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The Tangent Formula Program for the X-Ray Analysis of Noncentrosymmetric Crystals

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CONTENTS

Abstract	ii
Problem Status	ii
Authorization	ii
INTRODUCTION	1
BASIC DESCRIPTION OF THE PROGRAM	1
INSTRUCTION INPUT	3
Description of the Input Data	3
Sequence of Input Data — The Preparation and Arrangement of All the Input Data for Processing the Tangent Formula	8
OUTPUT DESCRIPTION	9
TAPE REQUIREMENTS	11
LIMITATIONS	11
ACKNOWLEDGMENTS	11
REFERENCES	11
APPENDIX A - Tangent Formula Program	13
APPENDIX B - Complete FORTRAN-63 Source Program Listing	14
APPENDIX C - Sample Input Control Cards	39
APPENDIX D - Program Output after Processing the Sample Input Control Cards in Appendix C	44

ABSTRACT

This report contains a description and operating instructions for the tangent-formula refinement program applicable to noncentrosymmetric crystals. This program is coded entirely in FORTRAN language for a large-sized memory computer and is completely listed in the Appendixes.

PROBLEM STATUS

This is a final report on one phase of the problem; work on the problem is continuing.

AUTHORIZATION

NRL Problem C07-03
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THE TANGENT FORMULA PROGRAM FOR THE X-RAY ANALYSIS OF NONCENTROSYMMETRIC CRYSTALS

INTRODUCTION

The uses of the tangent formula in x-ray crystal structure analysis are the refinement of the basic set of phases already determined and the generation of new phases associated with vectors whose normalized structure factors are fairly large (1). Utilization of the tangent formula also improves an approximate set of phases obtained from the partial structure of a crystal and provides additional phases through recycling processes from the original set (2). This formula was derived in 1956 by Karle and Hauptman (3). The current version requires high-speed-core storage equipment containing 65,536 48-bit words for data processing and is written entirely in FORTRAN-63 language designed to be run with the Drum Scope Monitor System on the Control Data 3800 computer located at the NRL Computation Center (4).

BASIC DESCRIPTION OF THE PROGRAM

The tangent-formula program consists of a main program and twelve subroutines, excluding the trigonometric and the computer system subroutines. The flow chart is illustrated in Appendix A, where most subroutines are grouped into three important sections, such as (a) symmetry transformation section, (b) sort section, and (c) sigma-2 calculation section.

TANGFORM is the main program, which not only reads in or lists out all the necessary information or data but also transfers proper controls to several subroutines which perform their own chores. The TANGFORM program manipulates the reflection data. These data contain the normalized structure factors, which are obtained from the experimental intensity data by several appropriate geometric corrections and a K-curve calculation (5). The K-curve calculation and geometric corrections are incorporated into the data reduction program written by H. Norment (6) and revised by Stephen Brenner. For each cycle of refinement in the TANGFORM program, the data containing fairly large magnitudes of the normalized structure factor are divided into two parts. The first one, labeled the basic set, comprises all the unique three-dimensional reflections with the phases associated with them; the second one comprises the vectors with no phases assigned. Each set can be read from the three different sources: (a) system card reader, (b) input tape read in either BCD or binary mode, and (c) tape generated from the last refinement. All or some reflections in the above two sets constitute the search deck, or $\vec{h}$ deck, chosen for the application of the two-vector interaction relationship.

The heart of the TANGFORM program is the utilization of the sigma-2 algorithm, whereby the $\vec{h}$ are obtained from the combinations of $\vec{k}$ and $\vec{h} - \vec{k}$. All the reflections in the basic set are expanded severalfold, depending on the space group, and this set comprises the $\vec{k}$, or $\vec{h} - \vec{k}$, deck and can be called the expanded deck. One of the most important features in the TANGFORM program is the provision for an automatic generation of symmetry-related vectors for most space groups. This operation is performed with the aid of the four routines comprised of TXPAND, GENCHK, GEN, and FLSFUN, giving the permutations of the Miller indices and the phase changes (7).

To speed up the sigma-2 interaction in the SEARCH routine, it is essential to sort all the expanded vectors lexicographically. TANGFORM calls for SRTSAB, SIFTUP, and EXCHG, all of which have the capacity of sorting thousands of three-dimensional data in a few seconds (8). To further speed up the sigma-2 interaction, the MKTBL routine prepares a pseudo address table for all the expanded Miller index values and also determines the maximum and minimum values of h, k, and l. For each search reflection $\vec{h}$ for which pairs $\vec{k}$ and $\vec{h} - \vec{k}$ are found, the ACTION routine performs three functions:

