SEE DESCRIPTION
PART).

14-21 DIGN2 NEW VALUE FOR THE IGNORANCE FACTOR
(ONLY NEEDED IF IGNO IS NOT 0).

22-29 SYSDEV ESTIMATED SYSTEMATIC ERROR IN PERCENT OF INTENSITY.
(ONLY NEEDED IF THE PARAMETER ISYS ON THE CONTROL
CARD IS NOT 0).

30-37 REJE MULTIPLE OF SIGMA(T) OR SIGMA(C) RESP. TO BE USED FOR
REJECTING REFLECTIONS.
(ONLY NEEDED IF THE PARAMETER IREJEC ON THE CONTROL
CARD IS NOT 0).

38-45 MU ABSORPTION COEFFICIENT
(ONLY NEEDED IF THE PARAMETER IABSO ON THE CONTROL
CARD IS NOT 0 AND TBAR IS NOT READ FROM CARDS).

46-53 SIGLT MULTIPLE OF THE STANDARD DEVIATION BELOW WHICH AN
INTENSITY SHOULD BE MARKED AS LESS THAN .
0 THE DEFAULT VALUE 3.0 IS USED
NOT 0 SIGLT IS THE MULTIPLE TO BE USED
FOR THIS MARKING THE STANDARD DEVIATION WHICH IS
WRITTEN ONTO THE OUTPUT FILE IS USED.

54-61 OFLOW WITH THIS VALUE ALL THE INTENSITIES AND SIGMA(C)
(SEE DESCRIPTION PART) ARE MULTIPLIED JUST AFTER
READING THE DATA.
(HELPFUL FOR EXAMPLE IF THERE ARE VERY HIGH
ABSORPTION FACTORS WHICH LEAD TO AN OVERFLOW OF THE
OUPUT FORMAT.)

62-69 FINTCU AVERAGE ONLY THE REFLECTIONS WITH INTENSITIES LESS
THAN FINTCU * SIGMA(INTENSITY). IF FINTCU=0, THEN
ALL REFLECTIONS ARE AVERAGED.

INPUT FORMAT CARD

(THIS CARD IS ONLY NEEDED IF THE HKL-CARDS CAN NOT BE READ USING
STANDARD FORMAT (SEE HKL-CARD DESCRIPTION)).

FORMAT (A4,1X,16A4,A3)

COLUMN NAME FUNCTION

1- 4 IBUFF LABEL FOR IDENTIFYING THE CARD TO BE THE INPUT FORMAT
CARD.

FORI LABEL OF THE INPUT FORMAT CARD.

6-72 IPFOR STANDARD FORTRAN NOTATION OF THE FORMAT TO BE USED
READING THE HKL-CARDS.
(THE FORMAT MUST START WITH (A3, IN ORDER TO
RECOGNIZE THE END CARD (SEE BELOW)).
(THE FORMAT MUST CORRESPOND WITH THE VERSION OF HKL-
CARDS SELECTED BY THE PARAMETER IFHKL ON THE
CONTROL CARD).

OUTPUT FORMAT CARD

(ONLY NECESSARY IF THE HKL-CARDS ON THE OUPUT FILE SHOULD NOT HAVE
STANDARD FORMAT).

FORMAT (A4,1X,4A1,1X,4A1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	IBUFF	LABEL FOR IDENTIFYING THE CARD TO BE THE OUPUT FORMAT CARD. FORO LABEL OF THE OUTPUT FORMAT CARD.
6- 9	IRMTI	NUMBER PART OF THE F-FORMAT FOR THE INTENSITY OUTPUT. (THE . MUST BE IN COLUMN7 OR 8)
11-14	IRMTS	NUMBER PART OF THE F-FORMAT FOR THE STANDARD DEVIATION OUTPUT. (THE . MUST BE IN COLUMN12 OR 13) EXAMPLE FORO 10.2 7.3 MEANS THAT THE OUTPUT FORMAT IS F10.2 FOR THE INTENSITY AND F7.3 FOR THE STANDARD DEVIATION.

ATTENTION

IF THIS CARD IS READ ALWAYS BOTH FORMATS MUST BE GIVEN, IRMTI AND IRMTS.

SCALE FACTOR CARD

(ONLY NECESSARY IF THERE ARE MORE THAN ONE SCALE GROUP IN THE DATA SET).

FORMAT (A4,1X,8F8.3)

COLUMN	NAME	FUNCTION
1- 4	IBUFF	LABEL FOR IDENTIFYING THE CARD TO BE THE SCALE FACTOR CARD. SCAL LABEL OF THE SCALE FACTOR CARD.
6-69	SCLFAK	SCALE FACTORS FOR THE DIFFERENT SCALE GROUPS IN THE SEQUENCE OF INCREASING SCALE GROUP NUMBERS USING EIGHT COLUMNS FOR EACH FACTOR. (THE INTENSITIES WILL BE CHANGED SO THAT THE SCALE FACTOR OF THE FIRST REFLECTION READ IS VALUABLE FOR THE WHOLE DATA SET.)

MATRIX CARD

(ONLY NECESSARY IF THE INDICEES OF THE REFLECTIONS SHOULD BE TRANSFORMED).

FORMAT (A4,1X,9F8.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	IBUFF	LABEL FOR IDENTIFYING THE CARD TO BE THE SCALE FACTOR CARD. MATR LABEL OF THE MATRIX CARD
6-53	TRAFO	ELEMENTS OF A 3*3 MATRIX LINE BY LINE USING EIGHT COLUMNS FOR EACH ELEMENT. EACH HKL-VECTOR WILL BE MULTIPLIED WITH THIS MATRIX BEFORE AVEARGING. (IF A NON INTEGER VALUE FOR ONE OF THE INDICES RESULTS THE REFLECTION

WILL BE REJECTED WITH A WARNING).

CELL CARD

(ONLY NECESSARY IF AFTER AVERAGING THE DATA SHOULD BE SORTED FOR INCREASING SIN(THETA) / LAMBDA).

FORMAT (A4,1X,6F8.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	IBUFF	LABEL FOR IDENTIFYING THE CARD TO BE THE CELL CARD.
		CELL LABEL OF THE CELL CARD.
6-53	CELL	CELL PARAMETERS A, B, C, ALPHA, BETA, AND GAMMA USING EIGHT COLUMNS FOR EACH VALUE. (A,B,C IN ANGSTROMS AND THE ANGLES IN DEGREES).

HKL CARDS

(ONLY NECESSARY HERE IF IKART ON THE CONTROL CARD IS 0 AND THEY ARE NOT READ FROM A FILE (PARAMETER INUNIT ON THE LABEL CARD)).

STANDARD FORMAT (ALTERNATIVE VALUES BELOW DEPENDING ON THE SELECTED VERSION).

(A3,10X,3I3,3X,I3,I3,F9.0,F9.5,F5.0,7X,F8.4)
3X 9X 8X

TABEL OF VERSIONS ACCEPTED BY THE PROGRAMME

VERSION NUMBER	LABEL	H,K,L	LESS THAN MARKING	SCALE GROUP	INTEN-SITY	TBAR	SIGMA	ASTAR
1	X	X	X		X		X	
2	X	X	X		X	X	X	
3	X	X	X	X	X		X	
4	X	X	X	X	X	X	X	
5	X	X	X		X		X	X
6	X	X	X		X	X	X	X
7	X	X	X	X	X		X	X
8	X	X	X	X	X	X	X	X

EXPLANATION OF THE TABLE

LABEL	ONLY FOR IDENTIFICATION OF THE END CARD. (IF THE LABEL OF THE CARD IS NOT END IT WILL BE TAKEN AS A HKL CARD).
H,K,L	MILLER INDECES
LESS THAN MARKING	1 NO LESS THAN REFLECTION 2 LESS THAN REFLECTION
SCALE GROUP	NUMBER OF THE SCALE GROUP TO WHICH THE REFLECTIONS BELONGS.

INTENSITY	IF THE VERSION NUMBER IS POSITIVE	INTENSITY (I(OBS))
	IF THE VERSION NUMBER IS NEGATIVE	STRUCTUR FACTOR (F)
TBAR	MEAN PATH LENGTH	
SIGMA	STANDARD DEVIATION	
	IF THE VERSION NUMBER IS POSITIVE	OF I(OBS)
	IF THE VERSION NUMBER IS NEGATIVE	OF F
ASTAR	ABSORPTION FACTOR	

REMARK

THE OUTPUT CARDS OF THE AVERAGING PROGRAMME ARE WRITTEN ACCORDING TO THE VERSION NUMBER 4 RESPECTIVELY (IF ABSORPTION FACTORS ARE READ BUT IABSO = 0 (SEE CONTROL CARD)) ACCORDING TO VERSION NO. 8 .

END CARD

(THIS CARD MUST ALWAYS BE THE LAST CARD BEFORE THE FINISH CARD OR THE CALLING CARD FOR THE NEXT PROGRAMME)

FORMAT (A3)

COLUMN	NAME	FUNCTION AND POSIBLE VALUES
1- 3	IBUFF	LABEL FOR IDENTIFYING THE CARD TO BE THE END CARD.
		END LABEL OF THE END CARD.

THE END CARD IS NECESSARY FOR RECOGNIZING THE END OF THE HKL-CARDS IF THESE ARE READ FROM THE STANDARD INPUT UNIT RESPECTIVELY FOR RECOGNIZING THE END OF THE INPUT CARDS IF THE HKL-CARDS ARE READ FROM A FILE OR A FOURIER FILE IS READ.

NOTATION OF THE LAUE AND CRYSTAL CLASSES

TO BE WRITTEN LEFT JUSTIFIED IN THE FORMAT A4,A1 ON THE CONTROL CARD.

TRICLINIC

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
P 1	(1)	1		5 BLANKS
P -1	(2)	-1	-1	-1

MONOCLINIC

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
		C-AXIS PERPENDICULAR		
P 2	(3)			
P 21	(4)			
B 2	(5)	2		2/MZA
P M	(6)			
P B	(7)			

B M	(8)			
B B	(9)	M		2/MZB
P 2/M	(10)			
P 21/M	(11)			
B 2/M	(12)			
P 2/B	(13)			
P 21/B	(14)			
B 2/B	(15)	2/M	2/M	2/MZ

B-AXIS PERPENDICULAR

P 2	(3)			
P 21	(4)			
C 2	(5)	2		2/MYA
P M	(6)			
P C	(7)			
C M	(8)			
C C	(9)	M		2/MYB
P 2/M	(10)			
P 21/M	(11)			
C 2/M	(12)			
P 2/C	(13)			
P 21/C	(14)			
C 2/C	(15)	2/M	2/M	2/MY

ORTHORHOMBIC

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
P 222	(16)			
P 221	(17)			
P 21212	(18)			
P 212121	(19)			
C 2221	(20)			
C 222	(21)			
F 222	(22)			
I 222	(23)			
I 212121	(24)	222		MMM A
P MM2	(25)			
P MC21	(26)			
P CC2	(27)			
P MA2	(28)			
P CA21	(29)			
P NC2	(30)			
P MN21	(31)			
P BA2	(32)			
P NA21	(33)			
P NN2	(34)			
C MM2	(35)			
C MC21	(36)			
C CC2	(37)			
A MM2	(38)			
A BM2	(39)			
A MA2	(40)			
A BA2	(41)			
F MM2	(42)			
F DD2	(43)			
I MM2	(44)			
I BA2	(45)			
I MA2	(46)	MM2		MMM B
P MMM	(47)			
P NNN	(48)			
P CCM	(49)			
P BAN	(50)			
P MMA	(51)			
P NNA	(52)			
P MNA	(53)			
P CCA	(54)			

P BAM	(55)			
P CCN	(56)			
P BCM	(57)			
P NNM	(58)			
P MMN	(59)			
P BCN	(60)			
P BCA	(61)			
P NMA	(62)			
C MCM	(63)			
C MCA	(64)			
C MMM	(65)			
C CCM	(66)			
C MMA	(67)			
C CCA	(68)			
F MMM	(69)			
F DDD	(70)			
I MMM	(71)			
I BAM	(72)			
I BCA	(73)			
I MMA	(74)	MMM	MMM	MMM

TETRAGONAL

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
P 4	(75)			
P 41	(76)			
P 42	(77)			
P 43	(78)			
I 4	(79)			
I 41	(80)	4		4/M A
P -4	(81)			
I -4	(82)	-4		4/M B
P 4/M	(83)			
P 42/M	(84)			
P 4/N	(85)			
P 42/N	(86)			
I 4/M	(87)			
I 41/A	(88)	4/M	4/M	4/M
P 422	(89)			
P 4212	(90)			
P 4122	(91)			
P 41212	(92)			
P 4222	(93)			
P 42212	(94)			
P 4322	(95)			
P 43212	(96)			
I 422	(97)			
I 4122	(98)	422		4/MMA
P 4MM	(99)			
P 4BM	(100)			
P 42CM	(101)			
P 42NM	(102)			
P 4CC	(103)			
P 4NC	(104)			
P 42MC	(105)			
P 42BC	(106)			
I 4MM	(107)			
I 4CM	(108)			
I 41MD	(109)			
I 41CD	(110)	4MM		4/MMB
P -42M	(111)			
P -42C	(112)			
P -421M	(113)			
P -421C	(114)			
I -42M	(121)			
I -42D	(122)	-42M		4/MMC

P -4M2	(115)			
P -4C2	(116)			
P -4B2	(117)			
P -4N2	(118)			
I -4M2	(119)			
I -4C2	(120)	-4M2		4/MMD
P 4/MMM	(123)			
P 4/MCC	(124)			
P 4/NBM	(125)			
P 4/NNC	(126)			
P 4/MBM	(127)			
P 4/MNC	(128)			
P 4/NMM	(129)			
P 4/NCC	(130)			
P 42/MMC	(131)			
P 42/MCM	(132)			
P 42/NBC	(133)			
P 42/NNM	(134)			
P 42/MBC	(135)			
P 42/MNM	(136)			
P 42/NMC	(137)			
P 42/NCM	(138)			
I 4/MMM	(139)			
I 4/MCM	(140)			
I 41/AMD	(141)			
I 41/ACD	(142)	4/MMM	4/MMM	4/MMM

TRIGONAL

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
		RHOMBOHEDRAL SETTING		
R 3	(146)	3		-3RHA
R -3	(148)	-3	-3	-3RHO
R 32	(155)	321		-3M A
R 3M	(160)			
R 3C	(161)	3M1		-3M B
R -3M	(166)			
R -3C	(167)	-3M1	-3M1	-3M
		HEXAGONAL SETTING		
P 3	(143)			
P 31	(144)			
P 32	(145)			
R 3	(146)	3		-3HEA
P -3	(147)			
R -3	(148)	-3	-3	-3HEX
P 312	(149)			
P 3112	(151)			
P 3212	(153)	312		-31MA
P 31M	(157)			
P 31C	(159)	31M		-31MB
P -31M	(162)			
P -31C	(163)	-31M	-31M	-31M

P 321	(150)			
P 3121	(152)			
P 3221	(154)			
R 32	(155)	321		-3M1A
P 3M1	(156)			
P 3C1	(158)			
R 3M	(160)			
R 3C	(161)	3M1		-3M1B
P -3M1	(164)			
P -3C1	(165)			
R -3M	(166)			
R -3C	(167)	-3M1	-3M1	-3M1

HEXAGONAL

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
P 6	(168)			
P 61	(169)			
P 65	(170)			
P 62	(171)			
P 64	(172)			
P 63	(173)	6		6/M A
P -6	(174)	-6		6/M B
P 6/M	(175)			
P 63/M	(176)	6/M	6/M	6/M
P 622	(177)			
P 6122	(178)			
P 6522	(179)			
P 6222	(180)			
P 6422	(181)			
P 6322	(182)	622		6/MMA
P 6MM	(183)			
P 6CC	(184)			
P 63CM	(185)			
P 63MC	(186)	6MM		6/MMB
P -6M2	(187)			
P -6C2	(188)	-6M2		6/MMC
P -62M	(189)			
P -62C	(190)	-62M		6/MMD
P 6/MMM	(191)			
P 6/MMC	(192)			
P 63/MCM	(193)			
P 63/MMC	(194)	6/MMM	6/MMM	6/MMM

CUBIC

SPACE GROUP		CRYSTAL CLASS	LAUE CLASS	NOTATION
P 23	(195)			
F 23	(196)			
I 23	(197)			
P 213	(198)			
I 213	(199)	23		M3 A
P M3	(200)			
P N3	(201)			

```
F M3     (202)
F D3     (203)
I M3     (204)
P A3     (205)
I A3     (206)    M3                  M3              M3


P 432    (207)
P 4232   (208)
F 432    (209)
F 4132   (210)
I 432    (211)
P 4332   (212)
P 4132   (213)
I 4132   (214)    432                                 M3M A

P -43M   (215)
F -43M   (216)
I 43M    (217)
P -43N   (218)
F -43C   (219)
I -43D   (220)    -43M                                M3M B

P M3M    (221)
P N3N    (222)
P M3N    (223)
P N3M    (224)
F M3M    (225)
F M3C    (226)
F D3M    (227)
F D3C    (228)
I M3M    (229)
I A3D    (230)    M3M                 M3M             M3M
```

CARD ORDER SUMMARY OF THE PROGRAM BONVIB

```
 TITLE           CARD

 CONTROL         CARD

 CELL VAR.-COVAR.CARDS


   NO CARD IS OPTIONAL
```

TITLE CARD

```
FORMAT (18A4)

COLUMN NAME    FUNCTION

 1-72  TITEL   ANY SEQUENCE OF SYMBOLS USED AS TITLE OF THE PROGRAM.
```

CONTROL CARD

```
FORMAT (3I1,3F8.0)

COLUMN NAME    FUNCTION AND POSSIBLE VALUES

    1  MBODAN  BOND DISTANCE, ANGLE SELECTOR
```

```
                0      NONE COMPUTED
                1      DISTANCES ONLY
                2      DISTANCES AND ANGLES COMPUTED

    2  MELVIB  THERMAL ELLIPSOID SELECTOR

                0      NO ELLIPSOIDS COMPUTED
                1      THERMAL ELLIPSOIDS COMPUTED FOR ANISOTRIPIC
                       ATOMS
  3  MTENSA  HIGHER ORDER ANALYSIS SELECTOR
           0      NO ANALYSIS
           1      ANALYSIS OF HIGHER ORDER THERMAL TENSORS
 4-11  DLIMIT(1)      MINIMUM BOND DISTANCE OUTPUT
12-19  DLIMIT(2)      MAXIMUM BOND DISTANCE USED IN ANGLES OUTPUT
20-27  DLIMIT(3)      MAXIMUM BOND DISTANCE OUTPUT
```

CELL VAR.-COVAR.CARDS

(THIS 4 CARDS CONTAIN THE CELL VARIANCE-COVARIANCE MATRIX)

REMARK
THIS MATRIX CAN NOT BE CALCULATED BY THE PROMETHEUS SYSTEM UP TO NOW.
IT IS COMPUTED E.G. BY THE PARAM PROGRAM OF THE XRAY-SYSTEM
(STEWARD ET. AL. 1967).
YOU CAN GIVE 0 RESP. BLANKS ON THESE CARDS. THIS MEANS THAT THE
EFFECT OF ERRORS IN THE CELL CONSTANTS ON THE DISTANCES ARE
NEGLECTED.

CARD 1

FORMAT (6E12.6)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-12		VARIANCE OF A (IN ANGSTROMS^2)
13-24		COVARIANCE OF A WITH B
25-36		COVARIANCE OF A WITH C
37-48		COVARIANCE OF A WITH ALPHA (IN ANGSTROMS-RADIANS)
49-60		COVARIANCE OF A WITH BETA
61-72		COVARIANCE OF A WITH GAMMA

CARD 2

FORMAT (6E12.6)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-12		VARIANCE OF B
13-24		COVARIANCE OF B WITH C
25-36		COVARIANCE OF B WITH ALPHA
37-48		COVARIANCE OF B WITH BETA
49-60		COVARIANCE OF B WITH GAMMA
61-72		VARIANCE OF C

CARD 3

FORMAT (6E12.6)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-12		COVARIANCE OF C WITH ALPHA
13-24		COVARIANCE OF C WITH BETA
25-36		COVARIANCE OF C WITH GAMMA
37-48		VARIANCE OF ALPHA (IN RADIANS^2)
49-60		COVARIANCE OF ALPHA WITH BETA
61-72		COVARIANCE OF ALPHA WITH GAMMA

CARD 4

FORMAT (6E12.6)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-12		VARIANCE OF BETA
13-24		COVARIANCE OF BETA WITH GAMMA
25-36		VARIANCE OF GAMMA

CARD ORDER SUMMARY OF THE PROGRAMME FOURIE

	TITLE	CARD
	INPUT-OUTPUT	CARD
*	ANGLE SELECTION	CARD(S)
*	HKL SELECTION	CARDS
*	PATTERSON TITLE	CARD
*	CELL	CARD
*	CELL TYPE	CARD
*	SYMMETRY	CARDS
*	FORMAT	CARD
*	HKL	CARDS
*	END	CARD
	CONTROL	CARD
*	MULTIPLICITY	CARD

* THESE CARDS ARE OPTIONAL

TITLE CARD

FORMAT (18A4)

COLUMN	NAME	FUNCTION
1-72	TITEL	ANY SEQUENCE OF SYMBOLS USED AS TITLE OF THE PROGRAMME

INPUT-OUTPUT CARD

FORMAT (8I3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	ISELEC	SHEER ANGLE OF THE PRINTED POINT ARRAY
		0 THE REAL ANGLE OF THE AXES LAYING IN THE PRINTED SECTION WILL BE THE SHEER ANGLE.
		NOT 0 THE VALUE OF ISELEC WILL BE THE SHEER ANGLE.
4- 6	ISTAT	SWITCH FOR PRINT THE REFLECTIONS USED FOR CALCULATION.