1. The phases are computed in the following manner:

$$\varphi_{\vec{h}} = \tan^{-1} \frac{\sum_{k_r} |E_{\vec{k}} E_{\vec{h}-\vec{k}}| \sin(\varphi_{\vec{k}} + \varphi_{\vec{h}-\vec{k}})}{\sum_{k_r} |E_{\vec{k}} E_{\vec{h}-\vec{k}}| \cos(\varphi_{\vec{k}} + \varphi_{\vec{h}-\vec{k}})}, \tag{1}$$

where the E values are the normalized structure factors and the φ values are the phases. For each vector $\vec{h}$, k_r is the total number of combinations of $\vec{k}$ and $\vec{h} - \vec{k}$ which are found. Phases are kept in a range $-\pi < \varphi \leq \pi$. This is taken care of automatically in the HEMIR routine. Phases whose vectors have particular symmetry properties, e.g., pure real, pure imaginary, or both, depending on the space group, are usually adjusted in the RESET routine.

2. The normalized structure factors are calculated in the following order:

$$A = \frac{\sigma_2}{\sigma_4^{1/2}} \sum_{k_r} E_{\vec{k}} E_{\vec{h}-\vec{k}} \cos(\varphi_{\vec{k}} + \varphi_{\vec{h}-\vec{k}}) \Big/ \text{No. of Contributors}, \tag{2}$$

$$B = \frac{\sigma_2}{\sigma_4^{1/2}} \sum_{k_r} E_{\vec{k}} E_{\vec{h}-\vec{k}} \sin(\varphi_{\vec{k}} + \varphi_{\vec{h}-\vec{k}}) \Big/ \text{No. of Contributors}, \tag{3}$$

$$E_c = (A^2 + B^2)^{1/2} \tag{4}$$

where

$$\sigma_n^m = \left(\sum_{j=1}^{N} Z_j^n \right)^m,$$

in which Z is the atomic number of j atoms and N is the total number of atoms in the unit cell.

3. The sums involved in the following R factors are accumulated for all search $\vec{h}$:

$$R_E = \frac{\Sigma \left| |E_{obs}| - |E_{calc}| \right|}{\Sigma |E_{obs}|}, \tag{5}$$

where R_E is the R factor for the normalized structure factors. At the end of each iterative cycle, all the calculated normalized structure factors are rescaled so as to be on the same level as the observed ones. Before going to the next cycle, each search reflection is subjected to three rejection criteria. The phases are rejected (a) if the

structure-factor magnitude $|E_h|_{calc}$ is too small, e.g., 0.3, (b) if the change in the phase value from one cycle to the next is too large, e.g., π, and (c) if the number of contributors is not large enough, e.g., 3. For criteria (a) and (c), the vector will be searched again in the following cycle, whereas for criterion (b), the vector will be discarded. After sufficient phases are generated, an E map may be computed employing the normalized structure factors as Fourier coefficients.

INSTRUCTION INPUT

The data input consists of several control cards and the vector data cards. These input cards are usually positioned at the end of the program cards, which together with the input cards are loaded from the system card reader. There are other vector data which are read from an auxiliary tape having a specific logical unit number.

Description of the Input Data

The input data are categorized into five main parts:

1. Symmetry transformation information
2. Reset phase information
3. Constant information for calculating normalized structure factors
4. Tape and rejection criteria information
5. Optional control information for manipulation of the reflection data and the vector card information

Symmetry Transformation Information — Description of the Input Data — A tabulation of the contents of card 1 is as follows:

Columns	1-5	6-10	11-72
Data	JSYM	CENTER	CMNT
Format	I5	F5.0	7A8,A6

Card 1 contains the following information:

1. For each space group, JSYM is the numbered sets of general equivalent positions for atoms not related by centric inversion or lattice translation.

2. CENTER determines whether the crystal is centrosymmetric or not. If it is centrosymmetric, CENTER is 0.0; otherwise, it is nonzero for noncentrosymmetric.

3. CMNT is the BCD information, which spells out the space group. For example, one can punch the following: P212121 D4/2 NO. 19 PAGE 385. A maximum of 62 characters is allowed.

A tabulation of the contents of card 2 is as follows:

Columns	1-5	6-10	11-15	16-20
Data	X	Y	Z	TRNSLTN
Format	I5	I5	I5	I5

Card 2 consists of symmetry matrix information for each space group. Each matrix contains three cards, listing a general equivalent position in terms of rotation and translation properties. The translation part can be expressed as an integer multiple of one-twelfth. For instance, if one has a general position, such as X + 1/2, -Y, -Z + 1/4, one can punch the following way:

1	0	0	6
0	-1	0	0
0	0	-1	3

The number of matrices is specified by JSYM in card 1.