0 DO NOT PRINT THE REFELCTIONS.
NOT 0 PRINT FOR ALL REFLECTIONS USED THE FOLLOWING VALUES
H,K,L,F(OBS),F(CALC),A(CALC),B(CALC),PHASE.

(H,K,L MILLER INDICES,
F(OBS) OBSERVED STRUCTURE FACTOR
F(CALC) CALCULATED STRUCTURE FACTOR
A(CALC) REAL PART OF F(CALC)
B(CALC) IMGINARY PART OF F(CALC)
PHASE PHASE ANGLE OF F(CALC) IN DEGREES.

7- 9 IFILE LOGICAL NUMBER OF THE INPUT FILE (FOURIER-FILE).

0 THE DEFAULT VALUE 13 WILL BE USED.
NOT 0 IFILE IS THE LOGICAL NUMBER OF THE INPUT FILE.

ATTENTION
THIS FILE IS ALSO NEEDED IF HKL-CARDS ARE READ (IPAT NOT 0). IN THIS CASE THE FILE IS TEMPORARILY USED TO STORE THE DATA INFORMATION.

10-12 IAUSG LOGICAL NUMBER OF THE OUTPUT FILE.

0 THE DEFAULT VALUE 11 WILL BE USED.
NOT 0 IAUSG IS THE LOGICAL NUMBER OF THE OUTPUT FILE.

13-15 IPAT SWITCH FOR READ HKL-CARDS INSTEAD OF A FOURIER FILE AND CALCULATE A PATTERSON SYNTHESIS.
(THE FOURIER FILE IN THIS CASE IS CREATED BY THE FOURIE PROGRAMME ITSELF).

0 THE DATA ARE READ FROM A FOURIER FILE.
NOT 0 READ HKL-CARDS AND CALCULATE A PATTERSON SYNTHESIS.

ATTENTION
IF HKL-CARDS ARE READ NO ANGLE SELECTION IS POSSIBLE AND THE PARAMETER IPART IS SET TO 0.

REMARK
A PATTERSON SYNTHESIS CAN ALSO BE CALCULATED FROM A FOURIER FILE, WITH HKL-CARDS HOWEVER ONLY A PATTERSON SYNTHESIS CAN BE CALCULATED.

16-18 IPART SWITCH FOR READ ANGLE SELECTION CARDS OR HKL SELECTION CARDS.

0 READ NO SELECTION CARDS.
NEG. READ ANGLE SELECTION CARD(S).
POS. READ HKL SELECTION CARDS.

19-21 IMINI IN THE PRINTED POINT ARRAY ALL VALUES BETWEEN IMINI
22-24 IMAXI ANS IMAXI ARE SUPPRESSED.

ANGLE SELECTION CARD(S)

(THIS CARD IS ONLY READ IF THE PARAMETER IPART ON THE INPUT-OUTPUT CARD IS LESS THAN 0).

FORMAT (2F8.5,I3)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1- 8 SINMIN ONLY THOSE REFLECTIONS WILL BE USED FOR CALCULATION
9-16 SINMAX FOR WHICH SIN(THETA) / LAMBDA IS GREATER THAN SINMIN AND LESS THAN SINMAX.

17-19 IMORE SWITCH FOR READ THE SECOND ANGLE SELECTION CARD.

0 THIS IS THE LAST ANGLE SELECTION CARD.
NOT 0 THE FOLLOWING CARD IS AGAIN AN ANGLE SELECTION CARD.

(AT MOST THERE CAN BE 2 ANGLE SELECTION CARDS).

HKL SELECTION CARDS

(THIS CARDS ARE ONLY READ IF THE PARAMETER IPART ON THE INPUT-OUTPUT CARD IS GREATER THAN 0).

FORMAT (A3,10X,3I3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	IMEHR	SWITCH FOR READ ONE MORE HKL SELECTION CARD. END THIS IS THE LAST HKL SELECTION CARD. NOT END THE FOLLOWING CARD IS AGAIN A HKL SELECTION CARD.
14-16	IHKL	USE THE REFLECTION WITH THE
17-19	JHKL	MILLER INDICES IHKL,JHKL, AND KHKL
20-22	KHKL	FOR THE CALCULATION.

ATTENTION
IN THE PRESENT VERSION THE PROGRAMME CAN READ AT MOST 100 HKL SELECTION CARDS.

PATTERSON TITEL CARD

(THIS CARD IS ONLY NECESSARY IF THE PARAMETER IPAT ON THE INPUT-OUTPUT CARD IS NOT ZERO).

FORMAT (3A4)

COLUMN	NAME	FUNCTION
1-12	LABEL	ANY SEQUENCE OF SYMBOLS USED AS LABEL OF THE FOURIER FILE TO BE CREATED.

CELL CARD

(ONLY NECESSARY IF IPAT IS NOT ZERO)

FORMAT (6F8.0)

COLUMN	NAME	FUNCTION
1- 8	A	LATTICE CONSTANTS
9-16	B	GIVEN IN
17-24	C	ANGSTROMS.
25-32	ALPHA	LATTICE ANGLES
33-40	BETA	GIVEN IN
41-48	GAMMA	DEGREES.

CELL TYPE CARD

(ONLY NECESSARY IF IPAT IS NOT ZERO)

FORMAT (2I3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	ICENT	FLAG FOR CETRIC OR ACENTRIC CELL 0 CENTRIC CELL 1 ACENTRIC CELL

4- 6	ICELL	INDICATOR FOR THE TYPE OF THE CELL
		0 PRIMITIVE
		1 A- CENTERED
		2 B- CENTERED
		3 C- CENTERED
		4 I- CENTERED
		5 F- CENTERED
		6 RHOMBOHEDRAL

SYMMETRY CARDS

(ONLY NECESSARY IF IPAT IS NOT ZERO)

FORMAT (3(3A3,1X),I4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	JTNS	TRANSLATIONAL PART OF X .
		HERE CAN APPEAR ONE OF THE OPERATORS DESCRIBED BELOW OR END TO INDICATE THAT ALL SYMMETRY CARDS WERE READ.
5- 6	IRMAT	FIRST POSITIONAL PART OF X .
8- 9	IRMAT	SECOND POSITIONAL PART OF X .
11-13		TRANSLATIONAL PART OF Y .
15-16		FIRST POSITIONAL PART OF Y .
18-19		SECOND POSITIONAL PART OF Y .
21-23		
25-26		SAME FOR Z .
28-29		
30-33	IEF	END OF SYMMTERY CARDS INDICATOR
		0 THE NEXT CARD IS A SYMMETRY CARD
		NOT 0 THIS IS THE LAST SYMMETRY CARD (THE CARD ITSELF MUST ALSO CONTAIN SYMMETRY INFORMATION)

THE TRANSLATIONAL OPERATORS MUST BE OF THE FOLLOWING FORM (B = BLANK)
BBB, 1/2, 1/3, 2/3, 1/4, 3/4, 1/6, OR 5/6 .
THE POSITIONAL OPERATOR MUST BE OF THE FORM (W = X, Y, OR Z)
+W, BW (=+W), OR -W.

ATTENTION
THE SYMMETRIY POSITION X Y Z MUST BE INCLUDED. THE MAXIMUM NUMBER OF SYMMETRY CARDS IS 24. SYMMETRY OPERATIONS INCLUDING THE INVERSION OR A TRANSLATION DUE TO LATTICE CENTERING ARE CREATED BY THE PROGRAM AND MUST NOT BE INCLUDED HERE.

FORMAT CARD

(ONLY NECESSARY IF IPAT IS NOT ZERO)

FORMAT (18A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-72	FRMT	INDICATOR FOR THE FORMAT OF THE HKL-CARDS.
1- 4		(A3, THIS BEGINNING IS NECESSARY TO RECOGNIZE THE END CARD AFTER THE LAST HKL-CARD
5-72		REST OF THE FORMAT IN STANDARD FORTRAN NOTATION THE DATA ON A HKL-CARD CAN ONLY BE READ IN THE SEQUENCE DEFINED IN HKL CARDS BELOW.

HKL CARDS

(ONLY NECESSARY IF IPAT IS NOT ZERO).

FORMAT (A3, (REST DEFINED IN THE FORMAT CARD ABOVE))

THE DATA ARE READ FROM EACH CARD IN THE FOLLOWING SEQUENCE

FLAG,H,K,L,MREJ,F(OBS),SIGMA

FLAG VARIABLE TO RECOGNIZE THE END CARD (SEE DESCRIPTION BELOW)
H,K,L MILLER INDECES
MREJ MARK FOR LESS THAN REFLECTIONS (REJECTION FLAG)
1 NO LESS THAN REFLECTION
2 LESS THAN REFLECTION
F(OBS) INTENSITY
SIGMA STANDARD DEVIATION OF THE INTENSITY

END CARD

(ONLY NECESSARY IF IPAT IS NOT ZERO, BUT THEN IS MUST FOLLOW AFTER THE LAST HKL CARD).

FORMAT (A3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	FLAG	HKL THIS IS A HKL CARD
		NOT HKL THIS IS THE END CARD AFTER THE LAST HKL CARD

CONTROL CARD

FORMAT (7I1,1X,9I4,2F8.0,A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	ITYPE	MAP TYPE INDICATOR.
		0 FOURIER MAP USING F-OBSERVED.
		1 DIFFERENCE FOURIER MAP.
		2 FOURIER MAP USING F-CALCULATED.
		3 PATTERSON MAP.
		4 PROJECTION ON A PLANE GIVEN BY ISECT FO-MAP
		5 " " " " DELTA
		6 " " " " FC-MAP

REMARK
IF ON THE INPUT,OUPUT CARD THE PARAMETER IPAT IS NOT ZERO
ITYPE IS SET TO BE 3 .

2	ISECT	SELECTION FLAG FOR DIFFERENT ORIENTATIONS OF THE SECTION(S) TO BE CALCULATED.

	ACROSS THE PAGE	DOWN THE PAGE	SECTION(S)	UP OR DOWN (SEE BELOW)
0	X	Y	Z	DOWN
1	X	Z	Y	UP
2	Y	X	Z	UP
3	Y	Z	X	DOWN
4	Z	Y	X	UP
5	Z	X	Y	DOWN

UP = THE SECTION COORDINATE INCREASES WITH INCREASIN
SECTION NUMBER
DOWN THE SECTION COORDINATE DECREASES WITH INCREASIN

SECTION NUMBER.
(THIS MEANS THAT THE SYSTEM IS ALWAYS RIGHT HANDED).

3 ICENT CENTRIC INDICATOR
(FOR SUBSTANCES WITH CENTRIC CELL AND HIGH ANOMALOUS DISPERSION IT IS NECESSARY HERE, TO DECLARE AN ACENTRIC CELL, BECAUSE IN THE FOURIE PROGRAMME FOR CENTRIC CELLS THE IMAGINARY PART OF THE STRUCTURE FACTOR IS ALWAYS NEGLECTED).

0 CENTRIC
1 ACENTRIC

4 KREJ SWITCH FOR INCLUDE THE REFLECTIONS WITH REJECTION FLAG SET IN THE CALCULATION.
(REJECTION FLAG SEE HKL-CARD DESCRIPTION).

0 IGNORE REJECTION FLAG AND INCLUDE ALL REFLECITONS.
1 DO NOT INCLUDE ANY REFLECTIONS WITH REFLECTION FLAG SET.

5 IPLT SWITCH FOR SAVE THE CALCULATED MAP FOR LATER PLOTTING (PLOTTE) OF CALCULATION OF AN ARBITRARY SECTION (ARBSEC).

0 DO NOT SAVE THE MAP.
NOT 0 SAVE THE MAP ON UNI CARD).

6 LSPC SWITCH FOR SINGLE- OR DOUBLE SPACED PRINTED OUPUT.

0 DOUBLE SPACED LINES.
1 SINGEL SPACED LINES.

7 NPNT SWITCH FOR PRINT THE CALCULATED POINT ARRAY.

0 PRINT THE POINT ARRAY
1 DO NOT PRINT THE POINT ARRAY

9-12 IX NUMBER OF DIVISIONS ALONG THE X-AXIS.
13-16 IXI INITIAL POINT ALONG THE X-DIRECTION.
17-20 IXF FINAL POINT ALONG THE X-DIRECTION.

21-24 IY NUMBER OF DIVISIONS ALONG THE Y-AXIS.
25-28 IYI INITIAL POINT ALONG THE Y-DIRECTION.
29-32 IYF FINAL POINT ALING THE Y-DIRECTION.

33-36 IZ NUMBER OF DIVISIONS ALONG THE Z-AXIS.
37-40 IZI INITIAL POINT ALONG THE Z-DIRECTION.
41-44 IZF FINAL POINT ALONG THE Z-DIRECTION.

45-52 EXXAG EXAGGERATION FACTOR (OUTPUT VALUES ARE MULTIPLIED BY EXXAG).

53-60 F000 NUMBER OF ELECTRONS IN THE UNIT CELL, NEEDED FOR FOURIER AND PATTERSON SYTHESES.
(CAN BE OMITTED DIFFERENCE FOURIER IS CALCULATED).

61-64 IWAHL SWITCH FOR READ OR CALCULATE MULTIPLICITIES.

CALC CALCULATE THE MULTIPLICITIES
NOT CALC READ MULTIPLICITIES FROM THE FOLLOWING MULTIPLICITY CARD

65-72 FMGNR MULTIPLICITY OF GENERAL REFLECTION

MULTIPLICITY CARD

(ONLY NECESSARY IF THE PARAMETER IWAHL ON THE CONTROL CARD IS NOT EQUAL CALC)

FORMAT (12F6.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES				
1- 6	FMULT	MULTIPLICITY OF	H00	OR	0K0	
7-12		MULTIPLICITY OF	00L			
13-18		MULTIPLICITY OF	HK			
19-24		MULTIPLICITY OF	H0L			
25-30		MULTIPLICITY OF	0KL			
31-36		MULTIPLICITY OF	HH			
37-42		MULTIPLICITY OF	H0H			
43-48		MULTIPLICITY OF	0KK			
49-54		MULTIPLICITY OF	HHH			
55-60		MULTIPLICITY OF	HHL			
61-66		MULTIPLICITY OF	HKK	OR	HKH	
67-72		MULTIPLICITY OF	HKL			

L I S T F C

CARD ORDER SUMMARY OF THE PROGRAMME LISTFC

LABEL	CARD
TITLE	CARD
CONTROL	CARD
* HKL	CARD(S)

* THESE CARDS ARE OPTIONAL

LABEL CARD

FORMAT (3A4,A3)

COLUMN	NAME	FUNCTION
1-12	LABEL	ANY SEQUENCE OF SYMBOLS USED AS PROGRAMME TITLE
13-15	INPUT	BLANK INPUT IS VIA FOURIER-FILE HKL INPUT IS VIA STANDARD HKL-CARDS

TITLE CARD

FORMAT (10A4)

COLUMN	NAME	FUNCTION
1- 40	TITLE	ANY SEQUENCE OF SYMBOLS USED AS PROGRAM TITLE

CONTROL CARD

FORMAT (3Il,I4,Al,I3,5(1X,Il),3(1X,Al),9(lX,Il).2X.
2(1X,Il),2F8.0)

COLUMN	NAME	FUNCTION
1	ISORH	(1)/(2)/(3) FOR H INDEX VARIES (MOST)/(NEXT MOST)/(LEAST) RAPIDLY (CODE TO TELL HOW INPUT DATA ARE SORTED)
2	ISORK	SORTING FREQUENCY FOR K INDEX
3	ISORL	SORTING FREQUENCY FOR L INDEX
4- 7	LINE	NUMBER OF LINES PER *LISTFC* PAGE
8	IAPAGE	(BLANK)/(A) FOR (DO)/(ABSOLUTELY DO NOT) INTERNALLY CHANGE THE VALUE OF THE NUMBER OF LINES IN ORDER TO MAKE THE BOTTOM OF THE LAST PAGE AS EVEN AS POSSIBLE
9-11	ICOLPP	NUMBER OF LIST COLUMNS PER *LISTFC* PAGE **N O T E** THE PRODUCT OF THE NUMBER OF LINES

AND THE NUMBER OF COLUMNS PER *LISTFC* PAGE CANNOT
EXCEED 3000. THAT IS, NO MORE THAN 3000 FOR THE TOTAL OF
REFLECTIONS AND HEADINGS (INCLUDING ALL SPACES), PER PAGE.

PREFATORY NOTICE PAY ATTENTION - ZERO (OR BLANK) IN ANY
OF THE NEXT FIVE FIELDS MEANS JUST THAT...

13	IBLNK	NUMBER OF BLANK PRINT COLUMNS BEFORE THE LISTFC COLUMN
15	IIN	NUMBER OF PRINT COLUMNS FOR THE MOST RAPIDLY CHANGING INDEX
17	IFOC	NUMBER OF PRINT COLUMNS FOR FO TIMES 10
19	IFCC	NUMBER OF PRINT COLUMNS FOR FC TIME5 10
21	IPHC	NUMBER OF PRINT COLUMNS FOR SIGFO TIMES 10
23	IFLLT	SPECIAL FLAG FOR LESS THANS (BLANK=*)
25	IFLEX	SPECIAL FLAG FOR EXTINCT REFLECTIONS (BLANK=E)
27	IFLSPC	SPECIAL FLAG FOR SPECIAL REFLECTIONS

PREFATORY NOTICE THE NEXT NINE FIELDS ARE (BLANK)/(l) FOR {DO NOT)/(DO)

29	ISIGNO	PRINT SYMBOLS FOR LESS THAN OR EXTINCT REFLECTIONS THIS SYMBOL SWITCH ADDS ONE MORE PRINT COLUMN
31	ISIGNC	FOR CENTRIC STRUCTURES ATTACH SIGN OF A TO FC
33	ISPACE	DOUBLE SPACE THE LINES
35	IRESTO	RESTORE EACH *LISTFC* PAGE TO BE THE TOP OF A PRINTER PAGE
37	ITIT	PRINT CURRENT TITLE AT TOP OF EACH PRINTER PAGE
39	IPNCH	PUNCH A SET OF =FCARD= (HAS H,K,L,FO,FC,A,B,JCODE, AND LEVEL INDICATORS) PUNCH UNIT AT PRESENT
41	NOT USED	
43	ISIGS	PRINT MINUS SIGN ON THE FO OF THE REFLECTIONS WHICH ARE LESS THANS
45	ITWOT	WRITE A SEPERATE COPY OF THE FC LIST ON UNIT
49	ITRY	NUMBER OF TIMES TO TRY TO GET HEADINGS AT THE TOP

CARD ORDER SUMMARY OF THE PROGRAMME PDFMAP

	TITLE	CARD
	CONTROL	CARD
	OUTPUT	CARD
*	SPECIAL PLANE	CARDS
	ATOM SELECTION	CARD

* THESE CARDS ARE OPTIONAL

TITLE CARD

FORMAT (17A4)

COLUMN	NAME	FUNCTION
1-68	TITEL	ANY SEQUENCE OF SYMBOLS USED AS PROGRAMME TITLE

CONTROL CARD

FORMAT (5I1,1X,6I1,10I5,F6.3,I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	IPDFF	SELECTION FLAGS FOR ORDERS OF THERMAL PARAMETERS TO BE INCLUDED IN THE PDF- OR POTENTIAL-CALCULATION. 0 DO NOT INCLUDE THIS ORDER 1 INCLUDE THIS ORDER
1		SECOND ORDER OF THERMAL PARAMETERS.
2		THIRD ORDER
3		FOURTH ORDER
4		FIFTH ORDER
5		SIXTH ORDER
7	IPDF	SELECTION FLAG FOR CALCULATE A NORMAL OR AN EXTENDED EDGEWORTH MAP. (EXTENDED MAP IS ONLY MEANINGFUL FOR THE EDGEWORTH EXPANSION). 0 CALCULATE A NORMAL MAP. 1 CALCULATE AN EXTENDED MAP.
8	ISECT	SELECTION FLAG FOR DIFFERENT ORIENTATIONS OF THE SECTION(S) TO BE CALCULATED.

	ACROSS THE PAGE	DOWN THE PAGE	SECTION(S)	UP OR DOWN (SEE BELOW)
0	X	Y	Z	DOWN
1	X	Z	Y	UP
2	Y	X	Z	UP
3	Y	Z	X	DOWN
4	Z	Y	X	UP
5	Z	X	Y	DOWN

UP = THE SECTION COORDINATE INCREASES WITH INCREASING SECTION NUMBER
DOWN THE SECTION COORDINATE DECREASES WITH INCREASING SECTION NUMBER.
(THIS MEANS THE SYSTEM IS ALWAYS RIGHT HANDED).

9	IPLT	SWITCH FOR SAVE THE CALCULATED MAP FOR LATER PLOTTING (PROGRAM PLOTTE). 0 DO NOT SAVE THE MAP 1 SAVE THE MAP NB: THE VAX-VMS VERSION WILL CREATE SEVERAL FILES FOR LATER PLOTTING: XXXX_PD.S2 CONTAINS THE PDF XXXX_PD.S4 CONTAINS THE ERROR-PDF XXXX_PD.S6 CONTAINS THE SIGNIFICANCE-MAP
10	LSPC	SWITCH FOR SINGLE- OR DOUBLE SPACED PRINTED OUPUT. 0 DOUBLE SPACED LINES. 1 SINGLE SPACED LINES.

11	NPNT	SWITCH FOR PRINT THE CALCULATED POINT ARRAY. 0 PRINT THE POINT ARRAY. 1 DO NOT PRINT THE POINT ARRAY.
12	IOR	SWITCH FOR DIFFERENT POSTIONS OF THE ATOM FOR WHICH THE PDFMAP IS CALCULATED WITHIN THE SECTION. 0 ATOM POSITION AT THE GRID COORDINATES 0,0,0 . 1 ORIGIN OF THE CELL AT THE GRID COORDINATES 0,0,0 .
13-17	IX	NUMBER OF DIVISIONS ALONG THE X-AXIS.
18-22	IXI	INITIAL POINT ALONG THE X-DIRECTION.
23-27	IXF	FINAL POINT ALONG THE X-DIRECTION.
28-32	IY	NUMBER OF DIVISIONS ALONG THE Y-AXIS.
33-37	IYI	INITIAL POINT ALONG THE Y-DIRECTION.
38-42	IYF	FINAL POINT ALONG THE Y-DIRECTION.
43-47	IZ	NUMBER OF DIVISIONS ALONG THE Z-AXIS. (IF IZ=0 THE SPECIAL PLANE CARDS WILL BE READ AND THE PDF (OR POTENTIAL) WILL BE CALCULATED ONLY IN THE PLANE DEFINED BY THESE CARDS).
48-52	IZI	INITIAL POINT ALONG THE Z-DIRECTION.
53-57	IZF	FINAL POINT ALONG THE Z-DIRECTION.
58-62	MC	NUMBER OF MONTE-CARLO LOOPS FOR ERROR CALCULATION (IF MC = 0 NO ERRORS WILL BE CALCULATED; IF MC > 0 ONLY ONE PLANE OR ONE SECTION MAY BE CALCULATED) A SAVE NUMBER FOR MC USUALLY IS 1000.
63-66	SIFA	SIGNIFICANCE LIMIT FOR MONTE-CARLO SIGNIFICANCE MAPS (SEE EQ.A6 IN W.F.KUHS ACTA CRYST.A (1992).
67-69	ISQ	0 MEAN SQUARE DEVIATIONS ARE CALCULATED (DEFAULT) 1 POSITIVE AND NEGATIVE DEVIATIONS ARE CALCULATED SEPARATELY

OUTPUT CARD

FORMAT (F9.0,3I5,I2,1X,I2,I5,F8.0,A1,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES.
1- 9	EXXAG	EXAGGERATION FACTOR (OUTPUT VALUES ARE MULTIPLIED BY EXXAG).
10-14	IMINI	IN THE PRINTED OUTPUT ALL VALUES BEWTEEN IMINI AND
15-19	IMAXI	IMAXI ARE SUPPRESSED.
20-24	ISELEC	SHEER ANGLE OF THE PRINTED POINT ARRAY. 0 APPROXIMATION OF THE REAL CRYSTAL ANGLE. NOT 0 ISELEC IS THE VALUE OF THE ANGLE IN DEGREES TO BE APROXIMATED.
25-26	IPLU	LOGICAL UNIT NUMBER OF THE PLOT-FILE TO BE WRITTEN (DEFAULT VALUE 11).
28-29	MAIN	LOGICAL UNIT NUMBER OF THE MAIN-FILE TO BE READ (DEFAULT VALUE 10).
30-34	ICCH	SELECTION FLAG FOR TREATEMENT OF THE MIXED PRODUCT OF THE THIRD ORDER TENSOR IN THE EDGEWORTH EXPANSION. (ONLY NEEDED IF THE EDGEWOTH EXPANSION IS SELECTED). 0 INCLUDE THE TERM C(I,J,K) * C(P,Q,R) * H(I,J,K,P,Q,R) (EINSTEIN SUMMATION CONVENTION USED). 1 DO NOT INCLUDE THIS TERM. 2 DO ONLY INCLUDE THIS TERM.

35-42 T TEMPERATURE AT WHICH THE DATA HAVE BEEN MEASURED.

0. CALCULATE THE PROBABILITY DENSITY FUNCTION (PDF).
NOT 0. INSTEAD OF THE PDF THE POTENTIAL WILL BE CALCULATED. THE NORMALISATION IS DONE BY USING THE MAXIMUM VALUE OF THE PDF OF THE FIRST CALCULATED SECTION IF THERE IS NOT GIVEN A VALUE FOR PNORM (PNORM SEE BELOW).

43 KELVIN UNIT OF THE TEMPERATURE T (ONLY NEEDED IF T IS NOT 0.)

K TEMPERATURE IS GIVEN IN KELVIN .
NOT K TEMPERATURE IS GIVEN IN CELSIUS.
(0. CELSIUS MUST BE GIVEN AS 273.16 K BECAUSE FOR T = 0. THE PDF WOULD BE CALCULATED).

44-51 PNORM VALUE OF THE PROBABILITY DENSITY FUNCTION (PDF) TO BE USED FOR THE NORMALISATION OF THE POTENTIAL (ONLY NEEDED IF T IS NOT 0.)

0. THE MAXIMUM VALUE OF THE FIRST CALCULATED SECTION OF THE PDF WILL BE USED FOR NORMALISATION.
NOT 0. PNORM WILL BE USED FOR NORMALISATION.

SPECIAL PLANE CARDS

(THESE CARDS ARE ONLY NECESSARY IF THE PARAMETER IZ ON THE CONTROL CARD IS ZERO).

FORMAT (A4,2X,3F8.0)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1- 6 MTYP SWITCH FOR DIFFERENT POSSIBILITIES OF DEFINITION OF A PLANE.

CENTER THE POINT GIVEN ON THIS CARD SHOULD BE THE CENTER OF THE PLANE CALCULATED.

CORNER THE POINT GIVEN ON THIS CARD SHOULD LAY ON AN EDGE OF THE PLANE.

7-14 E(1) X-COORDINATE OF THE POINT IN FRACTIONAL COORDINATES
15-22 E(2) Y-COORDINATE OF THE POINT IN FRACTIONAL COORDINATES
23-30 E(3) Z-COORDINATE OF THE POINT IN FRACTIONAL COORDINATES

THERE MUST BE EXACTY THREE SUCH CARDS .
(ONLY ONE OF THE POINTS CAN BE THE CENTER OF THE PLANE).

REMARK
THE FOLLOWING PARAMETERS ARE MEANINGLESS WHEN SPECIAL PLANE CARDS ARE GIVEN

ON THE CONTROL CARD ISECT,IOR,IZI, AND IZF.
ON THE OUTPUT CARD ISELEC.

ATOM SELECTION CARD

FORMAT (60I1)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1 IPLOT SWITCH FOR CALCUATION OF THE PDF (OR POTENTIAL) FOR THE FIRST ATOM

0 DO NOT CALCULATE A PDF (RESP. POTENTIAL)

1 CALCULATE THE PDF (OR POTENTIAL) FOR THE FIRST ATOM.

2 SAME FOR THE SECOND ATOM
3 SAME FOR THE THIRD ATOM
4 AND SO ON .

REMARK
THERE CAN BE MORE THAN ONE PARAMETER SET TO 1 .

P L O T T E

CARD ORDER SUMMARY OF THE PROGRAMME PLOTTE

INPUT-OUTPUT	CARD
TITLE	CARD
LAYOUT	CARD
CONTOUR-LINE	CARD(S)
* LINE DRAWING	CARD(S)
* CROSS	CARD(S)
* PDFMAP	CARD
SECTION	CARD(S)
* LABEL	CARD(S)
* CROSS CONTINUE	CARD(S)

* THESE CARDS ARE OPTIONAL

INPUT-OUTPUT CARD

FORMAT (A4,2X,4I2)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1- 4 IWAEHL INDICATOR FOR THE PROGRAMME WHICH HAS WRITTEN THE DATA FILE TO BE READ (FILE GENERATING PROGRAMME).

FOUR
PDFM
ARBS

5- 6 INRFIL LOGICAL NUMBER OF THE INPUT FILE.

0 DEPENDING ON THE VALUE OF IWAEHL THE FOLLOWING DEFAULT VALUES ARE USED.

IWAEHL	DEFAULT VALUE
FOURIE	11
ARBSEC	12

*** Note for PDFMAP_Files : no default value
take 31 for density

33 for Errmaps
35 for Signif.-maps

NOT 0 INRFIL IS THE LOGICAL NUMBER OF THE INPUT FILE.

9-10	IFRAC	INDICATOR FOR THE COORDINATES USED ON THE LINE DRAWING CARD(S), THE CROSS CARD(S), AND THE LINE LABEL CARD(S). 0 COORDINATES ARE GIVEN IN GRID COORDINATES. (ACCORDING TO THE GRID SELECTION IN THE FILE GENERATING PROGRAMME). 1 COORDINATES ARE GIVEN IN FRACTIONAL COORDINATES OF THE UNIT CELL, IF SECTIONS PARALLEL TO THE AXES ARE PLOTTED.
11-12	NRCROS	SWITCH FOR DIFFERENT POSSIBILITIES OF DRAWING CROSSES ON THE PLOTS. POS. FOR EACH PLOT NEW COORINATES FOR THE CROSSES TO BE DRAWN WILL BE READ FROM A CROSS (CONTINUE) CARD. 0 CROSSES WILL ONLY BE DRAWN ON THE FIRST PLOT AT THE POINTS GIVEN ON THE CROSS CARD. NEG. CROSSES WILL BE DRAWN ON THE NEXT NRCROS PLOTS AT THE POINTS GIVEN ON THE CROSS CARD.

TITLE CARD

FORMAT (8A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-32	ITITLE	ANY SEQUENCE OF SYMBOLS TO BE PRINTED AS A TITLE ON THE PLOT(S).

*** note for POSTSCRIPT following Charaters difficult to use
"(" , ")" , "\" , "Angstroem"
*** look at the POSTSCRIPT-Manual

LAYOUT CARD

FORMAT (F5.0,I5,3F5.0,4I5,F5.0,I5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	TLEHGT	HEIGHT OF THE LETTERS OF THE TITLE TO BE WRITTEN ON THE PLOT(S). NEG. NO TITLE WILL BE WRITTEN ON THE PLOT(S). 0 THE DEFAULT VALUE OF 1. CM IS USED. POS. TLEHGT IS THE HEIGHT OF THE LETTERS IN CM.

REMARK
IF THE TITLE GIVEN ON THE TITLE CARD WOULD BECOME LONGER THAN THE PAPER USING THE SELECTED DIMENSION OF THE LETTERS THIS DIMENSION IS NOT DECREASED AUTOMATICALLY.

6- 10	NLABL	NUMBER OF LABEL CARDS TO BE READ.
11-15 16-20	A B	THESE TWO VARIABLES ARE USED TO DETERMINE THE DIMENSION OF THE PLOT(S). (DEFINITION OF WIDTH AND LENGTH SEE PICTURE BELOW). A=0, B=0. FOR THE FIRST PLOT A SCALE FACTOR IS DETERMINED TO MAKE A = 16. CM . THE SAME FACTOR IS USED FOR B. FOR THE FOLLOWING PLOTS THE SCALE OF THE FIRST PLOT WILL BE USED PROVIDED THAT A IS LESS THAN 16. CM.

IF A WOULD BECOME GREATER THAN 16 CM A NEW SCALE FACTOR IS DETERMINED USING THE SAME PROCEDURE AS FOR THE FIRST PLOT.

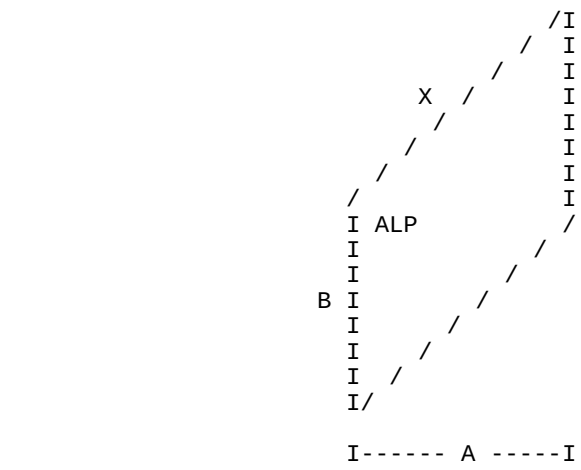
A LESS THAN -1 , B ARBITRARY BUT NOT 0 OR
A ARBITRARY BUT NOT 0 , B LESS THAN -1.
A NEW SCALE FACTOR WILL BE CALCULATED USING THE SAME PROCEDURE AS FOR THE FIRST PLOT IN THE CASE A=0, B=0 . (USEFUL FOR CHANGING THE SCALE IF THE CURRENT LAYOUT CARD IS NOT FOR THE FIRST PLOT).

A=0, B LESS THAN 0.
S = ABS(B) WILL BE USED AS SCALE FACTOR.
(ABS(B) IS THE SCALE OF THE PLOT IN CM/ANGSTROMS).

A GREATER THAN 0, B = 0 OR
A = 0 , B GREATER THAN 0.
A OR B WILL BE TAKEN AS THE WIDTH OR THE LENGTH OF THE PLOT IN CM RESPECTIVELY AND THE OTHER AXIS WILL BE PLOTTED IN THE SAME SCALE.

REMARK
WHENEVER THE INPUT LEADS TO A WIDTH (A) GREATER THAN 16. CM THE PLOT WILL BE SCALED TO A = 16. CM.

21-25 ALP ANGLE BETWEEN THE AXES DEFINED IN THE FOLLOWING PICTURE.



EXPLANATION OF THE SYMBOLS

X AXIS WHICH WAS PRINTED ACROSS THE PAGE IN THE POINT ARRAY OF THE FILE GENERATING PROGRAMME.
B LENGTH OF THE AXIS PLOTTED IN VERTICAL DIRECTION.(IN THIS DESCRIPTION ONLY CALLED LENGTH OF THE PLOT).
A WIDTH OF THE PLOT.
ALP ANGLE BETWEEN B AND X .

IF ALP IS 0 THE REAL ANGLE BETWEEN B AND X WILL BE PLOTTED.

26-30 NP NUMBER OF INTERPOLATION POINTS PER SPLINE.
(IF NP IS LESS THAN 6 THE DEFAULT VALUE NP=6 IS USED)

31-35 NCONT NUMBER OF CONTOUR-LINE CARDS TO BE READ.
(THE POSSIBLE MAXIMUM VALUE OF NCONT IS 10)

36-40 NLINE NUMBER OF LINE DRAWING CARDS TO BE READ AND SWITCH

FOR MAKE A FRAME AROUND THE PLOT.

0 MAKE A FRAME
POS. AROUND THE PLOT.

NEG. MAKE NO FRAME.

IABS(NLINE) IS THE NUMBER OF LINE DRAWING CARDS TO BE READ. (THE POSSIBLE MAXIMUM VALUE OF NLINE IS 20)

41-45 NCROSS NUMBER OF CROSS CARDS TO BE READ. (SEE ALSO THE PARAMETER NRCROS ON THE INPUT-OUTPUT CARD). (THE POSSIBLE MAXIMUM VALUE OF NCROSS IS 20).

46-50 SCROSS DIMENSION OF THE CROSSES.

0 THE DEFAULT VALUE 0.75 CM IS USED.
NOT 0 SCROSS IS THE DIMENSION IN CM.

51-55 NSECT NUMBER OF SECTION CARDS TO BE READ (THE POSSIBLE MAXIMUM VALUE OF NSECT IS 10).

CONTOUR-LINE CARD(S)

(THIS CARD MUST APPEAR NCONT TIMES (SEE LAYOUT CARD)).

FORMAT (3F5.0,I5)

COLUMN	NAME	FUNCTION
1- 5	SBEG	HEIGHT OF THE INITIAL CONTOUR-LINE (OF THE GROUPE OF OF LINES DEFINED ON THIS CARD).
6-10	CSTEP	STEP BETWEEN THE CONTOUR-LINES (DEF. ON THIS CARD).
11-15	SLIM	HEIGHT OF THE FINAL CONTOUR LINE (OF THE GROUP OF LINES DEFINED ON THIS CARD).
16-20	NSIG	NUMBER OF DIGITS AFTER DECIMAL POINT USED FOR WRITING THE HEIGHT AT EACH CONTOUR LINE.

NEG. DO NOT WRITE THE HEIGHTS ON THE PLOT.
0 ONLY INTEGER VALUES
POS. WRITE THE HEIGHTS WITH NSIG DIGITS.

LINE DRAWING CARD(S)

(THIS CARD MUST APPEAR ABS(NLINE) TIMES (SEE LAYOUT CARD)).

FORMAT (2F5.0)

COLUMN	NAME	FUNCTION AND POSSSIBLE VALUES
1- 5	XLINE	COORDINATES OF A POINT. LINES ARE DRAWN FROM THE POINT
6-10	YLINE	GIVEN IN THE LAST LINE DRAWING CARD TO THIS ONE (IF THIS IS NOT THE FIRST CARD) AND FROM THIS POINT TO THE ONE GIVEN IN THE NEXT LINE DRAWING CARD (IF THIS WAS NOT THE LAST CARD)

CROSS CARD(S)

(THIS CARD MUST APPEAR NCROSS TIMES (SEE LAYOUT CARD)).

FORMAT (2F5.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	BX	COORDINATES OF THE POINT, WHERE A CROSS SHOULD BE
6-10	BY	PLOTTED. (THE SECTION(S) ON WHICH A CROSS WILL BE DRAWN IS

DEFINED BY THE PARAMETER NRCROS ON THE INPUT-OUTPUT CARD. THE COORDINATES MUST BE GIVEN IN THE SYSTEM

DEFINED BY THE PARAMETER IFRAC ON THE SAME CARD)

SECTION CARD(S)

(THIS CARD MUST APPEAR NSECT TIMES (SEE LAYOUT CARD)).

FORMAT (3I5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	INITZ	FOR THE SECTIONS FROM SECTION NUMBER INITZ TO THE
6-10	ISTEPZ	SECTION NUMBER IFINZ IN STEPS OF ISTEPZ CONTOUR
11-15	IFINZ	MAPS WILL BE PLOTTED. (THE SECTIONS WERE NUMBERED BY THE FILE GENERATING PROGRAMME).

LABEL CARD(S)

(THIS CARD MUST APPEAR NLABL TIMES (SEE LAYOUT CARD)).

FORMAT (5F5.0,A6)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	WX	COORDINTES OF THE POINT WHICH SHOULD BE MARKED BY
6-10	WY	THE LABEL LABL GIVEN ON THIS CARD. (WX AND WY MUST BE GIVEN IN GRID COORDINATES. WX IS TAKEN ALONG THE X-AXIS AND WY ALONG THE B-AXIS DESCRIBED IN THE PICTURE UNDER THE LAYOUT CARD).
11-15	DX	PLOTTER OFFSET FROM THE POINT DEFINED BY WX AND WY
16-20	DY	FOR STARRING THE LABEL. (DX AND DY MUST BE GIVEN IN CM. DX IS TAKEN ALONG THE X-AXIS AND DY ALONG THE B-AXIS DESCRIBED IN THE PICTURE UNDER THE LAYOUT CARD). (IF DX=0. AND DY=0. THE DEFAULT VALUES DX=0.5 CM AND DY=0. CM ARE USEC).
21-25	HGT	HEIGHT OF THE SYMBOLS OF THE LABEL TO BE PLOTTED. (IF HGT=0. THE DEFAULT VALUE HGT=0.75 CM IS USED).
26-31	LABL	ANY SEQENCE OF SYMBOLS TO BE PLOTTED AT THE POINT AND IN THE DIMENSION DEFINED ON THIS CARD.

CROSS CONTINUE CARD(S)

(THIS CARD IS ONLY NECESSARY IF THE PARAMETER NRCROS ON THE INPUT-OUTPUT CARD IS POSITIV, BUT THEN IT MUST APPEAR (NRCROS * NCROSS) TIMES (NCROSS SEE LAYOUT CARD)).

THIS CARD HAS EXACTLY THE SAME FORM AS THE CROSS CARD.