Reset Phase Information — Adjustment Phase Card — A tabulation of the contents of card 3 is as follows:

Columns	1-27	28-72
Data	KIND	ALPH
Format	27I1	5A8,A5

Card 3 has the function of adjusting phases according to the special reflection type. Each Miller index is classified whether it is even (g), odd (u), or zero (0). Each vector type is located in the following column order:

Column	Vector Type	Column	Vector Type
1	0,0,0	15	g,g,u
2	0,0,g	16	g,u,0
3	0,0,7	17	u,0,0
4	0,g,0	18	g,u,u
5	0,g,g	19	u,0,0
6	0,g,u	20	u,0,g
7	0,u,0	21	u,0,u
8	0,u,g	22	u,g,0
9	0,u,u	23	u,g,g
10	g,0,0	24	u,g,u
11	g,0,g	25	u,u,0
12	g,0,u	26	u,u,g
13	g,g,0	27	u,u,u
14	g,g,g		

The KIND entry in the corresponding column position causes the phase to be adjusted in the following manner:

KIND	Function
1	REAL, e.g., 0 or PI
2	IMAGINARY, e.g., +PI/2 or -PI/2
3	No change
4	0
5	PI
6	+ PI/2
7	- PI/2
8	Between - PI and + PI
9	Between 0 and 2 * PI

ALPH is for input of Hollencth information, e.g., the name of the space group and its listing number in the International Tables. It mainly serves to identify this reset card.

Constant Information for Calculating Normalized Structure Factors — Constant Card — A tabulation of the contents of card 4 is as follows:

Columns	1-15	15-30
Data	SIG2	SIG4
Format	FI5.3	FI5.3

SIG2 and SIG4 are the σ_2 and σ_4 constants used for calculating A and B in Eqs. (2) and (3). The latter are used to compute the normalized structure factors. Note that the program will take the square root of SIG4 in the denominators for both the A and B parts.

Tape and Rejected Criteria Information Card — The control card provides information in the logical unit of several tapes, serves the option of listing necessary information, and gives specifically the rejection criteria for accepting phases.

A tabulation of the contents of card 5 is as follows:

Column	1-3	4-6	7-9	10-12	13-15	16-18	19-21	22-24	25-27	28-31	32-35	36-72
Data	IRMTR	IFLMTR	MTD	NTD	MTR	MTW	LISTX	LISTK	KCOUNT	ERJ	CHANGE	FMT
Format	I3	I3	I3	I3	I3	I3	I3	I3	I3	F4.2	F4.2	4A8, A5

Card 5 contains all the input parameters which are explained as follows:

1. IRMTR represents the binary cycle-tape rewind options for tape with the logical unit specified for MTR (card 5, part 5). The options are set up in the following table:

IRMTR	Options
-1, -2	Initial rewind only
-3	Initial rewind; IRMTR will be reset to zero before search technique takes place
0	Initial rewind before data are expanded and search technique takes place
+1, +2	No rewind
3	No initial rewind; IRMTR will be reset to zero before search technique occurs

These options are useful when distinct data are stacked on one tape having logical unit MTR.

2. IFLMTR refers to the number of the block deck to be skipped over after the IRMTR options. Note that each block is terminated with a 200 in the h field. If IFLMTR is blank or a negative number, this acts as a no operation code.

3. MTD is the logical unit number for the tapes containing all the data to be submitted for expansion. If MTD is positive, the tape will be rewound. Otherwise, it will

not be rewound. If MTD is zero or blank, this will be reset to the standard or system input number, which is 60.

4. NTD is the logical unit number for the tape containing all the data to be submitted for expansion. If NTD is positive, the tape will be rewound. If it is negative, rewinding will not take place. NTD will be automatically reset to logical unit 60, a standard input number, if NTD is zero or blank.

5. MTR is the logical number for the binary tape containing all the data to be used for expansion. It is a cycle tape. If MTR is zero or blank, the program will reset MTR equal to 25 automatically.

6. MTW is the binary output tape number. It will be reset to 25, if MTW equals to zero. If MTW is less than zero, the tape will be rewound; otherwise, no rewind will take place. Note usually MTW and MTR are one and the same tape if one data set is used in sequential cycles.

7. LISTX is the number of reflections for which symmetry mates are listed on the standard output.

8. LISTK is the number of reflections for which sigma-2 interactions are listed on the standard output.

9. KCOUNT is the rejection factor number. If the interaction count is less than the KCOUNT, a new phase value will not be assigned to the vector and will be redetermined in the next cycle.

10. ERJ is the normalized structure factor rejection factor. If the calculated normalized structure factor is less than ERJ, then the reflection associated with this calculated normalized structure factor will be rejected and will be entered again in the next cycle. For example, values between 0.3 and 0.5 can be used.