P O T C A L

CARD ORDER SUMMARY OF THE PROGRAM POTCAL

TITLE	CARD
CONTROL	CARD
DATA	CARD

DIRECTION CARD
ATOM SELECTION CARD

TITLE CARD

FORMAT (17A4)

COLUMN	NAME	FUNCTION
1-68	TITLE	ANY HOLLERITH TEXT AS PROGRAM TITLE

CONTROL CARD

FORMAT (10Il)

COLUMN	NAME		FUNCTION AND POSSIBLE VALUES
1	IDIR	0	DIRECTION GIVEN BY FRACTIONAL COORDINATES OF THE LAST POINT TO BE CALCULATED. CALCULATION IS REFERRED EITHER TO THE REFINED ATOM POSITION OR THE MAXIMUM IN PDF (S.VARIABLE ISRT)
		1	AS 0 BUT DIRECTION GIVEN BY A VECTOR (UVW).
		2	DIRECTION GIVEN BY A VECTOR (UVW). CALCULATION STARTS AT A GIVEN POINT (S.VARIABLE VE ON DIRECTION CARD).
2	ISRT	0	CALCULATION STARTS AT THE REFINED ATOM POSITION, AT THE MAXIMUM OF PDF OR AT A GIVEN POINT.
		1	CALCULATION STARTS AT A GIVEN POINT AND STOPS AT AN OTHER GIVEN POINT.
		2	CALCULATION STARTS IN THE OPPOSITE OF THE GIVEN DIRECTION, GOES THROUGH THE REFERENCE POINT AND STOPS AT THE GIVEN LAST POINT.
3	IRNM	0	NO SEARCH FOR LOCAL MAXIMA IN PDF
		1	(SEARCH FOR) + NO CALCULATION OF BONDS
		2	(LOCAL MAX-) + CALCULATION OF BOND DISTANCES
		3	(IMA IN PDF) + CALCUL. OF BONDS AND ANGLES
		4	AS 1 (ADDITIONAL REPLACE THE)
		5	AS 2 (REFINED ATOM POSITION)
		6	AS 3 (BY THE MAXIMUM IN PDF)
		7	READ MAXIMUM IN PDF AND NORMALIZE TO THIS VALUE (S. VARIABLE RNORM ON DATA CARD).
4	IPLT	0	NO PLOTTING OF THE CALCULATED POTENTIAL
		1	PLOT AND PRINT THE CALCULATED POTENTIAL
		2	ONLY PLOTTING OF THE CALCULATED POTENTIAL
5	IMOM	0	DO NOT CALCULATE MOMENTS AND CUMULANTS
		1	CALCULATE MOMENTS AND CUMULANTS NUMERICALLY ALONG A GIVEN DIRECTION (SEE DIRECTION CARD) OR ALONG THE SHIFT VECTOR IF DIRECTION IS NOT SPECIFIED (VA AND VE EQUAL TO ZERO).
6	IEXT	0	NORMAL EDGEWORTH-SERIES (AND GRAM-CHARLIER)
		1	EXTENDED EDGEWORTH-SERIES TO BE CALCULATED (PREREQUISITE IS THE PRESENCE OF THE HARMONIC DATA ON UNIT IHARMO).
7	IPRI	0	NO PRINT OF POINTS WITH ZERO OR NEGATIVE PDF
		1	PRINT ALL CALCULATED POINTS
		2	NO PRINT AT ALL
8	ISGL	0	SIGNIFICANCE LIMIT AUTOMATICALLY CALCULATED AT THE 1 P.C. POINT.
		1	SIGNIFICANCE LIMIT GIVEN BY THE USER (S. VARIABLE SIGLN ON DATA CARD).
9	IPLO	0	PLOTSCALES GIVEN BY THE USER, PLOTSIZE ACCORDINGLY (S. VARIABLES GRIDX AND GRIDY ON DATA CARD).
		1	PLOTSIZE GIVEN BY THE USER, PLOTSCALES ACCORDINGLY (S. VARIABLES GRIDX AND GRIDY ON DATA CARD).

10	IWHL	0	ENERGY IN THE PLOT IS GIVEN IN EV
		1	ENERGY IN THE PLOT IS GIVEN IN 10**-19 J.

DATA CARD

FORMAT (6F8.3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	TMPT	TEMPERATURE OF THE DIFFRACTION EXPERIMENT IN K
9-16	GRID	INTERVAL FOR PRINTED OUTPUT OF POTENTIAL IN AE (DEFAULT = 0.05 AE).
17-24	GRIDX	SCALE FOR DISPLACEMENT (X-AXIS) IN THE PLOT IN CM/AE (DEFAULT = 10.0 CM/AE) OR PLOTSIZE (X-AXIS) IN CM (DEFAULT = 10.0 CM).
25-32	GRIDY	SCALE FOR ENERGY (Y-AXIS) IN THE PLOT IN CM/EV OR CM/10**-19 J (DEFAULT = 50 CM/EV OR 50 CM/10**-19 J) OR PLOTSIZE (Y- AXIS) IN CM (DEFAULT = 10.0 CM).
33-40	SIGLN	SIGNIFICANCE LIMIT IN EV OR 10**-19 J (ACCORDING TO VARIABLE IWHL ON CONTROL CARD). ALL POINTS ABOVE THIS LIMIT WILL NOT BE PLOTTED.
41-48	RNORM	PDF AT THE MAXIMUM FOR NORMALIZATION OF THE POTENTIAL (TO SAVE THE TIME FOR REPEATED SEARCHING OF THE LOCAL MAXIMUM).

DIRECTION CARD

FORMAT (6F8.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES	
1- 8	VE(l)	(COORDINATES OF THE LAST)	FOR A-DIRECTION
9-16	VE(2)	(POINT TO BE CALCULATED)	FOR B-DIRECTION
17-24	VE(3)	(OR COMPONENT OF (UVW))	FOR C-DIRECTION
25-32	VA(l)	(COORDINATES OF THE FIRST)	FOR A-DIRECTION
33-40	VA(2)	(POINT TO BE CALCULATED)	FOR B-DIRECTION
41-48	VA(3)	(ONLY IF IDIR=2 OR ISRT=l)	FOR C-DIRECTION

ATOM SELECTION CARD

FORMAT (60I.l)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	ICALC	0 DO NOT CALCULATE POTENTIAL OF THIS ATOM
		1 CALCULATE POTENTIAL OF THIS ATOM
ETC		(SEQUENCE ACCORDING TO THE ORDER IN THE MAIN UNIT).

P R E D E S

CARD ORDER SUMMARY OF THE PROGRAMME PREDES

TITLE	CARD
TEXT	CARDS
END	CARD

NO CARD IS OPTIONAL

TITLE CARD

FORMAT (5Al,I3,lX,Al,lX,6Al)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 5	IT	THIS COLUMNS MUST CONTAIN THE WORD TITLE FOR RECOGNITION OF THIS CARD AS A TITLE CARD.
6- 8	NPAGE	STARTING NUMBER FOR NUMERATING THE PRINTED PAGES.
10	IPART	INDICATOR FOR THE PART OF THE SYSTEM DESCRIPTION TO WHICH THE PRINTED PAGES BELONG.
		BLANK GENERAL (ONLY THE SYMBOLS GIVEN IN COLUMN 12-17 FOR KENN ARE PRINTED IN THE PAGE HEADER.
		1 DESCRIPTION (DESCRIPTION OF THE FORMALISMS USED IN THE PROGRAMM. THE WORD DESCRIPTION IS INCLUDED IN THE PAGE HEADER).
		2 CARD ORDER (CARD ORDER SUMM (THE WORD CARD ORDER IS INCLUDED IN THE PAGE HEADER).
12-17	KENN	ANY SEQUENCE OF SYMBOLS TO BE PRINTED ON EACH PAGE AS A PAGE HEADER.

REMARK

ALTHOUGH THE TITLE CARD ALWAYS MUST BE THE FIRST CARD IT CAN BE REPEATED BETWEEN THE TEXT CARDS AS OFTEN AS THE PAGE HEADER MUST BE CHANGED.

TEXT CARDS

FORMAT (Al,71Al)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IT	THE SIGN IN THE FIRST COLUMN IS ALWAYS INTERPRETED AS A MONITORING SIGN AND NOT PRINTED IN THE OUTPUT.
		BLANK NORMAL PRINTING OF THE LINE (COLUMN 2 - 72).
		0 LIKE BLANK
		1 START A NEW PAGE WITH THIS LINE.
		+ PRINT THIS LINE ON THE SAME LINE AS THE ONE BEFORE. (NO LINEFEED)
		L LEAVE ONE BLANK LINE BEFORE PRINTING THIS LINE.
		R PRINT THIS LINE TWO TIMES WITHOUT LINEFEED. (IT THEN LOOKS DARKER THAN THE NORMAL TEXT).
		2 THE NEXT 4 LINES SHOULD NOT BE SEPARATED BY STARTING A NEW PAGE. IF THERE ARE LESS THAN 4 LINES LEFT ON THE CURRENT PAGE A NEW PAGE WILL BE STARTED WITH THIS LINE.
		3 SAME AS 2 FOR THE NEXT 6 LINES
		4 SAME AS 2 FOR THE NEXT 8 LINES AND SO ON
		9 SAME AS 2 FOR THE NEXT 18 LINES
		A SAME FOR 20 LINES
		B SAME FOR 22 LINES
		C SAME FOR 24 LINES
		D SAME FOR 26 LINES

END CARD

FORMAT (3Al)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	IT	IF IN THE FIRST THREE COLUMNS THE WORD END IS READ THIS MEANS THAT ALL THE TEXT CARDS ARE READ AND THE PRINTING IS NOW FINISHED.

CARD ORDER SUMMARY OF THE PROGRAMME REFINE

	LABEL	CARD
	CYCLE START	CARD
	MAIN CONTROL	CARD
*	CELL	CARD
*	BOND LIMITS	CARD
*	CELL TYPE	CARD
*	SYMMETRY	CARD(S)
*	SCAT.CURVE TYPE	CARD
*	EXPONENT. FORM	CARD
*	TABULATION FORM	CARDS
*	ANOMALOUS DISP.	CARD
*	SCALE FACTOR	CARD
*	EXTINCTION	CARD
*	ATOM SELECTION	CARD
*	ATOM PARAMETER	CARD(S)
*	SPECIAL PARAM.	CARD
*	SPECIAL VALUE	CARD(S)
*	ALPHA PARAMETER	CARD(S)
*	T-FACTOR TYPE	CARD
*	SCALE REFINE	CARD
*	EXTINC. REFINE	CARD
*	ALPHA REFINE	CARD
*	SPECIAL REFINE	CARD
*	ATOM REFINE	CARD(S)
*	NEW VALUE	CARD(S)
*	DEPENDENCY	CARD(S)
*	DIFFRACTOMETER	CARD
*	ORIENTATION	CARDS
*	FORMAT	CARD
*	DATA DEFINING	CARD

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* MEASUREMENT     CARD
* MONOCHROMATOR   CARD
* PARTIAL         CARDS
* HKL             CARDS
  CONTINUE        CARD

*   THESE CARDS ARE OPTIONAL
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LABEL CARD

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FORMAT (3A4,2X,I2)

COLUMN NAME    FUNCTION AND POSSIBLE VALUES

 1-12  LABEL   ANY SEQUENCE OF SYMBOLS TO BE USED AS LABEL OF THE
               PRINTED OUTPUT AND THE BINARY DATA FILE FOR ALL RUNS
               OF THE PROGRAMME REFINE AND ALL FOLLOWING RUNS OF
               PROGRAMMES READING A BINARY DATA FILE (FOURIE, PDFMAP,
               ETC.).
               (IF THE CURRENT CYCLE IS NOT AN -A PRIORI- CYCLE THE
                LABEL READ FROM THE -MAINFILE- FILE OVERWRITES THE
                LABEL GIVEN HERE).

15-16  ICFILE  LOGICAL NUMBER OF THE -MAINFILE- FROM WHICH RESULTS OF
               EARLIER RUNS HAVE TO BE READ IF THIS IS A -CONTINUE-
               CYCLE.

               0      THE DEFAULT VALUE 10 IS USED.
               NOT 0  ICFILE IS THE LOGICAL NUMBER OF THE MAINFILE.
```

CYCLE START CARD

```
FORMAT (18A4)

COLUMN NAME    FUNCTION AND POSSIBLE VALUES

 1-72  TITLE   ANY SEQUENCE OF SYMBOLS TO BE USED AS TITLE OF THE
               CURRENT CYCLE. IF OTHER PROGRAMMES WILL USE THE
               RESULTS OF THIS CYCLE, THIS TITLE IS USED AS A LABEL.
```

MAIN CONTROL CARD

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FORMAT (A1,3I1,1X,5I1,1X,8I1,3F8.0,1X,I1,1X,3I1,1X,I1)

COLUMN NAME    FUNCTION AND POSSIBLE VALUES

    1  IEEF    SWITCH FOR PRINTED OUTPUT

               P      PRINT THE OUTPUT ON THE STANDARD OUTPUT UNIT.
               T      PRINT ALL INFORMATIONS ONLY ON A TEMPORARY-
                      FILE (LOGICAL NUMBER 15 ).

    2  MFSEL   STRUCTURE FACTOR EQUATION SELECTOR.

               0      ONLY STRUCTURE FACTOR AND R-VALUE CALCULATION
                      FOR STRUCTURE FACTOR EQUATION (SF-EQ.) NO. 1 .
```

1 LEAST-SQUARES REFINEMENT FOR SF-EQ. NO. 1 .

2 SAME FOR
3 SF-EQ. NO. 2

4 SAME FOR
5 SF-EQ. NO. 3

6 SAME FOR
7 SF-EQ. NO. 4

THE STRUCTURE FACTOR EQUATIONS ARE

NO. 1 FOURIERTRANSFORM OF THE EDGEWORTH EXPANSION.
NO. 2 FOURIERTRANSFORM OF THE GRAM-CHARLIER EXPANSION.
NO. 3 MODIFIED EDGEWORTH EXPANSION.
NO. 4 ALPHA FORMALISM (MODIFIED GRAM-CHARLIER EXPANSION).

REMARK
A CHANGE OF THE STRUCTURE FACTOR EQUATION USED DURING THE REFINEMENT IS ONLY POSSIBLE BY SETTING IOVER (SEE BELOW) NOT EQUAL 0 . THEREFORE IN -CONTINUE- CYCLES USING THE SAME SF-EQ. YOU MUST ONLY CHOSE BETWEEN MFSEL=0 FOR STRUCTURE FACTOR CALCULATION AND MFSEL=1 FOR REFINEMENT.

3 MREF SWITCH FOR DIFFERENT REFINEMENT TYPES.

0 DO NOT CHANGE THE CURRENT REFINEMENT TYPE.
(IN AN -A PRIORI- CYCLE 0 IS OVERWRITTEN BY 1).
1 REFINE R(W) (WEIGHTED R-VALUE) ON F.
(F = STRUCTURE FACTOR)
2 REFINE R(U) (WEIGHTED R-VALUE BUT USING UNIT WEIGHTS) ON F.
3 REFINE R(W) ON F**2.
4 REFINE R(U) ON F**2.

4 IREJ SWITCH FOR DIFFERENT REJECT POSSIBILITIES.

0 DO NOT CHANGE THE FORMALISM USED FOR REJECTING REFLECTIONS.
(IN AN -A PRIORI- RUN IREJ=0 IS INTERPRETED TO BE 1).
1 INCLUDE ALL REFLECTIONS.
2 REJECT REFLECTIONS MARKED ON THE HKL-CARDS AS LESS THAN.
IF DELMAX (THIS CARD COL.36-43) IS NOT EQUAL 0, ALL REFLECTIONS WITH A RATIO I/SIGMA(I) (OR F/SIGMA(F)) SMALLER THAN DELMAX WILL BE REJECTED.
3 REJECT ALL REFLECTIONS MARKED AS LESS THAN AND IN ADDITION ALL REFLECTIONS WITH

ABS(F(OBS)-F(CALC)) GREATER THAN (DELMAX*SIGMA)

EXPLANATION
F(OBS) = OBSERVED STRUCTURE FACTOR.
F(CALC) = CALCULATED STRUCTURE FACTOR.
DELMAX = FACTOR WHICH CAN BE GIVEN ON THIS CARD (SEE BELOW).
IF THIS IS NOT AN -A PRIORI- CYCLE AND IF IN THIS CYCLE A FOURIER FILE HAS BEEN CREATED, DELMAX IS COMPUTED TO BE 9 TIMES THE VALUE FOR WHICH EXACTLY HALF OF THE REFLECTIONS WOULD BE REJECTED.
SIGMA = STANDARD DEVIATION OF F(OBS) IF THE THE PARAMETER IWT ON THE DATA DEFINING CARD IS NOT EQUAL 2 .
(FOR IWT = 2 SIGMA IS CALCULATED FROM THE WEIGHTS).
REMARK
WHEN REFINING ON F**2, NEVERTHELESS THE FUNCTION ABOVE IS CALCULATED USING F AND THE

STANDARD DEVIATION OF F.

4 LIKE 3 BUT NO SPECIAL CONDITION FOR LESS THAN REFLECTIONS.

5 LIKE 3 BUT NO SPECIAL COMPUTATION OF DELMAX . (DELMAX MUST BE GIVEN ON THIS CARD).

6 LIKE 4 BUT NO SPECIAL COMPUTATION OF DELMAX . (DELMAX MUST BE GIVEN ON THIS CARD).

7 REJECT ALL REFLECTIONS MARKED AS LESS THAN AND IN ADDITION THOSE LAYING OUTSIDE THE INTERVAL OF SIN(THETA)/LAMBDA DEFINED BY THE PARAMETERS UNTEN AND OBEN (SEE BELOW).

8 REJECT ALL REFLECTIONS MARKED AS LESS THAN BUT THOSE FOR WITH F(CALC) LESS THAN F(OBS) .

9 LIKE 8 BUT IN ADDITION REJECT ALL REFLECTIONS LAYING OUTSIDE THE INTERVALL OF SIN(THETA)/LAMBDA DEFINED BY THE PARAMETERS UNTEN AND OBEN (SEE BELOW).

(COLUMN 5 IS EMPTY)

6 MSF STRUCTURE FACTOR OUPUT SELECTOR.

0 NO STRUCTUR FACTOR OUTPUT.

1 PRINTED LIST OF STRUCTURE FACTORS CONTAINING THE FOLLOWING INFORMATION

H,K,L = MILLER INDICES
F(OBS) = OBSERVED STRUCTURE FACTOR (REFLECTIONS MARKED AS LESS THAN SQUAREROOT(Y * (A*A + B*B)) ON THE INPUT CARDS ARE MARKED HERE WITH LT PRINTED BEHIND F(OBS)
F(CALC) = CALCULATED STRUCTURE FACTOR
A(CALC) = REAL PART OF F(CALC)
B(CALC) = IMAGINARY PART OF F(CALC)
DELTA F = F(OBS) - F(CALC)
DELT/WEIGHT = (DELTA F) / WEIGHT
EXT. FACTOR = EXTINCTION FACTOR Y DEFINED BY F(CALC) =
SINT/LAM = SIN(THETA) / LAMBDA (REJECTED REFLECTIONS ARE MARKED BY RJ PRINTED BEHIND SINT/LAM).

2 STRUCTURE FACTORS PRINTED ON OUTPUT AND WRITTEN ON THE FOURIER FILE . THIS FILE IS THE DATA FILE FOR THE PROGRAMMES FOURIE, ERRMAP, LISTFC, OR AVERAG.

3 STRUCTURE FACTORS WRITTEN ON FOURIER FILE ONLY.

4/5 LIKE 1/2 BUT SHORT STRUCTURE FACTOR LIST.

7 MCORR CORRELATION MATRIX OUTPUT SELECTOR

0 CORRELATION MATRIX NOT PRINTED. (THE VALUES OF THE 20 LARGEST OFF-DIAGONAL CORRELATION COEFFICIENTS ARE PRINTED FOR EVERY LEAST-SQUARES CYCLE).

1 ENTIRE CORRELATION MATRIX PRINTED.

2/3 LIKE 0/1 BUT ALSO OUTPUT TO A LEVERAGE FILE.

ATTENTION

The leveredge file is only created if this cycle is a refinement cycle or a calc. of structure factors.

8 MBODAN BOND DISTANCES AND ANGLES SELECTOR.

0 NO DISTANCES AND ANGLES COMPUTED.
1 ONLY DISTANCES BETWEEN DMIN AND DMAX COMPUTED. (DMIN AND DMAX SEE BOND LIMITS CARD).
2 DISTANCES BETWEEN DMIN AND DMAX AND CORRESPONDING ANGLES COMPUTED. (DMIN AND DMAX SEE BOND LIMITS CARD).

REMARKS
THE PROGRAMME REFINE CALCULATES DISTANCES AND ANGLES WITHOUT STANDARD DEVIATIONS. FOR CALCULATION WITH STANDARD DEVIATIONS CALL PROGRAMME BONVIB .
THE BOND LIMITS (DMIN,DMAX) MAY NOT BE READ IN THE CURRENT CYCLE IF DONE BEFORE (THEY MUST BE READ IN AN -A PRIORI- CYCLE INDEPENDENT FROM THE VALUE GIVEN FOR MBODAN).

9 MELVIB SELECTOR FOR COMPUTATION OF ELLIPSOIDS OF VIBRATION.

0 NO ELLIPSOIDS COMPUTED.
1 THERMAL ELLIPSOIDS COMPUTED FOR ATOMS WITH AT LEAST ANISOTROPIC TEMPERATURE FACTORS. (ONLY IN THE CASE OF HARMONIC REFINEMENT THE THERMAL ELLIPSOIDS REPRESENT THE MEAN SQUARE DISPLACEMENTS OF THE ATOMS ALONG THE PRINCIPAL AXES. WHEN REFINING ANHARMONIC TEMPERATURE FACTORS THE ELLIPSOIDS COULD BE CALCULATED AS A TEST FOR THE POSITIVITY OF THE SECOND ORDER TENSOR. THIS POSITIVITY IS A PREREQUISITE FOR THE EXISTENCE OF THE PROBABILITY DENSITY FUNCTION)
2 LIKE 1 AND IN ADDITION THERMAL CORRECTIONS OF THE BOND LENGTHS COMPUTED.

10 IFILE READ AND REWRITE DATA SET INDICATOR.

0 DATA SET REWRITTEN ON THE MAINFILE IF THIS IS THE LAST CYCLE OF THE CURRENT RUN.
1 DATA SET NOT REWRITTEN.
2 LIKE 0 BUT IN ADDITION (DURING INPUT) READ THE STANDARD DEVIATIONS OF PARAMETERS REFINED IN PREVIOUS CYCLES FROM THE MAINFILE (SEE REMARK BELOW).
3 LIKE 1 BUT IN ADDITION (DURING INPUT) READ THE STANDARD DEVIATIONS OF PARAMETERS REFINED IN PREVIOUS CYCLES FROM THE MAINFILE (SEE REMARK BELOW).

REMARK
2 OR 3 ARE ONLY NECESSARY, IF CALCULATION IS NOT A FULL MATRIX LEAST SQUARES FIT.

(COLUMN 11 IS EMPTY)

ATTENTION

IN AN -A PRIORI- CYCLE ALL THE FOLLOWING VARIABLES NEW(1)-NEW(8) MUST BE NOT EQUAL 0 .

12 NEW(1) READ NEW CELL PARAMETERS (CELL CARD).

0 DO NOT.
1 DO.

13 NEW(2) READ NEW BOND DISTANCE LIMITS USED IN CALCULATION OF BONDS (BOND LIMITS CARD).

0 DO NOT.
1 DO.

14 NEW(3) READ NEW SYMMETRY INFORMATION (CELL TYPE CARD AND SYMMETRY CARDS).

0 DO NOT.

1 DO.

15 NEW(4) READ NEW SCATTERING FACTORS (SCAT.CURVE TYPE CARD(S) AND EXPONENT. FORM CARD(S) OR TABULATION FORM CARD(S) PLUS ANOMALOUS DISP. CARD(S) IF NEEDED).

0 DO NOT.
1 DO.

16 NEW(5) SELECTOR FOR READ NEW PARAMETER VALUES (SCALE FACTOR CARD, EXTINCTION CARD, ATOM PARAMETER CARD(S), SPECIAL PARAM. CARD, AND ALPHA PARAMETER CARD(S)).

0 DO NOT READ ANY NEW PARAMETER VALUE.
1 READ ENTIRE PARAMETER LIST OF PARAMETER VALUES (SEE LIST OF CARDS IN BRACKETS ABOVE).
2 READ ONLY NEW SCALE FACTORS (SCALE FACTOR CARD)
3 READ ONLY NEW EXTINCTION PARAMETERS (EXTINCTION CARD).
4 READ ONLY NEW ATOM PARAMETERS (ATOM PARAMETER CARD(S)) SELECTED BY ATOM SELECTION CARD(S
5 READ ONLY NEW SPECIAL PARAMETERS (SPECIAL PARAM. CARD).
6 READ ONLY NEW ALPHA PARAMETER(S) (ALPHA PARAMETER CARD(S)).

17 NEW(6) READ NEW TEMPERATURE FACTOR TYPES (T-FACTOR TYPE CARD)

0 DO NOT.
1 DO.

18 NEW(7) READ NEW PARAMETER SELECTIONS AND DEPENDENCIES (SCALE REFINE CARD, EXTINC. REFINE CARD, ALPHA REFINE CARD SPECIAL REFINE CARD, ATOM REFINE CARD(S), NEW VALUE CARD(S), AND DEPENDENCY CARD(S)).

REMARK
THE EXTINC. REFINE CARD IS ONLY NEEDED IF EXTINCTION CORRECTION IS SELECTED, AS WELL THE ALPHA- AND THE SPECIAL REFINE CARD CAN BE OMITTED. THE NEW VALUE CARD(S) ARE ONLY NEEDED FOR SPECIAL VALUES OF THE PARAMETERS GIVEN ON THE ATOM REFINE CARD(S).

19 NEW(8) INDICATOR FOR DIFFERENT TYPES OF HKL-CARDS TO BE READ (FORMAT SPECIFIED BY THE FORMAT CARD) AND SWITCH FOR READ DIFFRACTOMETER CARD AND ORIENTATION CARDS.

0 DO NOT READ HKL-CARDS. (I.E. READ MAIN UNIT)
NOT 0 READ HKL CARDS. THE VALUES 1-9 CORRESPOND TO VARIOUS OPTIONS FOR THE ORDER OF THE LIST, AS EXPLAINED BELOW. IF THE VALUES IN BRACKETS ARE USED (6-9) IN ADDITION THE DIFFRACTOMETER CARD AND THE ORIENTATION CARDS ARE READ.

TABEL OF VERSIONS OF HKL-CARDS ACCEPTED BY THE PROGRAMME

NEW(8)	LABEL	IH	MREJ	ISG	FOBS	TBAR	SIGMA
1 (6)	X	X	X		X		X
2 (7)	X	X	X		X	X	X
3 (8)	X	X	X	X	X		X
4 (9)	X	X	X	X	X	X	X
5	X	X					

EXPLANATION OF THE TABLE

LABEL HKL CARD DESIGNATOR. IT IS ONLY NEEDED TO INDICATE THE END OF THE LIST.
END THE LAST HKL-CARD WAS READ. (NO FURTHER

INFORMATION IS READ FROM THE CARD WITH THE LABEL = END).

NOT END THIS CARD IS AN HKL=CARD.

IH MILLER INDICES.

MREJ DESIGNATOR FOR REFLECTIONS USED AS OBSERVED OR LESS THAN REFLECTIONS.
1 OBSERVED REFLECTION
2 LESS THAN REFLECTION

ISG NUMBER OF THE SCALE GROUP TO WHICH THE REFLECTION BELONGS.

FOBS INTENSITY OR STRUCTURE FACTOR (SEE PARAMETER IFOBS ON THE DATA DEFINING CARD).

TBAR ABSORPTION WEIGHTED MEAN PATH LENGTH OF THE BEAM THROUGH THE CRYSTAL.

SIGMA STANDARD DEVIATION OR WEIGHT OF THE PARAMETER FOBS DEPENDING ON THE VALUE OF IWT ON THE DATA DEFINING CARD.

REMARK

NEW(8)=5 CAN BE USED FOR READING ONLY MILLER INDICES FOR STRUCTURE FACTOR CALCULATION.

20-27 UNTEN
28-35 OBEN
LOWER AND UPPER LIMIT OF THE INTERVAL OF SIN(THETA)/LAMBDA NEEDED FOR THE REJECTION OF CERTAIN REFLECTIONS IF THE PARAMETER IREJ ON THIS CARD (SEE ABOVE) IS 7 OR 9 .

36-43 DELMAX FACTOR NEEDED FOR THE REJECTION OF CERTAIN REFLECTIONS IF THE PARAMETER IREJ ON THIS CARD (SEE ABOVE) IS 2 (IN SOME CASES), 3, 4, 5, OR 6 .

(COLUMN 44 IS EMPTY)

45 IPART PARTIAL STRUCTURE FACTOR CALCULATION SELECTOR

0 CALCULATE STRUCTURE FACTORS FOR THE COMPLETE STRUCTURE.

ATTENTION
THE VALUES IPART = 1 AND 2 ARE ONLY POSSIBLE IF THE PARAMETER NEW(8) ON THIS CARD IS NOT EQUAL 0.

1 CALCULATE STRUCTURE FACTORS ONLY FOR A PARTIAL STRUCTURE BY DELETING ATOM(S) SELECTED BY PARTIAL CARD(S).
(SEE REMARK BELOW).

2 LIKE 1 BUT NOW F(OBS) IS OVERWRITTEN BY F(CALC) OF THE COMPLETE STRUCTURE.
(USING THIS PROCEDURE ONE CAN CALCULATE THE MAXIMUM INFLUENCE OF THE SELECTED ATOM(S) ON THE R-VALUE).

REMARK
IF IPART=1 OR 2 NO REFINEMENT IS POSSIBLE AND THE DATA SET CANNOT BE REWRITTEN.
WHEN THE CALCULATION OF PARTIAL STRUCTURE FACTORS IS SELECTED BY SETTING IPART=1 OR 2 THE PHASE WILL BE CALCULATED USING THE COMPLETE STRUCTURE. IF THE PHASE SHOULD BE CALCULATED TOO ONLY USING THE PARITAL STRUCTURE TOO, THE ATOMS MUST BE DELETED BY SETTING THE OCCUPANCIES TO ZERO. (THEN THE PARAMETER IPART IS NOT NEEDED).

(COLUMN 46 IS EMPTY)

47 IHARM SELECTOR FOR WRITE A HARMONIC-FILE FOR CALCULATION OF AN EXTENDED EDGEWORTH MAP.
(ONLY NEEDED IF AN EXTENDED EDGEWORTH MAP SHOULD BE CALCULATED WITH THE PROGRAMME PDFMAP).

```
                0      DO NOT WRITE A HARMONIC-FILE.
                1      WRITE A HARMONIC-FILE.
                       (LOGICAL NUMBER OF THE HARMONIC-FILE = 9 ).

   48  JXPAR   INDICATOR FOR THE USE OF SPECIAL PARAMETERS.

                0      DO NOT USE SPECIAL PARAMETERS.
                1      USE SPECIAL PARAMETERS.
                       (FOR SPECIAL PARAMETERS SEE DESCRIPTION PART).

   49  IFSGEN  ORIENTATION DETERMINATION SELECTOR.
               (ORIENTATION  MEANS THE TWO DIFFERENT ORIENTATIONS OF
                ENANTIOMORPHIC STRUCTURES)

                0      DO NOT DETERMINE THE ORIENTATION.
                1      CHANGE TO THE ORIENTATION WITH LOWER  R(W) .

(COLUMN 50 IS EMPTY)

   51  IOVER   INDICATOR FOR CHANGE OF THE STRUCTURE FACTOR EQUATION.

                0      DO NOT ALLOW A CHANGE OF THE STRUCTURE FACTOR
                       EQUATION IF THE CURRENT CYCLE IS NOT AN
                       -A PRIORI- CYCLE.
                1      ALLOW THE CHANGE OF THE STRUCTURE FACTOR
                       EQUATION ALTHOUGH THE CURRENT CYCLE IS NOT AN
                       -A PRIORI- CYCLE.
```

CELL CARD

(ONLY NEEDED IF NEW(1) NOT EQUAL 0).

FORMAT (6F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	AG	LATTICE CONSTANTS
9-16	BG	A, B, AND C
17-24	CG	GIVEN IN ANGSTROMS.
25-32	WINKEL	LATTICE ANGLES
33-40	WINKEL	ALPHA, BETA, AND GAMMA
41-48	WINKEL	GIVEN IN DEGREES.

BOND LIMITS CARD

(ONLY NEEDED IF NEW(2) IS NOT EQUAL 0).

FORMAT (2F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	DMIN	MINIMUM BOND DISTANCE IN ANGSTROMS.
9-16	DMAX	MAXIMUM BOND DISTANCE IN ANGSTROMS. (DMIN AND DMAX ARE ONLY USED FOR THE CALCULATION OF BOND DISTANCES AND ANGELS IF THE PARAMETER MBODAN ON THE MAIN CONTROL CARD IS 1 OR 2).

CELL TYPE CARD

(ONLY NEEDED IF NEW(3) IS NOT EQUAL 0).

FORMAT (A4,25X,2A1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES

1- 4	ICENT	FLAG FOR CENTRIC OR ACENTRIC CELL
		CENT CENTRIC CELL
		ACEN ACENTRIC CELL
22,23	ICELL	INDICATOR FOR THE TYPE OF THE CELL (CAN BE WRITTEN IN COLUMN 22 OR 23).
		P PRIMITIVE
		A A- CENTERED
		B B- CENTERED
		C C- CENTERED
		I I- CENTERED
		F F- CENTERED
		R RHOMBOHEDRAL

REMARK
BECAUSE OF THE SPECIAL FORMAT THIS CARD CAN BE WRITTEN IN THE FORM

CENTRIC CELL OF TYPE I
OR
ACENTRIC CELL OF TYPE P
AND SO ON.

SYMMETRY CARDS

(ONLY NEEDED IF NEW(3) IS NOT EQUAL 0).

FORMAT (3A3,1X,3A3,1X,3A3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	JTNS	TRANSLATIONAL PART OF X .
		HERE ONE OF THE OPERATORS DESCRIBED BELOW OR THE WORD END TO INDICATE THAT ALL SYMMETRY CARDS WERE READ MUST APPEAR.
5- 6	IRMAT	FIRST POSITIONAL PART OF X .
8- 9	IRMAT	SECOND POSITIONAL PART OF X .
11-13		TRANSLATIONAL PART OF Y .
15-16		FIRST POSITIONAL PART OF Y .
18-19		SECOND POSITIONAL PART OF Y .
21-23		
25-26		SAME FOR Z .
28-29		

THE SYMMETRY OPERATIONS MUST BE WRITTEN IN THE FORM USED IN THE INTERNATIONAL TABLES OF CRYSTALLOGRAPHY. THIS MEANS THAT
THE TRANSLATIONAL OPERATORS ARE OF THE FOLLOWING FORM (B = BLANK)
BBB, 1/2, 1/3, 2/3, 1/4, 3/4, 1/6, OR 5/6 .
THE POSITIONAL OPERATOR ARE OF THE FORM (W = X, Y, OR Z)
+W, BW (=+W), OR -W.

ATTENTION
THE SYMMETRY POSITION X Y Z MUST BE INCLUDED.

REMARK
THERE CAN BE A MAXIMUM OF 24 SYMMETRY CARDS, BECAUSE POSITIONS RELATED BY A CENTER OF INVERSION OR LATTICE CENTERING MAY NOT BE INCLUDED.

SCAT.CURVE TYPE CARD

(ONLY NEEDED IF NEW(4) IS NOT EQUAL 0).

FORMAT (A1,3A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IFLAG	ANOMALOUS DISPERSION INDICATOR AND END FLAG

		BLANK NO ANOMALOUS DISPERSION CORRECTION TO BE USED. A ANOMALOUS DISPERSION CORRECTION TO BE READ FOR THIS SCATTERING CURVE (ANOMALOUS DISP. CARD) E END FLAG INDICATING THAT ALL SCATTERING CURVES WERE READ.
2- 9	L	ANY SEQUENCE OF SYMBOLS TO BE USED AS A LABEL FOR THIS SCATTERING CURVE.
10-13	ITABLE	INDICATOR FOR THE REPRESENTATION OF THE SCATTERING CURVE TO BE READ. BLANKS ON THE FOLLOWING CARD THE COEFFICIENTS FOR THE EXPONENTIAL REPRESENTATION OF THE SCATTERING CURVE ARE GIVEN. (EXPONENT. FORM CARD). TABLE ON THE FOLLOWING CARDS THE SCATTERING CURVE IS GIVEN IN TABULATION FORM. (TABULATION FORM CARDS).

REMARK
FOR EACH SCATTERING CURVE THERE MUST BE A SCAT.CURVE TYPE CARD FOLLOWED BY AN EXPONENT. FORM CARD OR BY TABULATION FORM CARDS PLUS (IF IFLAG=A) AN ANOMALOUS DISP. CARD.
THE END OF THE LIST MUST BE INDICATED BY AN END CARD CONTAINING ONLY THE WORD END TYPED IN COLUMNS 1-3 .

EXPONENT. FORM CARD

(ONLY NEEDED IF FOR THE PARAMETER ITABLE ON THE SCAT.CURVE TYPE CARD JUST WRITTEN ONLY BLANKS WERE TYPED).

FORMAT (9F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	A(1)	IF X-RAY DATA ARE REFINED THESE COEFFICIENTS MUST
9-16	B(1)	SATISFY THE FOLLOWING EQUATION
17-24	A(2)	$F(X) = C + \sum_{I=1}^{4} (A(I) * EXP(-B(I) * X * X))$
25-32	B(2)	
33-40	A(3)	
41-48	B(3)	WITH X = SIN(THETA) / LAMBDA
49-56	A(4)	
57-64	B(4)	IF NEUTRON DATA ARE REFINED C MUST BE THE SCATTERING
65-72	C	LENGTH. (A(I) AND B(I) ARE MEANINGLESS).

TABULATION FORM CARDS

(ONLY NEEDED IF THE PARAMETER ITABLE ON THE SCAT.CURVE CARD JUST WRITTEN IS EQUAL TABLE).

FORMAT (2F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	X	SIN(THETA) / LAMBDA
9-16	Y	CORRESPONDING VALUE OF THE SCATTERING CURVE.

REMARKS
FOR ONE SCATTERING CURVE THERE MAY BE A MINIMUM OF 10 AND CAN BE A MAXIMUM OF 35 TABULATION CARDS.
THE END OF THE LIST IS INDICATED BY X=0. AND Y=0. .
THE VALUES OF X MUST INCREASE MONOTONICALLY WHILE THE VALUES OF Y SHOULD DECREASE MONOTONICALLY. A 5 PERCENT DEVIATION FROM THE MONOTONY OF Y IS ALLOWED.

ANOMALOUS DISP. CARD

(ONLY NEEDED IF THE PARAMETER IFLAG ON THE LAST SCAT.CURVE TYPE CARD IS EQUAL A).

FORMAT (2F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	ANOM1	REAL PART OF ANOMALOUS DISPERSION CORRECTION
9-16	ANOM2	IMAGINARY PART OF ANOMALOUS DISPERSION CORRECTION

SCALE FACTOR CARD

(ONLY NEEDED IF NEW(5)=1 OR 2).

FORMAT (10F7.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 7	SCALE(1)	
8-14	.	
15-21	.	A MAXIMUM OF 10 SCALE FACTORS
22-28	.	CAN BE GIVEN.
29-35		(IF MORE THAN ONE SCALE FACTOR IS GIVEN ON THIS
36-42		CARD, EACH HKL CARD MUST CONTAIN THE NUMBER OF
43-49		THE SKALE FACTOR TO BE USED FOR THE REFLEC-
50-56		TION (NEW(8) = 3(8) OR 4(9))).
57-63		
64-70	SCALE(10)	

EXTINCTION CARD

(ONLY NEEDED IF NEW(5)=1 OR 3).

FORMAT (2I1,7F8.4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	NIEXT	INDICATOR FOR THE EXTINCTION MODEL TO BE USED.
		0-6 EXTINCTION CORRECTION BASED ON THE CALCULATIONS OF BECKER AND COPPENS.
		0 NO EXTINCTION CORRECTION
		1 ISOTROPIC EXTINCTION CORRECTION TYPE 1
		2 ISOTROPIC EXTINCTION CORRECTION TYPE 2
		3 ISOTROPIC EXTINCTION CORRECTION GENERAL CASE
		4 ANISOTROPIC EXTINCTION CORRECTION TYPE 1
		5 ANISOTROPIC EXTINCTION CORRECTION TYPE 2
		6 ANISOTROPIC ECTINCTION CORRECTION GENERAL CASE
		8 ISOTROPIC ZACHARIASEN CORRECTION OR ANISOTROPIC COPPENS AND HAMILTON CORRECTION. (SEE PARAMETER NDISTR).
2	NDISTR	DISTRIBUTION AND EXTINCTION CHANGE INDICATOR. (THIS PARAMETER HAS DIFFERENT MEANINGS DEPENDING ON THE EXTINCTION MODEL INDICATOR NIEXT).
		FOR NIEXT LESS EQUAL 6 (BECKER AND COPPENS EXTINCTION)
		0 (2) DISTRIBUTION OF MOSAIC SPREAD IS GAUSSIAN.
		1 (3) DISTRIBUTION OF MOSAIC SPREAD IS LORENTZIAN. (IF NDISTR=0 OR 1 AN AUTOMATIC DAMPING ROUTINE IS USED IF PARAMETERS BECOME UNPHYSICAL AND IF NO FIXED DAMPING FACTORS ARE SELECTED ON THE EXTINC. REFINE CARD. IF NDISTR=2 OR 3 NO AUTOMATIC DAMPING IS USED).

FOR NIEXT = 8
(ZACHARIASEN OR HAMILTON AND COPPENS EXTINCTION)

0 ISOTROPIC , DO NOT CHANGE.

1 ANISOTROPIC TYPE I , DO NOT CHANGE.

2 ANISOTROPIC TYPE II, DO NOT CHANGE.

3 ISOTROPIC , CHANGE TO ANISOTROPIC TYPE I

4 ISOTROPIC , CHANGE TO ANISOTROPIC TYPE II

5 ANISOTROPIC TYPE I , CHANGE TO ISOTROPIC

6 ANISOTROPIC TYPE II, CHANGE TO ISOTROPIC

7 ANISOTROPIC TYPE I , CHANGE TO ANISOTROPIC TYPE II

8 ANIXOTROPIC TYPE II, CHANGE TO ANISOTROPIC TYPE I

9 DO NOT CHANGE TYPE BUT RESET PARAMETER TO ZERO.

3-58 RNEUEX INITIAL VALUES FOR THE EXTINCTION PARAMETERS TO BE USED MULTIPLIED WITH A FACTOR OF 10000 .(SO THE VALUES GIVEN HERE ARE IDENTICAL WITH THOSE IN THE OUTPUT BECAUSE THERE THEY ARE PRINTED WITH THE SAME FACTOR).