11. CHANGE is the phase rejection factor. A vector will be rejected and will not be used again in the program, if the change in the phase values from one cycle to the other is greater than the CHANGE magnitude. If CHANGE is zero or blank, it will be reset to π.

12. FMT is the format specification for the BCD data loaded from the standard input system. The specification list includes the left and right parentheses and also contains editing codes, such as:

Iw = decimal integer conversion,

Fw·d = single precision floating point without exponent,

and

wX = intraline spacing,

where w and d are unsigned integer constants. As a typical example for a vector card containing the Miller indices, the normalized structure factor, and the phase information, the format specification can be punched as (3I5, F10.3, F5.1).

Optional Control Information for Manipulation of the Reflection, Data and the Vector Card Information – This control card contains many options for handling data checks and is usually read from the system input source. The data deck is input either from the system or auxiliary source, as determined by the tape and rejected criteria information card. The data deck is logically divided into two parts. The first part consists of vectors with the attached phases, and the second part consists of vectors whose phases have

not been assigned. The amount of each logical type of data and the interpretation of the actual data are controlled by two features: (a) certain information on the control card and (b) the position of the optionally included control cards within the deck. A card within the data is recognized as a control card by the occurrence of 200 in the h (Miller index) field. The control function instigated by the appearance of the 200 card in the data deck overrides specifications provided by the initial control card. This control card (card 6) is described as follows:

Columns	1-4	5-8	9-12	13-16	17-20	21-24	25-28	29-30	31-32	33-72
Data	INE	IDE	INS	IDS	INEP	IDER	INSP	JFMTB	LSQ	TITLE
Format	I4	I4	I4	I4	I4	I4	I4	I2	I2	5A8

The variable INE is a number to indicate how much input data is read from the binary tape to be submitted for the symmetry expansion. If INE is greater than 0, all data in the binary tape will be read up to 200 in the h field. If INE is equal to 0, there are no input data. If INE is less than 0, the number of vectors read from the binary tape is equal to the magnitude of INE.

The variable IDE is a number to indicate how much input data can be read from the standard input source to be submitted for the symmetry expansion. If IDE is greater than 0, all data from the standard input source will be read up to 200 in the h field. If IDE is equal to 0, there are no standard input data. If IDE is less than 0, only the magnitude of IDE will be stored into the memory from the standard input system.

The variable INS is a number to indicate how many vectors in the disk are to be used for the search technique. If INS is greater than 0, the number of reflections is the sum of the IDE and INE as described above. If INS is equal to 0, no data deck will be searched at all. If INS is less than 0, the input on count will be equal to the magnitude of INS.

The variable IDS is a number to indicate how much input data can be read from the standard input source to be submitted for the search technique. If IDS is greater than 0, all the data will be loaded from the system input up to the 200 card. If IDS is equal to 0, there are no data to be used for searching. If IDS is less than 0, the magnitude of IDS will be stored into the memory from the standard input equipment.

INEP deals with the disposition of vectors input from the binary tape. If the INEP indicator is 0, all reflections will be submitted for expansion, and none of them will be passed by. However, if INEP is any number other than 0, the vectors will be first read in from the binary tape according to the magnitude of INE (e.g., INE is less than 0), and then the remaining vectors up to the 200 termination record will be copied into the disk and will not be submitted for expansion.

IDER is the test flag to indicate whether the rejected reflections should be read in. If IDER is equal to 0, no rejected vectors will be introduced. If IDER is greater than 0, input rejected reflections (up to the 200 card) will be read in before the BCD input data, specified by IDE, are submitted for expansion.

INSP deals with the disposition of vectors input from the disk. If INSP is equal to 0, each vector from the disk will be submitted for search. If INSP is greater than 0, the data will be copied from the disk to the binary cycle tape (up to the 200) without performing any search. If it is less than 0, the number of data on the basis of the magnitude of INSP will be copied from the disk to the binary cycle tape. The remaining vectors will be submitted to search or discard, depending on the value of INS.

A test flag JFMTB indicates which control card is to be read in the next cycle. If JFMTB is 0, 1, or 4, the manipulating data card will be read next. If JFMTB is 2 or 5, the tape and rejected criteria information card will be read next. If JFMTB is greater than 3, no conversion of the phase angle values to radians is required. However, in the BCD input data, all phase angle values are assumed to be in degrees and will be converted automatically to radians.

LSQ is the indicator variable for processing the following options: (a) if LSQ is 0 or 1, the tangent-formula calculation will be performed and (b) if LSQ is 3, normalized-structure-factor calculation by the tangent formula will be performed without phase adjustment.

TITLE is the Hollerith information. A maximum of 40 characters are allowed. It is useful for the purpose of naming the crystals and specifying which cycle the tangent-formula program performs.

NOTE: The entire calculation will be terminated if control card 7 is entirely 0 or blank.

Card 7 or the reflection card contains the following information:

Data	h	k	l	E	P_1	P_2	P_3	P_N	. . .

The vector card comprises (a) the Miller indices, e.g., h, k, l, which are typically punched in the fixed-point mode (I), (b) the observed normalized structure factor E, and (c) the phases P, both of which are in the floating-point mode.

In cases where several phase possibilities are assigned for a particular reflection, one may punch in as many fields as there are on a card. A particular phase to be read in can easily be handled by specifying the variable format described by card 5, part 12.

Note that the phase are usually expressed in degrees. If the phase contains a number greater than the radian value 15, the vector associated with it will be rejected and will be reused in the next cycle of refinement.

A termination card, or 200 card, is defined as a card with a number 200 in the h field. It is generally used at the end of every vector data set so as to let the program give the total count automatically.

Sequence of Input Data — The Preparation and Arrangement of All the Input Data for Processing the Tangent Formula

The composite data deck is set up in the following way:

1. Transformation matrices
2. Phase reset information
3. Constant card
4. Tape and rejected criteria information card
5. Manipulating data card
6. Reject vector cards (if required)
7. BCD data cards including phase information (if required)
8. Binary data with phase information from tape (if required)
9. Pass binary data with phase information from tape (if required)
10. BCD data card excluding phase information (if required)

11. Pass binary data with no phase information
12. Binary tape with no phase information

etc.

The information control card for every new cycle, except the first one, usually begins with one of the control cards, such as 4 or 5, so as to continue the cycling processes. It is noted that the vector data in 7, 8, and 9 contain not only reflections and normalized structure factors but also has phase angle information. These data are to be used for expansion and searching. On the other hand, the vector data in 10, 11, and 12 have no phase values assigned to them and are used for the searching process only. The binary data in 8, 9, 11, and 12 are usually generated by the program from the last cycle in the course of the refinement process. Thus, the only vector data that can be prepared by the user would be in 6, 7, and 10, since the data are easily punched on cards. It is noted that the data cards in 6, 7, and 10 all use the same variable format described in card 5, part 12.

OUTPUT DESCRIPTION

Most of the output is self-explanatory. The output consists of nine parts (consult Appendix D concurrently with reading the following information):

1. The leading one-page output occurs immediately after reading the symmetry, reset, and constant cards. The preliminary output consists of:

A. Matrix number
B. Rotation matrix
C. Translation vector in twelfths
D. Holerith information
E. Phase adjustment entries
F. Sigma-2 and sigma-4 values

2. On the next page is a line output, which occurs immediately after reading the manipulating data card and before any data vectors are read. Usually, it prints the summary of the following results from the previous cycle:

A. Elapsed time in minutes
B. INEC (total number of binary input vectors for expansion)
C. IDEC (total number of BCD vectors submitted for expansion)
D. NBRJ (total number of reflections rejected from the rejected criteria)
E. NCSAVE (total number of expanded reflections)
F. INSC (total number of pass search binary data)
G. IDSC (total number of search BCD data)
H. INSN (total number of search binary data)
I. NBASIC (total number of reflections used for expansion)

3. The next line is a printout of the tape and rejected criteria information card, and all the variables have already been described in "Tape and Rejected Criteria Information." This output line serves the purpose for the user to verify his punching control card correctly.

4. This output lists the symmetry expansion of the basic reflections. This output is not always obtained, as it depends on the option of the program user. This output for each basic reflection consists of:

A. Miller indices h, k, l
B. Observational normalized structure factors
C. Phases

5. This section prints out the vectors rejected on the basis of the three criteria described in the description of the program. For each rejected vector, the list is as follows:

A. Miller indices h, k, l
B. Normalized structure factors
C. Phases in radians
D. Calculated structure factors
E. Calculated phases in radians
F. Total number of contributors

6. The output is mainly a listing of the tape and rejected criteria information card and a brief summary of the result of the expansion process:

A. Title of the manipulating data card
B. NC (total number of expanded vectors in the current cycle)
C. INEC (total number of binary data for expansion)
D. IDEC (total number of BCD data for expansion)
E. LSQ - option
F. NBRJ (total number of rejected vectors due to criteria)
G. NBASIC (total number of vectors with attached phases)
H. IRMTR - option for MTR tapes
I. IFLMTR - option for MTR tapes
J. MTD - option for expanded data tape
K. NTD - option for search data tape
L. MTR - option for binary input tape
M. MTW - option for binary output tape
N. ERJ (normalized structure factor rejection value)
O. CHANGE (upper limit for phase changes)
P. KCOUNT (upper limit for the number of contributors)

7. This section is a typical sigma-2 listing. The output prints out the list of $\vec{k}$, $E_{\vec{k}}$ and $\vec{h} - \vec{k}$, $E_{\vec{h}-\vec{k}}$ for each $\vec{h}$, $E_{\vec{h}}$. This output either is or is not obtained at the option of the program user.