3-10 PARAMETER 1
11-18 .
19-26 .
27-34 .
35-42
43-5
51-58 PARAMETER 7

WHEN BECKER AND COPPENS EXTINCTION IS USED THESE PARAMETERS HAVE THE FOLLOWING MEANING

PARAM. NO.	.....I S O T R O P I C.... TYPE 1	TYPE 2	GENERAL CASE	***A N I S O T R O P I C*** TYPE 1	TYPE 2	GENERAL CASE
1	G	R	R	Z(11)	Z(11)	Z(11)
2			G	Z(22)	Z(22)	Z(22)
3				Z(33)	Z(33)	Z(33)
4				Z(12)	Z(12)	Z(12)
5				Z(13)	Z(13)	Z(13)
6				Z(23)	Z(23)	Z(23)
7						R

REMARK
IF THE TYPE OF THE EXTINCTION IS CHANGED, THE CYCLE IS NOT AN -A PRIORI- CYCLE, AND THERE ARE NO VALUES GIVEN FOR RNEUEX (RNEUEX = 0.), THE PROGRAMME CONVERTS THE PARAMETER(S) REFINED BEFORE INTO THE NEW ONE(S). A CONVERSION FROM ISOTROPIC TO ANISOTROPIC IS ONLY POSSIBLE IF THE ORIENTATION MATRIX WAS READ OR WILL BE READ. (SEE NEW(8) ON THE MAIN CONTROL CARD).

ATTENTION
A CONVERSION FROM THE ZACHARIASEN (RESP. COPPENS AND HAMILTON) MODEL TO THE BECKER AND COPPENS MODEL OR VICE VERSA IS NOT POSSIBLE. FOR CHANGING THE MODEL AN -A PRIORI- CYCLE MUST BE STARTED.

ATOM SELECTION CARD(S)

PREFATORY NOTICE (CONCERNING THIS AND THE ATOM PARAMETER CARDS).

THERE ARE TWO POSSIBILITIES OF READING ATOM PARAMETER CARDS. IN AN -A PRIORI- CYCLE THE ENTIRE ATOM PARAMETER LIST FOR ALL ATOMS HAS TO BE READ AND NO ATOM SELECTION CARD CAN BE GIVEN. THE END OF THE LIST MUST BE INDICATED BY AN END CARD WHICH CONTAINS ONLY THE WORD END IN COLUMNS 1-3 .
IF IN A -CONTINUE CYCLE- YOU WANT TO CHANGE PARAMETERS OF CERTAIN ATOMS OR ADD SOME ATOMS TO THE CURRENT LIST, YOU MUST USE THE ATOM SELECTION CARD(S).

(THE ATOM SELECTION CARD IS ONLY NEEDED IF NEW(5) = 4).

FORMAT (I2)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 2	I	NUMBER OF THE ATOM FOR WHICH NEW ATOM PARAMETERS SHOULD BE READ (ATOM PARAMETER CARD(S)). (THE ATOMS ARE NUMBERED IN THE -A PRIORI- RUN FROM 1 TO NATOM ACCORDING TO THE SEQUENCE THEY ARE LISTED ON THE ATOM PARAMETER CARDS. THE NUMBER GIVEN FOR I HERE CAN BE GREATER THAN NATOM , BUT THEN I MUST INCREASE MONOTONICALLY STARTING WITH I = NATOM+1). (AS MENTIONED ABOVE THE END OF THE LIST OF ATOM SELECTION CARDS MUST BE INDICATED BY I = 0).

ATOM PARAMETER CARD(S)

(ONLY NEEDED IF NEW(5) = 1 OR 4).

PREFATORY NOTICE
THE ATOM PARAMETER CARD FOR ONE ATOM IN REALITY CONSISTS OF AT LEAST 2 CARDS AND AT MOST OF 11 CARDS DEPENDING ON THE ORDER OF THERMAL TENSORS TO BE READ.

CARD 1

FORMAT (A1,2A3,I4,2X,2F6.4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IFLAG	INDENTIFIER FOR THE END OF ATOM PARAMETER LIST.
		BLANK THERE ARE MORE ATOM PARAMETER CARDS TO BE READ.
		NOT BLANK THE ATOM PARAMETER CARDS WERE READ FOR ALL ATOMS. (ATTENTION.. THIS CARD IDENTIFIING THE END OF THE ATOM PARAMETER CARDS IS AN ADDITIONAL CARD. IT S CONTENS IS NO MORE READ.)
2- 7	TAG	ANY SEQUENCE OF SYMBOLS USED AS IDENTIFIER FOR THE ATOM.
8-11	SITE	MULTIPLICITY OF THE POSITION OCCUPIED BY THE ATOM.
14-19	OCCUP	TOTAL OCCUPANCY OF THE SITE.
20-25	OCCA	OCCUPANCY OF SPECIES A (SEE CARD 2) IN THIS SITE. (OCCA IS ONLY NEEDED IF MULTIPLE OCCUPANCY IS USED).

CARD 2

FORMAT (2I2,1X,A2,1X,9F7.5,I2)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 2	ISCAT1	NUMBER OF THE SCATTERING CURVE FOR SPECIES A . (THE SCATTERING CURVES ARE NUMBERED ACCORDING TO THE SEQUENCE THEY WERE READ).
3- 4	ISCAT2	NUMBER OF THE SCATTERING CURVE FOR SPECIES B . (ONLY NEEDED IF THERE IS A MULTIPLE OCCUPANCY OF TWO DIFFERENT ATOMS IN THIS POSITION).
6- 7	BTYP	TEMPERATUR FACTOR TYPE B BETA NOTATION U CRUICKSHANK NOTATION (MULTIPLIED BY 100) BU INPUT BETA, OUTPUT U UB INPUT U, OUTPUT BETA DEFAULT IS B.
9-15	XYZ(1)	X COORDINATE FOR THE ATOM
16-22	XYZ(2)	Y COORDINATE GIVEN IN
23-29	XYZ(3)	Z COORDINATE FRACTIONAL COORDINATES.
30-71	BETA	VALUES OF THE ELEMENTS FO THE THERMAL TENSOR OF SECOND ORDER (ANISOTROPIC TEMPERATURE FACTOR) RESP. ISOTROPIC B-VALUE.
30-36		BETA(11) OR THE B-VALUE IF ONLY ISOTROPIC THERMAL VIBRATONS ARE REFINED.)
37-43		BETA(22))
44-50		BETA(33)) OR U(IJ)*100 DE-
51-57		BETA(12)) PENDING ON BTYP
58-64		BETA(13))
65-71		BETA(23))
72-73	IEF	INDICATOR FOR THIRD ORDER CUMULANTS TO BE READ FROM THE FOLLOWING CARD. 0 DO NOT READ THIRD ORDER CUMULANTS, THIS IS THE LAST PARAMETER CARD FOR THIS ATOM. 1 READ THIRD ORDER CUMULANTS (CARD 3).

CARD 3

FORMAT (10F7.0,I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 70	CR	VALUES OF THE ELEMENTS OF THE THIRD ORDER CUMULANT MULTIPLIED WITH 1000. (THIS MEANS THAT THE VALUES GIVEN HERE ARE IDENTICAL WITH THOSE PRINTED IN THE OUTPUT).
1- 7		C(111)
8-14		C(222)
15-21		C(333)
22-28		C(112)
29-35		C(122)
36-42		C(113)
43-49		C(133)
50-56		C(223)
57-63		C(233)
64-70		C(123)
71	IEF	INDICATOR FOR FOURTH ORDER CUMULANTS TO BE READ FROM THE FOLLOWING TWO CARDS. 0 DO NOT READ FOURTH ORDER CUMULANTS. THIS IS THE LAST PARAMETER CARD FOR THIS ATOM. 1 READ FOURTH ORDER CUMULANTS.

CARD 4 AND CARD 5

FORMAT CARD 4 (10F7.0)

CARD 5 (5F7.0,35X,I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-70	DR	VALUES OF THE ELEMENTS OF THE FOURTH ORDER TENSOR MULTIPLIED WITH 10 000 LIKE ON THE OUTPUT.

	CARD 4	CARD 5
1- 7	D(1111)	D(1233)
8-14	D(2222)	D(1333)
15-21	D(3333)	D(2223)
22-28	D(1112)	D(2233)
29-35	D(1113)	D(2333)
36-42	D(1122)	
43-49	D(1123)	
50-56	D(1133)	
57-63	D(1222)	
64-70	D(1223)	

71	IEF	(CARD 5 ONLY)	INDICATOR FOR FIFTH ORDER CUMULANTS TO BE READ FROM THE NEXT THREE CARDS.
		0	DO NOT READ FIFTH ORDER CUMULANTS THIS IS THE LAST PARAMETER CARD FOR THIS ATOM.
		1	READ FIFTH ORDER CUMULANTS.

CARD 6, CARD 7, AND CARD 8

FORMAT CARD 6 (10F7.0)
CARD 7 (10F7.0)
CARD 8 (F7.0,63X,I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-70	ER	VALUES OF THE ELEMENTS OF THE FIFTH OREDER TENSOR MULTIPLIED WITH 100 000 LIKE ON THE OUTPUT.

	CARD 6	CARD 7	CARD 8
1- 7	E(11111)	E(11233)	E(23333)
8-14	E(22222)	E(11333)	
15-21	E(33333)	E(12222)	
22-28	E(11112)	E(12223)	
29-35	E(11113)	E(12233)	
36-42	E(11122)	E(12333)	
43-49	E(11123)	E(13333)	
50-56	E(11133)	E(22223)	
57-63	E(11222)	E(22233)	
64-70	E(11223)	E(22333)	

71	IEF		INDICATOR FOR SIXTH ORDER CUMULANTS TO BE READ FROM THE NEXT THREE CARDS (IEF MAY APPEAR ONLY ON CARD 8).
		0	DO NOT READ SIXTH ORDER CUMULANTS. THIS IS THE LAST PARAMETER CARD FOR THIS ATOM.
		1	READ SIXTH ORDER CUMULANTS.

CARD 9, CARD 10, AND CARD 11

FORMAT CARD 9 (10F7.0)
CARD 10 (10F7.0)
CARD 11 (8F7.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-70	FR	VALUES OF THE ELEMENTS OF THE SIXTH ORDER TENSOR MULTIPLIED WITH 1000 000 LIKE ON THE OUTPUT.

	CARD 9	CARD 10	CARD 11
1- 7	F(111111)	F(111233)	F(122333)
8-14	F(222222)	F(111333)	F(123333)
15-21	F(333333)	F(112222)	F(133333)
22-28	F(111112)	F(112223)	F(222223)
29-35	F(111113)	F(112233)	F(222233)
36-42	F(111122)	F(112333)	F(222333)
43-49	F(111123)	F(112222)	F(223333)
50-56	F(111133)	F(122222)	F(233333)
57-63	F(111222)	F(122223)	
64-70	F(111223)	F(122233)	

REMARK
IF THERE ARE MORE ATOMS TO BE READ, START AGAIN WITH AN ATOM SELECTION CARD RESP. WITH CARD 1 OF THE ATOM PARAMETER CARDS.

ATTENTION
IF THIS WAS THE LAST ATOM OF THE LIST THIS MUST BE INDICATED BY AN END CARD CONTAINING ONLY THE WORD END IN COLUMNS 1-3 .

SPECIAL PARAM. CARD

(ONLY NEEDED IF ON THE MAIN CONTROL CARD JXPAR NOT EQUAL 0 OR NEW(5) = 5).

FORMAT (2X,I2)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
3- 4	NPAR	NUMBER OF SPECIAL PARAMETERS TO BE USED.

SPECIAL VALUE CARD(S)

(THERE MUST BE NPAR SPECIAL VALUE CARDS CONTAINING THE NAMES, INITIAL VALUES, AND IDENTIFIERS OF THE SPECIAL PARAMETERS).

FORMAT (2A4,3I2,F10.4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	PARNAM	NAME OF SPECIAL PARAMETER, UP TO 8 ALPHANUMERIC CHARACTERS.
9-10	ITEM(1)	TYPE OF SPECIAL PARAMETER 0 LINEAR FUNCTION WITH COEFFICIENT GIVEN ON DEPENDENCY CARD. 1 RIGID BODY SYSTEM. 2 DEFINED BY USER IN SUBROUTINES SPVAL AND SPDERI (SEE DESCRIPTION PART).
11-12	ITEM(2)	INTEGER INDICATING WHICH RIGID-BODY-SYSTEM, IF MORE THAN ONE, THIS PARAMETER REFERS TO.
13-14	ITEM(3)	PARAMETER DESIGNATOR. IF THE TYPE IS 1 THE CODE IS AS FOLLOWS 1 X COORDINATE OF ORIGIN (IN CRYSTAL AXES SYSTEM) 2 Y COORDINATE OF ORIGIN 3 Z COORDINATE OF ORIGIN 4 OMEGA ANGLE FOR TRANSFORMATION TO STANDARD, ORTHONORMAL COORDINATE SYSTEM. 5 CHI ANGLE FOR TRANSFORMATION. 6 PHI ANGLE FOR TRANSFORMATION. 7 X COORDINATE OF AN ATOM IN THE SPECIAL SYSTEM. 8 Y COORDINATE OF AN ATOM.

	9	Z COORDINATE OF AN ATOM.
	10	T11
	11	T22
	12	T33
	13	T12
	14	T13
	15	T23
	16	L11
	17	L22
	18	L33
	19	L12
	20	L13
	21	L23
	22	S11
	23	S22
	24	S33
	25	S12
	26	S13
	27	S23
	28	S21
	29	S31
	30	S32
15-24 PAR		INITIAL VALUE OF THIS PARAMETER.

ALPHA PARAMETER CARD(S)

(ONLY NEEDED IF NEW(5)=1 OR 6 AND THE STRUCTURE FACTOR EQUATION NO. 3 OR 4 IS USED).

FORMAT (9F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8		VALUE OF ALPHA FOR THE FIRST ATOM (ATOM NUMBER ACCORDING TO THE SEQUENCE OF ATOMS ON THE ATOM PARAMETER CARDS).

ATTENTION
ALPHA VALUES ARE READ FOR ALL ATOMS, NOT ONLY FOR THOSE WHICH ARE REFINED WITH ANHARMONIC TEMPERATURE FACTORS. YOU HAVE TO TYPE 0. OR LEAVE EIGHT BLANKS FOR ATOMS WHICH DO NOT NEED AN ALPHA.

9-16		VALUE OF ALPHA FOR THE SECOND ATOM.
17-24	.	THIRD ATOM.
25-32	.	
33-4		
41-48		
49-56		
57-64		
65-72		VALUE OF ALPHA OF THE NINETH ATOM.

REMARKS
IF THE NUMBER OF INITIAL VALUES (= NUMBER OF ATOMS) IS GREATER THAN 9, ADD AS MANY OF ALPHA PARAMETER CARDS AS YOU NEED.
IN THE CURRENT VERSION OF THE PROGRAMME NO DEPENDENCIES BETWEEN ALPHA-PARAMETERS ARE POSSIBLE.

T-FACTOR TYPE CARD

(ONLY NEEDED IF NEW(6) NOT EQUQL 0).

FORMAT (60I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	ISOT	INDICATOR FOR THE TEMPERATURE FACTOR TYPE TO BE USED FOR ATOM NUMBER 1 (NUMBER ACCORDING TO THE SEQUENCE OF THE ATOMS ON THE ATOM PARAMETER CARDS).

0	NOW ISOTROPIC	, DO NOT CHANGE.
1	NOW ANISOTROPIC	, DO NOT CHANGE.
2	NOW ISOTROPIC	, CHANGE TO ANISOTROPIC.
3	NOW ANISOTROPIC	, CHANGE TO ISOTROPIC.
4	NOW 3RD ORDER	, DO NOT CHANGE.
5	NOW ANISOTROPIC	, CHANGE TO 3RD ORDER.
6	NOW 3RD ORDER	, CHANGE TO ANISOTROPIC
7	NOW 4TH ORDER	, DO NOT CHANGE.
8	NOW 3RD ORDER	, CHANGE TO 4TH ORDER.
9	NOW 4TH ORDER	, CHANGE TO 3RD ORDER.
A	NOW 5TH ORDER	, DO NOT CHANGE.
B	NOW 4TH ORDER	, CHANGE TO 5TH ORDER.
C	NOW 5TH ORDER	, CHANGE TO 4TH ORDER.
D	NOW 6TH ORDER	, DO NOT CHANGE.
E	NOW 5TH ORDER	, CHANGE TO 6TH ORDER.
F	NOW 6TH ORDER	, CHANGE TO 5TH ORDER.

2 SAME FOR ATOM NUMBER 2 .
3 SAME FOR ATOM NUMBER 3 .
4 AND SO ON .

ATTENTION

60 ATOMS IN THE ASSYMMETRIC UNIT ARE ALLOWED AS LONG AS ONLY TEMPERATURE FACTORS UP TO 4TH ORDER ARE REFINED.
IF TEMPERATURE FACTORS ARE REFINED IN HIGHER THAN 4TH ORDER THE SITUATION IS AS FOLLOWS
ONLY THE FIRST SIX ATOMS GIVEN ON THE ATOM PARAMETER CARDS CAN BE REFINED WITH 5TH OR (AND) 6TH ORDER.
THE ATOMS WITH THE NUMBERS 7 TO 40 CAN BE REFINED WITH TEMPERATURE FACTORS UP TO 4TH ORDER.
THE ATOMS WITH THE NUMBERS 41 TO 60 MUST BE RESTRICTED TO ANISOTROPIC TEMPERATURE FACTORS.

SCALE REFINE CARD

(ONLY NEEDED IF NEW(7) NOT EQUAL 0).

FORMAT (10I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IBUFF	REFINEMENT SWITCH FOR SCALE FACTOR NUMBER 1 .
	0	PARAMETER IS FIXED, DO NOT REFINE.
	1	REFINE THE PARAMETER.
	5	REFINE PARAMETER, BUT DAMP THE SHIFT BY MULTI-MULTIPLYING THE CALCULATED VALUE WITH 0.1
	6	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.25
	7	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.5
	8	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.75
	9	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.9
2		SAME FOR SCALE FACTOR NUMBER 2 .
3		SAME FOR SCALE FACTOR NUMBER 3 .
4		AND SO ON .

EXTINC. REFINE CARD

(ONLY NEEDED IF NEW(7) NOT EQUAL 0 AND EXTINCTION IS SELCTED)
FORMAT (A1,6I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IBUFF	REFINEMENT SWITCH FOR THE FIRST EXTINCTION PARAMETER.
		FOR THE FUNCTION OF THE VALUES SEE SCALE REFINE CARD. (JUST ABOVE).

2 SAME FOR THE SECOND EXTINCTION PARAMETER (IF NEEDED).
3 AND SO ON .

REMARK
IF IN CASE OF BECKER AND COPPENS EXTINCTION THE REFINEMENT SWITCH(ES) ARE SET TO 1 AN AUTOMATIC DAMPING CAN BE SELECTED (SEE PARAMETER NDISTR ON THE EXTINCTION CARD).

ALPHA REFINE CARD

(ONLY NEEDED IF NEW(7) NOT EQUAL 0 AND THE STRUCTURE FACTOR EQUATION NUMBER 3 OR 4 IS USED AND AT LEAST ONE ATOM IS REFINED WITH ANHARMONIC TEMPERATURE FACTORS).

FORMAT (65I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IBUFF	REFINEMENT SWITCH FOR THE ALPHA PARAMETER OF THE ATOM NUMBER 1 . FOR THE MEANING OF THE VLAUES SEE SCALE REFINE CARD .
2		SAME FOR ATOM NUMBER 2 .
3		AND SO ON . (THERE MUST BE AS MANY REFINEMENT SWITCHES AS ATOMS WERE GIVEN ON THE ATOM PARAMETER CARDS. THE ATOM NUMBERS CORRESPOND TO THE SEQUENCE OF THE ATOMS ON THESE CARDS).

SPECIAL REFINE CARD

(ONLY NEEDED IF NEW(7) NOT EQUAL 0 AND SPECIAL PARAMETERS ARE USED).

FORMAT (65I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IRPAR	REFINEMENT SWITCH FOR THE FIRST SPECIAL PARAMETER. MEANING OF THE VALUES SEE SCALE REFINE CARD .
2		SAME FOR THE SECOND SPECIAL PARAMETER.
3		AND SO ON. (THERE MUST BE NPAR (SEE SPECIAL PARAM. CARD) REFINEMENT SWITCHES).

ATOM REFINE CARD(S)

(ONLY NEEDED IF NEW(7) NOT EQUAL 0).

PREFATORY NOTICE
LIKE THE ATOM PARAMETER CARD THE ATOM REFINE CARD CONSISTS OF SEVERAL CARDS (UP TO 5) FOR EACH ATOM.