8. The output lists the results for all the reflections in each cycle. The printout for each vector is as follows:

A. Miller indices h, k, l
B. Observed phases
C. Calculated phases
D. Observed normalized structure factors
E. Calculated normalized structure factors
F. Real part A of the normalized structure factors
G. Imaginary part B of the normalized structure factors
H. Total number of interactions

9. The tangent-formula statistics are printed out just before the end of every cycle. The output result is:

A. R factors for the normalized structure factors
B. Scale factors for the calculated normalized structure factors
C. The overall scale factors

D. Total number of reflections processed
E. Total number of reflections bypassed

TAPE REQUIREMENTS

All the tapes available for operating the tangent-formula program are listed in the following table:

Symbol	Logical Unit	Description
MR	60	Standard input
MW	61	Standard output
MTR	25	Binary cycle tape
MTW	25	Auxiliary binary cycle tape
MTD	60	BCD tape for expansion
NTD	60	BCD tape for search
IDISK	2	Special auxiliary tape
ISK	3	Special auxiliary tape

At the NRL Computation Center under the CDC 3800 Drum Scope Monitor, the physical equipment for L.U. 60 is the card reader and that for L.U. 61 is the on-line printer. L.U. 02 and 03 sources could either be magnetic tapes or disks. The only tape that must be saved is the binary cycle tape (L.U. 25) and can be used as an input tape for the Fourier program. Note that the user may use different logical unit numbers for MTR, MTW, MTD, and NTD.

LIMITATIONS

There are only two restrictions imposed on this program for a computer containing 65,536 words: (a) the program will accommodate no more than 4650 expanded reflections and (b) the total number of rejected input vectors must not be greater than 100. For the computer whose memory size is less than 65,536 words, one can modify this program by reducing the dimension size in common block of /1/, REFLCT and EXPAND.

ACKNOWLEDGMENTS

We are indebted to Dr. Jerome Karle for his suggestions regarding the development of the program for the application of the tangent formula. We also thank Drs. Holden and Stewart for furnishing us the general space group transformation routines.

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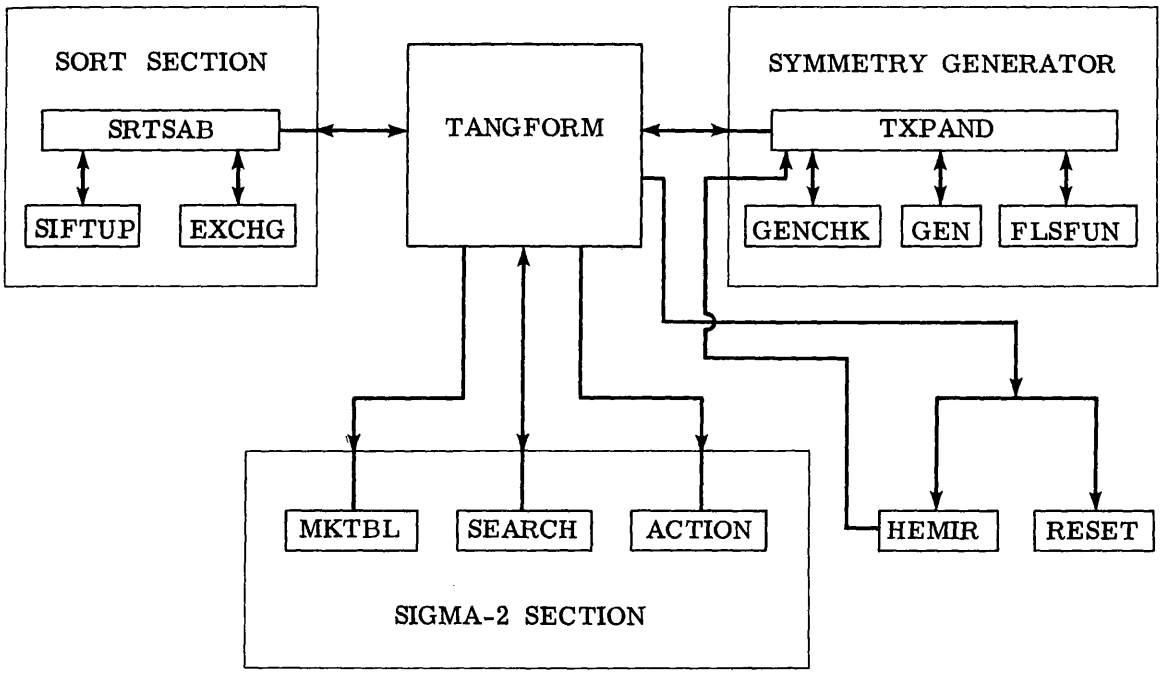
Appendix A

TANGENT FORMULA PROGRAM



Appendix B

COMPLETE FORTRAN-63 SOURCE PROGRAM LISTING

The complete FORTRAN source program listings are reproduced in this appendix.

```
      PROGRAM TANGFORM
C XTAN   SIGMA-2 TANGENT FORMULA SCHEDULAR
C        STEPHEN BRENNER,NRL  VERSION 11/09/67
      COMMON ISPARE(25),F(50)
      BANK,(1),/REFLCT/,(0),TANGFORM,/1/
      COMMON /REFLCT/ H(4650),K(4650),L(4650),E(4650),R(4650),FC(4650)
      COMMON /1/        AP(4650),BP(4650),CNTRB(4650)
      DIMENSION  HREJ(100),KREJ(100),LREJ(100)
      DIMENSION HKL(3),IT(150),TITLE(9),FMT(9)
      LOGICAL TZ,TP,T,BINSW
      LOGICAL EZW,CYCLE,SFCPT
      INTEGER H,HKL,HE,HLT,HREJ
      EQUIVALENCE (F(1),FE),(F(2),FR),(F(3),BE),(F(4),BR),(F(5),BN)
      EQUIVALENCE (F(6),PA),(F(7),PB)
      EQUIVALENCE (F(50),SCLALL),(F(49),CHANGE),(ISPARE(5),LISTK)
      EQUIVALENCE (F(48),CEZW)
      EQUIVALENCE (HKL(1),IH),(HKL(2),IK),(HKL(3),IL)
C              SYMMETRY GENERATER STORAGES
      COMMON/GENRTR/KTURE,JSYM,JGEN,KK,JDESIG,CENTER,TJ,I3,ME
     1              ,MSYM(3,4,48),JGENER(146),IDENT(48),JHP(3,48)
     2              ,IBLONG(48),ID(96),INDXP(3)
      DIMENSION KKK(48),JSIGN(48)
      EQUIVALENCE (ID(1),KKK(1)),(ID(49),JSIGN(1)),(I3,I4)
C                 CALLING PROGRAM DEPENDENT
      COMMON/EXPAND/HE(96),KE(96),LE(96),EE(96),RE(96),EX(96),AX(96),
     1BX(96)
     2              ,JH,JK,JL,FI,RI,CE,RA,RB
      COMMON/ATOMS/SIG2,SIG4
C        ***********************************************
      MR=50
      MW=61
      IDISK=4
      ISK=3
      ITLWD=5
      HLT=200
      LIMITH=500
      LIMITK=500
      LIMITL=500
      INSC1=0
C
      IDIMS=4650
      NCOS=1000
      B=100.
      SCLALL=0.0
      PI=3.1415926535898
```

```
      CNVRT=-7.
C     CNVRT=3.3
      CYCLE=.TRUE.
      EZW=.FALSE.
      I3=MW
      TIME1= TIMEF(XX)
C
C                          READ SYMMETRY MATRICES
            CALL TXPAND
C         READ FIXED PHASE ADJUSTMENT TABLE
            B=RESET(HKL,B)
C
      READ 2,SIG2,SIG4
    2 FORMAT (2F15.3)
      WRITE (MW,3) SIG2,SIG4
    3 FORMAT ( * SIG2=*,F15.3,* SIG4=*,F15.3)
      IF(SIG2.LT.1.0) SIG2=1.0
      IF(SIG4.LT.1.0) SIG4=1.0
      SIG4=SQRT(SIG4)
C                                          INPUT PARAMETERS FOR WHOLE JOB
   25 CONTINUE
C
      READ(MR,55)IRMTR,IFLMTR,MTD,NTD,MTR,MTW,LISTX,LISTK,KCOUNT
     1,ERJ,CHANGE,(FMT(I),I=1,5)
   55 FORMAT (9I3,2F4.2,4A8,A5)
C
      IF(PRJ.EQ.0.0)PRJ=PI
      IF (MTR.EQ.0) MTR=25
      IF (MTW.EQ.0) MTW=25
      ITEMP=MTW
      MTW=IABS(MTW)
      IF(ITEMP.LT.0) REWIND MTW
      ISPARE(1)=MTW
      ISPARE(2)=MTR
      IF( IRMTR.LE.0) REWIND MTR
      ITEMP=MTD
      MTD=IABS(MTD)
      IF(MTD.EQ.0) MTD=MR
      IF(ITEMP.GT.0.AND.MTD.NE.MR) REWIND MTD
      ITEMP=NTD
      NTD=IABS(NTD)
      IF(NTD.EQ.0) NTD=MR
      IF(ITEMP.GT.0.AND.NTD.NE.MR) REWIND NTD
   60 IF(IFLMTR.LE.0) GO TO 65
   61 READ(MTR) JH
      IF(JH.LT.HLT) GO TO 61