CARD 1

FORMAT (10I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IPARA	REFINEMENT SWITCH FOR THE TOTAL OCCUPANCY OF THE SITE RESP. FOR THE OCCUPANCY OF SPECIES A IF MULTIPLE OCCUPANCY IS USED (SEE ATOM PARAMETER CARD). 0 PARAMETER IS FIXED, DO NOT REFINE. 1 REFINE THE PARAMETER.

2	DO NOT REFINE AND SET BACK THE PARAMETER TO 0.
3	DO NOT REFINE BUT READ NEW PARAMETER VALUE FROM A NEW VALUE CARD (THE NEW VALUE CARD(S) FOLLOW AFTER THE ENTIRE LIST OF ATOM REFINE CARDS).
4	LIKE 3 BUT NOW REFINE THE NEW PARAMETER.
5	REFINE THE PARAMETER, BUT CAMP THE SHIFT BY MULTIPLYING THE CALCULATED VALUE WITH 0.1
6	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.25
7	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.5
8	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.75
9	REFINE PARAMETER, BUT DAMP WITH THE FACTOR 0.9

REMARK
THIS POSSIBLE PARAMETER VALUES HAVE THE SAME MEANING IN ALL REFINEMENT SWITCHES ON THE ATOM REFINE CARDS .

2	X	REFINEMENT SWITCH FOR THE X-COORDINATE OF THE ATOM.
3	Y	REFINEMENT SWITCH FOR THE Y-COORDINATE.
4	Z	REFINEMENT SWITCH FOR THE Z-COORDINATE.
5-10		REFINEMENT SWITCHES FOR THE ELEMENTS OF THE SECOND ORDER TENSOR (ANISORPIC TEMPERATURE FACTOR) RESP. FOR THE ISOTROPIC B-VALUE.
5		B-VALUE RESP. BETA(11)
6		BETA(22)
7		BETA(33)
8		BETA(12)
9		BETA(13)
10		BETA(23)

CARD 2

(ONLY NEEDED IF FOR THIS ATOM AT LEAST 3RD ORDER CUMULANTS ARE SELECTED (SEE T-FACTOR TYPE CARD).

FORMAT (10I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-10	IPARA	REFINEMENT SWITCHES FOR THE 10 REFINABLE ELEMENTS OF THE 3RD ORDER THERMAL TENSOR. SEQUENCE OF THE ELEMENTS SEE ATOM PARAMETER CARDS OR DEPENDENCY CARDS. POSSIBLES VALUES OF THE SWITCHES SEE CARD 1 OF THE ATOM REFINE CARDS.

CARD 3

(ONLY NEEDED IF FOR THIS ATOM AT LEAST 4TH ORDER CUMULANTS ARE SELECTED (SEE T-FACTOR TYPE CARD).

FORMAT (15I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-15	IPARA	REFINEMENT SWITCHES FOR THE 15 REFINABLE ELEMENTS OF THE 4TH ORDER THERMAL TENSOR. SEQUENCE OF THE ELEMENTS SEE ATOM PARAMETER CARDS OR DEPENDENCY CARDS. POSSIBLES VALUES OF THE SWITCHES SEE CARD 1 OF THE ATOM REFINE CARDS.

CARD 4

(ONLY NEEDED IF FOR THIS ATOM AT LEAST 5TH ORDER CUMULANTS ARE
SELECTED (SEE T-FACTOR TYPE CARD).

FORMAT (21I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-21	IPARA	REFINEMENT SWITCHES FOR THE 21 REFINABLE ELEMENTS OF THE 5TH ORDER THERMAL TENSOR. SEQUENCE OF THE ELEMENTS SEE ATOM PARAMETER CARDS OR DEPENDENCY CARDS. POSSIBLES VALUES OF THE SWITCHES SEE CARD 1 OF THE ATOM REFINE CARDS.

CARD 5

(ONLY NEEDED IF FOR THIS ATOM 6TH ORDER CUMULANTS ARE
SELECTED (SEE T-FACTOR TYPE CARD).

FORMAT (28I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-28	IPARA	REFINEMENT SWITCHES FOR THE 28 REFINABLE ELEMENTS OF THE 6TH ORDER THERMAL TENSOR. SEQUENCE OF THE ELEMENTS SEE ATOM PARAMETER CARDS OR DEPENDENCY CARDS. POSSIBLES VALUES OF THE SWITCHES SEE CARD 1 OF THE ATOM REFINE CARDS.

NEW VALUE CARD(S)

(ONLY NEEDED IF NEW(7) NOT EQUAL 0 AND AT LEAST ONE OF THE
REFINEMENT SWITCHES ON THE ATOM REFINE CARDS IS 3 OR 4).

FORMAT (F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 8	---	NEW VALUE FOR THE PARAMETER FOR WHICH THE REFINEMENT SWITCH ON THE ATOM REFINE CARDS WAS SET TO 3 OR 4. --- THE NAME DEPENDS ON THE SELECTED PARAMETER.

REMARK
THERE MUST BE ONE NEW VALUE CARD FOR EACH REFINEMENT SWTICH SET TO 3 OR 4 . THE SEQUENCE OF THE PARAMETER VALUES ON THE NEW VALUE CARDS MUST CORRESPOND WITH THE SEQUENCE OF THE SELECTED PARAMETERS ON THE ATOM REFINE CARDS.

DEPENDENCY CARD(S)

(ONLY NEEDED IF NEW(7) NOT EQUAL 0).

FORMAT (A1,I2,I3,5(2I3,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	LABEL	DEPENDENCY CHANGE SELECTOR N THIS IS A NEW LIST OF DEPENDENCIES. IF DEPENDENCIES WERE READ IN AN EARLIER CYCLE THEY ARE OVERWRITTEN BY THIS NEW LIST. IF THE LABEL=N IS USED IT MUST APPEAR ON THE FIRST DEPENDENCY CARD. THE END OF THE LIST MUST

		BE INDICATED BY LABEL=E (SEE BELOW). ALL CARDS BETWEEN THE LABEL=N AND THE LABEL=E CARD MUST START WITH LABEL=BLANK.
	O	USE AGAIN THE OLD LIST OF DEPENDENCIES READ IN EARLIER CYCLES. IF LABEL=O IS USED NO FURTHER DEPENDENCY CARDS ARE ALLOWED. (O IS ONLY SENSEFUL IF THE CURRENT CYCLE IS NOT AN -A PRIORI- CYCLE).
	A	USE THE OLD LIST OF DEPENDENCIES, AND ADD THE FOLLOWING DEPENDENCIES. (FOLLOWING DEPENDENCIES ARE.. THE DEPENDENCY ON THE CARD WITH LABEL=A ITSELF PLUS THE DEPENDENCIES ON THE FOLLOWING CARDS IF THESE CARDS START WITH LABEL=BLANK (OR LABEL=A). IF NO OTHER LABEL-FUNCTION IS USED THE LIST MUST BE TERMINATED WITH LABEL=E, BUT IT CAN ALSO BE FOLLOWED BY A LIST OF DEPENDENCIES TO BE DELETED (LABEL=D). (LABEL=A IS DESIGNED FOR ADDING DPENDENCIES TO A CURRENT LIST DURING A -CONTINUE CYCLE-).
	D	USE THE OLD LIST OF DEPENDENCIES, BUT DELETE THE FOLLOWING DEPENDENCIES. (FOR FURTHER EXPLANATIONS SEE LABEL=A. CARDS WITH LABEL=A AND LABEL=D CAN BE ARBITRARILY MIXED).
	P	LIKE LABEL=O BUT IN ADDITION THE DEPENDENCY-LIST WILL BE PRINTED. (NO FURTHER DEPENCY CARD IS ALLOWED).
	E	THIS IS THE END OF THE LIST (END CARD) (THE LAST DEPENDECY MUST BE GIVEN ON THE CARD BEFORE THE END CARD. THERE IS NO DEPENDENCY READ FROM THE END CARD ITSELF).
	BLANK	LABEL=BLANK HAS DIFFERENT MEANINGS DEPENDING ON THE LAST LABEL READ BEFORE. LABEL=BLANK ON THE FIRST DEPENDENCY CARD IS INTERPRETED AS LABEL=N. LABEL=BLANK AFTER LABEL=A OR LABEL=D IST INTERPRETED AS A OR D RESPECTIVELY. NOT ONLY LABEL=BLANK BUT ALSO BLANKS IS COLUMN 2 AND THREE IS INTERPRETED AS LABEL=E. (ALL CARDS AFTER LABEL=N TILL THE END CARD MUST START WITH LABEL=BLANK).
2- 3	IDPAR1	NUMBER OF THE ATOM TO WHICH THE DEPENDANT PARAMETER BELONGS.
5- 6	IDPAR2	NUMBER OF THE DEPENDANT PARAMETER (SEE TABLE BELOW).
7- 9	INPAR	NUMBER OF THE ATOM THE FIRST INDEPENDANT PARAMETER BELONGS TO. (SPECIAL PARAMETERS ARE ARBITRARILY INDICATED AS ATOM NUMBER 0).
10-12	INPAR	PARAMETER NUMBER OF THE FIRST INDEPENDANT PARAMETER. (ATOM NUMBER 0 AND PARAMETER NUMBER 0 DESIGNATES AN INITIALIZING CONSTANT ON A LINEAR DEPENDENCY FUNCTION).
13-20	CNPAR	COEFFICIENT OF FIRST RELATIONSHIP.
21-23	INPAR	ATOM NUMBER OF SECOND INDEPENDENT PARAMETER.
24-26	INPAR	SECOND INDEPENDENT PARAMETER NUMBER.
27-34	CNPAR	SECOND COEFFICIENT
35-37 38-40 41-48		SAME FOR THE THIRD INDEPENDENT PARAMETER.
49-51 52-54 55-62		SAME FOR THE FOURTH INDEPENDENT PARAMETER.
63-65 66-68 69-76		SAME FOR THE FIFTH INDEPENDENT PARAMETER.

REMARK
IF THE INDEPENDENT ATOM NUMBER IS ZERO, DESIGNATING A SPECIAL PARAMETER, AND THE CONSTRAINTS ARE NON LINEAR, THE SECOND AND FOURTH INDEPENDENT PARAMETER NUMBERS MAY BE NEGATIVE TO DENOTE THE END OF AN INCLUSIVE LIST BEGINNING WITH THE FIRST (THIRD) INDEPENDENT PARAMETER NUMBER.

ATTENTION

IF A LIST OF DEPENDENCIES IS READ THE END OF THE LIST MUST BE INDICATED BY AN END CARD. (SEE LABEL E IN COLUMN 1).

IF THERE ARE NO DEPENDENCIES THE END CARD MUST BE GIVEN.

TABLE OF THE PARAMETER NUMBERS

PARAM. NO.	PARAMETER	PARAM. NO.	PARAMETER	PARAM. NO.	PARAMETER
1	OCCUPANCY(OCCA) (SEE REMARK BELOW)	2	X	5	B OR BETA(11)
		3	Y	6	BETA(22)
		4	Z	7	BETA(33)
				8	BETA(12)
				9	BETA(13)
				10	BETA(23)
11	C(111)	21	D(1111)	36	E(11111)
12	C(222)	22	D(2222)	37	E(22222)
13	C(333)	23	D(3333)	38	E(33333)
14	C(112)	24	D(1112)	39	E(11112)
15	C(122)	25	D(1113)	40	E(11113)
16	C(113)	26	D(1122)	41	E(11122)
17	C(133)	27	D(1123)	42	E(11123)
18	C(223)	28	D(1133)	43	E(11133)
19	C(233)	29	D(1222)	44	E(11222)
20	C(123)	30	D(1223)	45	E(11223)
		31	D(1233)	46	E(11233)
		32	D(1333)	47	E(11333)
		33	D(2223)	48	E(12222)
		34	D(2233)	49	E(12223)
		35	D(2333)	50	E(12233)
				51	E(12333)
				52	E(13333)
				53	E(22223)
				54	E(22233)
				55	E(22333)
				56	E(23333)
57	F(111111)	67	F(111233)	77	F(122333)
58	F(222222)	68	F(111333)	78	F(123333)
59	F(333333)	69	F(112222)	79	F(133333)
60	F(111112)	70	F(112223)	80	F(222223)
61	F(111113)	71	F(112233)	81	F(222233)
62	F(111122)	72	F(112333)	82	F(222333)
63	F(111123)	73	F(113333)	83	F(223333)
64	F(111133)	74	F(122222)	84	F(233333)
65	F(111222)	75	F(122223)		
66	F(111223)	76	F(122233)		

REMARK
IN THE CURRENT VERSION OF THE PROGRAM NO DEPENDENCIES BETWEEN TOTAL OCCUPANCIES OF SITES ARE POSSIBLE. HOWEVER THIS MAY BE ACCOMPLISHED IN THE FOLLOWING WAY..
- YOU DEFINE A NULL SCATTERING CURVE ON AN ADDITIONAL SCAT. CURVE TYPE AND EXPONENT. FORM CARD.
- ON THE ATOM PARAMETER CARDS OF THE ATOMS WHO S OCCUPANCIES SHOULD

BE DEPENDANT YOU WRITE THE NUMBER OF THIS SCATTERING CURVE FOR SPECIES B (COLUMNS 3-4 ON CARD 2 OF THE ATOM PARAMETER CARDS).
- ON CARD 1 OF THE ATOM PARAMETER CARDS OF THESE ATOMS YOU HAVE TO WRITE FOR OCCUP (TOTAL OCCUPANCY) THE MAXIMUM OCCUPANCY WHICH IS POSSIBLE FOR SPECIES A ON THIS SITE.
  FOR OCCA YOU HAVE TO SET THE STARTING VALUE FOR THE OCCUPANCY OF SPECIES A.
- NOW YOU CAN DEFINE DEPENDENCIES BETWEEN THE PARAMETERS NO. 1 OF THESE ATOMS, E.G. DEPENDENCIES BETWEEN THE OCCUPANCIES OF SPECIES A. (THE DIFFERENCE TO THE MAXIMUM OCCUPANCY OF EACH SITE IS ALWAYS FILLED WITH THE NULL SCATTERING CURVE).

EXAMPLE

```
SCATTERING LENGTHS.. (NEUTRON DIFFRACTION)
 AG
0.      0.      0.      0.      0.      0.      0.      0.      6.02
 NULL
0.      0.      0.      0.      0.      0.      0.      0.      0.

 ATOM PARAMETER CARDS
 AG1     12  .3333 .26564
 1 2    .25    .0     .5     3.
 AG2      6  .6667 .13575
 1 2    .0     .5     .5     2.5

 ATOM REFINE CARDS
10001
00001
 DEPENDENCY CARDS
N 2  1  0  0 .6667    1  1 -2.
E
```

EXPLANATION
THE OCCUPANCY PER SITE OF AG2 ON 0,1/2,1/2 IS 2/3 MINUS TWO TIMES THE OCCUPANCY PER SITE OF AG1 ON 1/4,0,1/2.
(A LATER VERSION OF PROMETHEUS WILL BE CHANGED IN THIS POINT).

DIFFRACTOMETER CARD

(ONLY NEEDED IF NEW(8) IS GREATER THAN 5).

FORMAT (A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	MACHIN	INDICATOR FOR THE DEFINITION OF THE COORDINATE SYSTEM ON THE DIFFRACTOMETER USED FOR THE MEASUREMENT.
		BUSI THE COORDINATE SYSTEM DEFINITION OF BUSING AND LEVY IS USED. (SEE DESCRIPTION PART).
		DUMM A SPECIAL DEFINITION IS USED WHICH HAS TO BE PROGRAMMED BY THE USER. FOR DETAIL SEE DESCRIPTION PART.
		ANYTHING ELSE THE COORDINATE SYSTEM DEFINITION OF THE PHILIPS PW1100 DIFFRACTOMETER IS USED. (SEE DESCRIPTION PART).

ORIENTATION CARDS

(NEEDED ONLY IF NEW(8) IS GREATER THAN 5).

FORMAT OF EACH CARD (3F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES

CARD 1

1- 8	UB(1)	U11	COMPONENTS OF THE FIRST LINE OF THE
9-16	UB(2)	U12	ORIENTATION MATRIX. (DEFINITION OF THE
17-24	UB(3)	U13	ORIENTATION MATRIX SEE DESCRIPTION PART).

CARD 2

1- 8	UB(4)	U21	
9-16	UB(5)	U22	SECOND LINE.
17-24	UB(6)	U23	

CARD 3

1- 8	UB(7)	U31	
9-16	UB(8)	U32	THIRD LINE.
17-24	UB(9)	U33	

FORMAT CARD

(ONLY NEEDED IF NEW(8) NOT EQUQL 0).

FORMAT (18A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-72	FRMT	INDICATOR FOR THE FORMAT OF THE HKL-CARDS.
1- 4	STAN	THE HKL-CARDS ARE READ WITH THE STANDARD FORMAT (A3,10X,3I3,3X,I3,3X,F9.0,9X,F5.0) (SEQUENCE OF VARIABLES SEE HKL-CARDS BELOW OR NEW(8) ON THE MAIN CONTROL CARD). IF STAN IS TYPED IN COLUMNS 1-4 NO FURTHER MUST BE GIVEN ON THIS CARD.
	(A3,	THE HKL-CARDS TO BE READ HAVE NO STANDARD FORMAT. BEHIND (A3, THERE MUST FOLLOW THE REST OF THE FORMAT TO BE USED, WRITTEN IN STANDARD FORTRAN NOTATION. (THE BEGINNING WITH (A3, IS NECESSARY TO RECOGNIZE THE END CARD INDICATING THE END OF THE HKL-CARDS).

DATA DEFINING CARD

(ONLY NEEDED IF NEW(8) NOT EQUAL 0).

FORMAT (I2,2I1F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 2	ITEMP	INPUT UNIT INDICATOR
		0 HKL CARDS ARE ON STANDARD INPUT UNIT (IN).
		NOT 0 ITEMP IS THE LOGICAL NUMBER OF THE INPUT UNIT CONTAINING THE HKL-CARDS..
3	IFOBS	INTENSITY OR STRUCTURE FACTOR INDICATOR
		0 INTENSITIES IN CARDS.
		1 STRUCTURE FACTORS ON CARDS.
4	IWT	STANDARD DEVIATION INDICATOR
		0 STANDARD DEVIATION OF I ON CARDS. (I = INTENSITY).
		REMARKS
		IF THE STANDARD DEVIATION IS MODIFIED BY AN IGNORANCE FACTOR (PARAMETER WTFAC ON THIS CARD) THE FOLLOWING

EQUATION IS USED

SIGMA(F*F) = SQRT ((SIGMA(I))**2 + (WTFAC*I)**2)

TO CALCULATE THE STANDARD DEVIATION OF F THE FORMALISM OF REES IS USED (SEE DESCRIPTION PART).

1 STANDARD DEVIATION OF F ON CARDS.

REMARK
MODIFICATION BY AN IGNORANCE FACTOR (PARAMETER WTFAC ON THIS CARD) IS DONE IN THE FOLLOWING WAY

SIGMA(F) = SQRT((SIGMA(F))**2 + (WTFAC * F)**2)

2 WEIGHT ON CARDS.
IF REFINEMENT IS REQUESTED ON F THE PROGRAMME PRESUMES
WEIGHT = 1 / (SIGMA(F) **2)
(THIS PRESUMPTION IS USED IF SIGMA(F) IS MODIFIED BY AN IGNORANCE FACTOR AS DESCRIBED UNDER IWT = 1).
IF REFINEMENT IS REQUESTED ON F*F THE PROGRAMME PRESUMES
WEIGHT = 1 / (SIGMA(I) **2)
AND A MODIFICATION BY AN IGNORANCE FACTOR IS DONE AS DESCRIBED UNDER IWT = 0 .

3 LIKE IWT=0 BUT FOR CALCULATION OF THE STANDARD DEVIATION OF F INSTEAD OF THE FORMALISM OF REES THERE IS USED THE FORMULA
SIGMA(F) = 0.5 * SIGMA(I) / F

4 STANDARD DEVIATION OF I ON CARDS.
CALCULATION OF THE STANDARD DEVIATION OF F ACCORDING TO THE FORMULA OF REES.
THE VALUE OF SIGMA(F) CAN IN ADDITION BE MODIFIED BY THE ROUTINE WEIGHT TO BE WRITTEN BY THE USER.

5 STANDARD DEVIATION OF F ON CARDS.
THE STANDARD DEVIATION CAN BE MODIFIED BY THE ROUTINE WEIGHT TO BE WRITTEN BY THE USER.

5	IREJL	0/1	DO NOT READ/READ REFLECTIONS NOT TO BE INCLUDED IN THE REFINEMENT FROM REJECT-FILE
6-12	WTFAC	IGNORANCE FACTOR	

0. THE STANDARD DEVIATION WILL NOT BE MODIFIED BY AN IGNORANCE FACTOR.
NOT 0. THE STANDARD DEVIATION WILL BE MODIFIED BY THE IGNORANCE FACTOR WTFAC AS DESCRIBED UNDER THE PARAMETER IWT ABOVE.

MEASUREMENT CARD

(ONLY NEEDED IF NEW(8) NOT EQUAL 0).

FORMAT (2I1,2F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	INEUT	RADIATION AND MONOCHROMATOR INDICATOR

0 REFLECTIONS WERE MEASURED WITH XRAY-RADIATION USING A GRAPHITE MONOCHROMATOR MOUNTED ON THE DIFFRACTOMETER WITH A DIHEDRALE ANGLE OF 9 DEGREES. (IF NO MO-K-ALPHA RADIATION WAS USED INEUT MUST BE 2).
1 REFLECTIONS WERE MEASURED WITH NEUTRON

RADIATION.
2 REFLECTIONS WERE MEASURED WITH XRAY-RADIATION. READ IN THE MONOCHROMATOR DATA (MONOCHROMATOR CARD).

2 LPCORP LORENTZ AND POLARISATION CORRECTION SELECTOR

0 DO NOT CALCULATE A CORRECTION.
1 CALCULATE A LORENTZ AND POLARISATION CORRECTION (IF INEUT=1 ONLY LORENTZ CORRECTION).

3-10 WVLNGT WAVELENGTH IN ANGSTROMS

11-18 TBAR ABSORPTION WEIGHTED MEAN PATH LENGTH IN MICROMETERS TO BE USED FOR ALL REFLECTIONS. THE VALUE GIVEN HERE IS OVERWRITTEN, IF TBAR IS READ FROM THE HKL-CARDS (NEW(8) = 2 (7) OR 4 (9)).
(FOR A SPHERE TBAR MUST BE 3/2 TIMES THE RADIUS).

0 THE DEFAULT VALUE OF 300 MICROMETERS IS USED.
NOT 0 TBAR IS THE PATH LENGTH IN MICROMETERS.

MONOCHROMATOR CARD

(ONLY NEEDED IF NEW(8) NOT EQUAL 0 AND THE PARAMETER INEUT ON THE MEASUREMENT CARD EQUAL 2).

FORMAT (2F8.0,I2)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1- 8 DIHED DIHEDRALE ANGLE IN DEGREES.

9-16 TM IF ICOS = 0 TM = MONOCHROMATOR ANGLE IN DEGREES.
18 ICOS IF ICOS = 1 TM = SQUARE OF THE COSINE OF THE MONOCHROMATOR ANGLE.

PARTIAL CARDS

(ONLY NEEDED IF THE PARAMETER IPART ON THE MAIN CONTROL CARD IS NOT EQUAL 0 AND NEW(8)=0).

FORMAT (I2)

COLUMN NAME FUNCTION AND POSSIBLE VALUES

1- 2 I NUMBER OF THE ATOM TO BE DELETED .

0 INDICATOR THAT ALL PARTIAL CARDS WERE READ.
NOT 0 NUMBER OF AN ATOM. THE NEXT CARD WILL BE AGAIN A PARTIAL CARD.

HKL CARDS

(ONLY NEEDED IF NEW(8) NOT EQUAL 0 AND THE HKL-CARDS SHOULD BE READ FROM STANDARD INPUT UNIT (PARAMETER TEMP ON THE DATA DEFINING CARD EQUAL 0)).
THE INFORMATION READ FROM THE HKL-CARDS IS DESCRIBED UNDER THE PARAMETER NEW(8) ON THE MAIN CONTROL CARD, AND THE FORMAT OF THESE CARDS DEPENDS ON THE INPUT GIVEN ON THE FORMAT CARD.

CONTINUE CARD

FORMAT (4I1)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1	IEF	NEW CYCLE SELECTOR
		0 CALCULATE NO MORE CYCLE. END OF THE PROGRAMME REFINE.
		1 CALCULATE ONE MORE CYCLE. (THE CYCLE IS STARTED WITH READING THE CYCLE START CARD).
2	NFLAG	PARAMETER OUTPUT SELECTOR
		0 DO NOT PRINT ANY ATOM PARAMETERS ON THE UNIT WITH THE LOGICAL NUMBER IPUN (IPUN=04).
		1 PRINT UIJ-ATOMCARD OF XRAY SYSTEM. (FOR UIJ-ATOMCARD SEE XRAY SYSTEM).
		2 PRINT THE FOLLOWING CARDS
		SCALE FACTOR CARD EXTINCTION CARD ATOM PARAMETER CARDS SPECIAL PARAM. CARD (ODER SPECIAL VALUE CARD ALPHA PARAMETER CARD T-FACTOR TYPR CARD
		3 PRINT THE CARDS DESCRIBED UNDER NFLAG=1 PLUS THOSE UNDER NFLAG=2.
3-4	ISC1	LOGICAL NUMBER OF THE MAINFILE TO BE WRITTEN IF THIS IS THE LAST CYCLE OF THE CURRENT RUN.
		0 THE DEFAULT VALUE 10 WILL BE USED.
		NOT 0 ISC1 IS THE LOGICAL NUMBER OF THE MAINFILE.

S P H E R E

CARD ORDER SUMMARY OF THE PROGRAM SPHERE

TITLE	CARD
LABEL	CARD
INPUT UNIT	CARD
OUTPUT UNIT	CARD
ABSORPTION	CARD
CELL CONSTANT	CARDS
FORMAT	CARDS
LIST SELECTOR	CARD

NO CARD IS OPTIONAL

REMARK

THE CARD ORDERS OF SPHERE AND TDSCOR DIFFER FROM THOSE OF THE OTHER PROGRAMS OF THE SYSTEM PROMETHEUS. SPACE IS LEFT TO WRITE THE MEANING OF EACH PARAMETER IN FRONT OF ITS POSITION ON THE CARD SO THAT THE USER CAN INSERT OR CHANGE PARAMETERS WITHOUT HAVING TO REFER TO THE CARDORDER. (THE PARAMETERS ARE READ FORM THE CARDS WITH A FORMAT THAT AGREES WITH THE THE POSITIONS IN THE EXAMPLE BELOW)

EXAMPLE OF A CALL OF THE PROGRAM SPHERE

```
TITEL                     =LIKSO4 022C
LABEL                     =LIK022
INPUT -UNIT OF HKL CARDS  =1
OUTPUT-UNIT OF HKL CARDS  =11
```

```
MUE*R   =0.57707  RADIUS  = 0.335      WAVELENGTH = .71069
A       = 5.145          B       = 5.145          C       = 3.632
ALPHA   = 90.            BETA    = 90.               GAMMA= 120.
INPUT FORMAT (A3,10X,3I3,3X,2I3,F9.0,9X,F5.0)
OUTPUT FORMAT(A3,4X,A4,A2,3I3,3X,2I3,F9.0,F9.5,F5.0,7X,F8.4)
LISTING OF HKL CARDS=YES
```

FORMAT (7X,16A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
8-72	TITLE	ANY SEQUENCE OF SYMBOLS USED AS TITLE OF THE PROGRAM

LABEL CARD

FORMAT (7X,A4,A2)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
8-14	LABEL	ANY SEQUENCE OF SYMBOLS USED TO LABEL THE HKL CARDS

INPUT-UNIT CARD

FORMAT(25X,I5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
26-30	NUIN	LOGICAL NUMBER OF THE INPUT FILE CONTAINING THE HKL CARDS
		NOT 0 NUIN IS THE LOGICAL NUMBER OF THE INPUT FILE

OUTPUT-UNIT CARD

FORMAT (25X,I5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
26-30	NUOUT	LOGICAL NUMBER OF THE OUTPUT FILE
		0 THE DEFAULT VALUE 02 WILL BE USED
		NOT 0 NUOUT IS THE LOGICAL NUMBER OF THE OUTPUT FILE

ABSORPTION CARD

FORMAT (7X,F10.5,8X,F10.5,12X,F10.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
8-17	UMR	ABSORPTION COEFFICIENT * RADIUS OT THE CRYSTAL
27-36	RADIUS	RADIUS OF THE SPHERE IN MILLIMETERS
48-57	WLGTH	WAVELENGTH OF THE RADIATION IN ANGSTROEMS
		0 THE DEFAULT VALUE 0.71069 ANGSTROEM IS USED
		NOT 0 WLGTH IS THE WAVELENGTH IN ANGSTROEMS

CELL CONSTANT CARDS

CARD 1

FORMAT (7X,F10.5,6X,F12.5,7X,F10.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
8-17	A	LENGTH OF THE A-AXIS IN ANGSTROEMS
24-35	B	LENGTH OF THE B-AXIS

43-52	C	LENGTH OF THE C-AXIS

CARD 2

FORMAT (7X,F10.5,6X,F12.5,7X,Fl0.5)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
8-17	ALPHA	VALUE OF ALPHA IN DEGREES
24-35	BETA	VALUE OF BETA
43-52	GAMMA	VALUE OF GAMMA

FORMAT CARDS

CARD 1

FORMAT (13X,13A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
14-65	FORMIN	INPUT FORMAT FOR HKL CARDS THE FOLLOWING PARAMETERS ARE READ BY THE PROGRAM THE LABEL HKL, THE MILLER INDICES H, K, L, THE REJECT FLAG, THE SCALE GROUP. THE INTENSITY OR FOBS AND SIGMA 0 DEFAULT FORMAT USED IS (A3,10X,3I3,3X,2I3,F9.0,9X,F5.0) NOT 0 FORMIN IS THE INPUT FORMAT

CARD 2

FORMAT (13X,13A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
14-65	FOROUT	OUTPUT FORMAT FOR HKL CARDS 0 DEFAULT FORMAT USED IS (A3,4X,A4,A2,3I3,3X,2I3,F9.0,F9.5,F5.0,7X,F8.4) NOT 0 FOROUT IS THE OUTPUT FORMAT

LIST SELECTOR CARD

FORMAT (9X,A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
10-13	LIS	SWITCH FOR PRINT A LIST OF REFLECTIONS YES A LIST IS PRINTED NOT YES NO LIST IS PRINTED

T D S C O R

CARD ORDER SUMMARY OF THE PROGRAM TDSCOR

TITLE	CARD
INPUT-UNIT	CARD
OUTPUT-UNIT	CARD
TENSOR TYPE	CARD
TENSOR VALUE	CARDS
DETECTOR	CARD
SCAN	CARD
WAVELENGTH	CARD
TEMPERATURE	CARD
SPECIFIC WEIGHT	CARD
LIST SELECTOR	CARD
INTEGRATION	CARD
CELL	CARDS

```
  ROTATION            CARDS
* HKL                 CARDS
* END                 CARD


*   THESE CARDS ARE OPTIONAL
```

REMARK

THE CARDS FOR THE PROGRAM TDSCOR LIKE THOSE OF THE PROGRAM SPHERE DIFFER FROM THE CARDS OF THE OTHER PARTS OF THE SYSTEM PROMETHEUS. TEXT CAN BE INCLUDED ON THE CARDS WHICH EXPLAINS THE MEANING OF THE PARAMETERS. THE USER CAN INSERT HIS PARAMETER VALUES WITHOUT HAVING TO REFER TO THE CARD ORDER. (THE CARDS ARE NOT READ UNFORMATED. THE FORMAT IS ONLY CHOSEN SO THAT THE VALUES ARE READ AT THE POSITIONS SHOWN IN THE EXAMPLE BELOW).

EXAMPLE OF A CALL OF THE PROGRAM TDSCOR..

```
TDSCOR

THIS IS THE TITLE CARD FOR THE PROGRAM  TDSCOR
INPUT-UNIT OF HKL CARDS=            01
OUTPUT-UNIT OF HKL CARDS=        02
STIFFNESS

            1.15   0.39    0.18    0.00    0.00    0
                   1.15    0.18    0.00    0.00    0
                           1.18    0.00    0.00    0
                                   0.17    0.00    0
                                           0.17    0
                                                   0.38
DET-HEIGHT= 1.5  WIDTH=  2.
OMEGA-SCAN TILL  60. DEGREE   (PARAMETER SCT OF PW1100)
WAVELENGTH                     =0.70169
TEMPERATURE(C)                 = 615.
SPECIFIC WEIGHT                = 1.293
LISTING OF HKL-CARDS           = YES
NUMBER OF GRIDS FOR INTEGRATION =       2
    A= 3.7235 B= 3.7235  C= 3.881
ALPHA= 90. BETA= 90. GAMMA= 120.
ROTATION ANGLE OF CRYSTALL    LEFT    TILL MAXIMUM=      1.5
ROTATION ANGLE OF CRYSTALL    RIGHT   TILL MAXIMUM=      1.5
FINISH
```

TITLE CARD

FORMAT (18A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-72	TITEL	ANY SEQUENCE OF SYMBOLS USED AS A TITLE OF THE PROGRAM

INPUT-UNIT CARD

FORMAT (25X,Il0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
26-35	INUNIT	LOGICAL NUMBER OF THE INPUT FILE CONTAINING THE HKL-CARDS. 0 THE DEFAULT VALUE 01 WILL BE USED. NOT 0 INUNIT IS THE LOGICAL NUMBER OF THE INPUT FILE. (INPUT FILE CAN ALSO BE THE STANDARD INPUT UNIT).

OUTPUT-UNIT CARD

FORMAT (25X,Il0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES

26-35	OTUNIT	LOGICAL NUMBER OF THE OUTPUT FILE. 0 THE DEFAULT VALUE 02 WILL BE USED. NOT 0 OTUNIT IS THE LOGICAL NUMBER OF THE OUTPUT FILE

TENSOR TYPE CARD

FORMAT (A4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
l- 4	ITYPE	INDICATOR FOR COMPLIANCE OR STIFFNESS TENSOR GIVEN ON THE FOLLOWING TENSOR VALUE CARDS.
	COMP	COMPLIANCE TENSOR
	STIF	STIFFNESS TENSOR

TENSOR VALUE CARDS

THE FOLLOWING SIX CARDS CONTAIN THE VALUES OF THE TENSOR ELEMENTS.
(UNIT IN CASE OF STIFFNESS
GRAMMS*10**12/(CM*S**2) = 10**12 DYN/(CM**2)
AND THE INVERSE IN CASE OF COMPLIANCE).
BECAUSE BOTH TENSORS (COMPLIANCE TENSOR AND STIFFNESS TENSOR) ARE SYMMETRIC, ONLY THE DIAGONAL ELEMENTS AND THE ELEMENTS ABOVE THE DIAGONAL ARE READ BY THE PROGRAM.

CARD 1

FORMAT (6F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1-48	RMAT	VALUES OF THE FIRST LINE OF THE TENSOR. 1- 8 C(11) RESP. S(ll) 9-16 C(12) 17-24 C(13) 25-32 C(14) 33-40 C(15) 41-48 C(16)

CARD 2

FORMAT (8X,7F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
9-48	RMAT	VALUES OF THE SECOND ROW OF THE TENSOR STARTING WITH THE DIAGONAL ELEMENT. 9-16 C(22) RESP. S(22) 17-24 C(23) 25-32 C(24) 33-40 C(25) 40-48 C(26)

CARD 3

FORMAT (16X,4F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
17-48	RMAT	VALUES OF THE THIRD LINE OF THE TENSOR STARTING WITH THE DIAGONAL ELEMENT. 17-24 C(33) RESP. S(33) 25-32 C(34) 33-40 C(35) 40-48 C(36)

CARD 4

FORMAT (24X,3F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
25-48	RMAT	VALUES OF THE FOURTH LINE OF THE TENSOR STARTING WITH THE DIAGONAL ELEMENT. 25-32 C(44) RESP. S(44) 33-40 C(45) 41-48 C(46)

CARD 5

FORMAT (32X,2F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
32-48	RMAT	VALUES OF THE FIFTH LINE OF THE TENSOR STARTING WITH THE DIAGONAL ELEMENT. 32-40 C(55) RESP. S(55) 41-48 C(56) RESP. S(56)

CARD 6

FORMAT (40X,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
41-48	RMAT	C(66) RESP. S(66)

DETECTOR CARD

FORMAT (llX,F6.0,6X,F6.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
12-17	DCHI	HIGHT OF DETECTOR APERTURE IN DEGREES.
24-29	DNY	WIDTH OF DETECTOR APERTURE IN DEGREES.

SCAN CARD

FORMAT (15X,F6.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
16-21	SCT	SCATTERING ANGLE IN DEGREES FOR THE TRANSITION FROM MEASUREMENTS WITH THE OMEGA SCAN (BELOW SCT) TO MEASUREMENTS WITH THE THETA-TWO THETA SCAN (ABOVE SCT). (THIS ANGLE IS IDENTICAL WITH THE PARAMETER SCT OF THE PHILIPS PW1100 FOUR CIRCLE DIFFRACTOMETER).

WAVELENGTH CARD

FORMAT (llX,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
12-19	WVLNTH	WAVELENGTH IN ANGSTROMS. 0 THE DEFAULT VALUE 0.71069 ANGSTROMS IS USED. (MO-K(ALPHA) RADIATION) NOT 0 WVLNTH IS THE WAVELENGTH IN ANGSTROMS.

TEMPERATURE CARD

FORMAT (12X,A1,3X,F8.O)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
13	ITEMP	IDENTIFIER FOR THE UNIT OF THE TEMPERATURE C TEMPERATURE IS GIVEN IN DEGREES CELSIUS. NOT C TEMPERATURE IS GIVEN IN KELVIN.
17-24	T	MEASURING TEMPERATURE IN THE UNIT DEFINED BY ITEMP.

SPECIFIC WEIGHT CARD

FORMAT (16X,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
17-24	RHO	SPECIFIC WEIGHT IN GRAMMS/(CM**3).

LIST SELECTOR CARD

FORMAT (21X,4Al)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
22-25	IPUT	SELECTOR FOR PRINT A LIST OF THE HKL-CARDS WITH THE CORRECTED INTENSITIES. IF IN ONE OF THE FOUR COLUMNS A Y IS READ THE LIST WILL BE PRINTED (Y = YES). IF NO Y IS READ THE LIST WILL NOT BE PRINTED.

INTEGRATION CARD

FORMAT (32X,I8)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
33-40	IGRID	NUMBER OF GRIDS TO BE USED FOR THE GAUSSAIN INTEGRATION. 0 THE DEFAULT VALUE 20 WILL BE USED. NOT 0 IGRID IS THE NUMBER OF GRIDS TO BE USED.

CELL CARDS

THE FOLLOWING TWO CARDS CONTAIN THE PARAMTERS OF THE UNIT CELL.

CARD 1

FORMAT (3(2X,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
3-10	CELL	LENGTH OF THE A-AXIS IN ANGSTROMS
13-20		B-AXIS
23-30		C-AXIS

CARD 2

FORMAT (6X,F8.0,5X,F8.0,6X,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
7-14	CELL	VALUE OF ALPHA IN DEGREES
20-27		BETA
34-41		GAMMA

ROTATION ANGLE CARDS

THESE TWO CARDS ARE ALWAYS READ, BUT IF ONE OF THE TWO VALUES IS
THE INDIVIDUEL ROTATION ANGLES FOR EACH REFLECTION MUST BE GIVEN
ON THE HKL-CARDS.

FORMAT (51X,F8.0)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
52-59	SCMOG	CARD 1 ROTATION ANGLE OF THE CRYSTALL LEFT TILL PEAK IF ALGORITHMS LIKE THE LEHMANN-LARSON (ACTA-CRYST. A30,580(74)) ARE USED FOR THE DETERMI-NATION OF THE INTEGRATED INTENSITIES, SCMOG IS THE WIDTH OF THE CALCULATED REFLECTION PRO-FILE FROM THE LEFT (RIGHT) SIDE TO THE PEAK-MAXIMUM. 0 SCMOG IS INDIVIDUALLY GIVEN FOR EACH REFLECTION ON THE HKL-CARDS NOT 0 SCMOG IS GIVEN HERE
52-59	SCMOG	CARD 2 ROTATION ANGLE OF THE CRYSTALL RIGHT TILL PEAK (SEE AB0VE)

HKL-CARDS

(ONLY NECESSARY HERE IF ON THE INPUT UNIT CARD THE LOGICAL NUMBER OF
THE STANDARD INPUT UNIT WAS SELECTED).

FORMAT (A4,9X,3I3,3X,2I3,2F9.0.F5.0,lX,F6.4.lX,F6.4)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 4	LAB	LABEL TO RECOGNIZE THE END CARD (SEE BELOW).
14-22	IH	MILLER INDICES. 14-16 H 17-19 K 20-22 L
26-28	MREJ	INDICATOR FOR LESS THAN REFLECTIONS THE INDICATOR IS NOT USED IN THIS PROGRAM. IT IS ONLY REWRITTEN ON THE OUTPUT FILE.
29-31	ISC	SCALE GROUP THE SCALE GROUP IS NOT USED IN THIS PROGRAM. IT IS ONLY REWRITTEN ON THE OUTPUT FILE.
32-40	FI	INTENSITY
41-49	TBAR	ABSORPTION WEIGHTED MEAN PATH LENGTH (ONLY REWRITTEN ON THE OUTPUT FILE).
50-54	SIGMAI	STANDARD DEVIATION OF THE INTENSITY.
56-61	RU	WIDTH OF THE PEAK LEFT FROM MAXIMUM IN DEGREES.
63-68	RO	WIDTH OF THE PEAK RIGHT FROM MAXIMUM IN DEGREES. (RU AND RO ARE ONLY READ IF ROTATION ANGLE CARDS ARE EMPTY).

END CARD

(THIS CARD IS ONLY NECESSARY IF THE HKL CARDS ARE READ FROM THE
STANDARD INPUT UNIT).

FORMAT (A3)

COLUMN	NAME	FUNCTION AND POSSIBLE VALUES
1- 3	LAB	IDENTIFIER OF THE CARD END THE LAST HKL CARD WAS READ. THE INPUT STREAM OF THE PROGRAM IS TERMINATED.