      IFLMTR=IFLMTR-1
      GO TO 60
   65 CONTINUE
C                READ CONTROL INFORMATION, INITIALIZE EACH SET
   75 CONTINUE
C
  100 READ(MR,105)INE,IDE,INS,IDS,INEP,IDER,INSP,IFMTB,LSQ,
     1(TITLE(I),I=1,ITLWD)
C
  105 FORMAT(7I4,2I2,5A8)
C
      RADNS=PI/180.
      IF (IFMTB.GE.3) RADNS=1.0
      IFMTB=MOD(IFMTB,3)
      IF(IFMTB.LT.1) IFMTB=1
      IF(LSQ.LT.1) LSQ=1
      ISPARE(3)=LSQ
      CLOCK= TIMEF(XX)
      ELAPSE= (CLOCK-TIME1)/60000.
```

```
      TIME1= CLOCK
  106 CONTINUE
      WRITE(MW    ,120)ELAPSE,INEC,IDEC,NBRJ,NCSAVE,INSC,IDSC,INSN,NBASIC
     1,(TITLE(I),I=1,ITLWD),INE,IDE,INS,IDS,INEP,IDER,INSP,IFMTB,LSQ
  120 FORMAT(17H1ELAPSED MINUTES=F9.3,2H*,//56H   INEC   IDEC   NBRJ NCS
     1AVE   INSC   IDSC   INSN NBASIC,/8I7,////1H 5A8 //  63H    INE
     2IDE   INS    IDS    INER   IDER   INSP   IFMTB   LSQ  , /9I7)
C
C                                          INITIALIZE  IO
      REWIND IDISK
      IF(IRMTR.EQ.0) REWIND MTR
      IF(IABS(IRMTR).GE.3) IRMTR=0
C                                          COUNTS
C AFTER FIRST CALL, SSWF VALUE ALTERED ONLY BY SIGNAL KEY AT CONSOLE
      IF (SENSE SWITCH 4) 123,124
  123 STOP
  124 IF(INE.EQ.0.AND.IDE.EQ.0.AND.INEP.EQ.0) RETURN
C
      NC=0
      INEC=0
      IDEC=0
      INSC=0
      IDSC=0
      JH=0
      NBASIC=(
      NBRJ=0
C                                          READ REJECTS
  125 NREJ=0
      IF(IDER.EQ.0) GO TO 140
  130 NREJ=NREJ+1
      READ(MR,FMT) HREJ(NREJ),KREJ(NREJ),LREJ(NREJ)
      IF(HREJ(NREJ).LT.HLT) GO TO 130
      NREJ=NREJ-1
  140 CONTINUE
C                                          INPUT TO EXPANSION
      IF(INE.EQ.0) GO TO 200
C                                          BINARY INPUT
  150 INBR=1
      INM=IDIMS
      IF(INE.LT.0) INM=IABS(INE)
  160 INEC=INEC+1
      IF(INEC.GT.INM) GO TO 190
      READ(MTR) JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
      IF(JH.LT.HLT) GO TO 250
  190 INEC=INEC-1
  200 CONTINUE
C                                          BINARY PASSING INPUT
      IF(INEP.EQ.0.OR.JH.GE.HLT) GO TO 209
      INBR=3
  201 INEC=INEC+1
      READ(MTR) JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
      IF(JH.LT.HLT) GO TO 250
      INEC=INEC-1
  209 CONTINUE
      IF(IDE.EQ.0) GO TO 245
C                                          BCD INPUT
      INBR=2
      INM=IDIMS
      IF(IDE.LT.0) INM=IABS(IDE)
  210 IDEC=IDEC+1
      IF(IDEC.GT.INM) GO TO 240
      READ(MTD,FMT) JH,JK,JL,EI,RI
              IF( JH.GE.HLT ) GO TO 240
C                                   VARIABLE FORMAT
```

```
C         PHASE IS ASSUMED GIVEN IN RADIANS, UNLESS INPUT VALUE
C              EXCEEDS * CNVRT=3.3 * IN WHICH CASE CONVERSION
C              FACTOR FROM DEGREES TO RADIANS IS APPLIED.
      IF( ABS(RI) .GT. CNVRT) RI=RI*RADNS
      CE=EI
      BR=RI
      BN=0.0
      RA=0.0
      RB=0.0
C             REJECT ENCODED PHASE REFLECTIONS
         IF(RI.GE.6.3) GO TO 256
C        REFLECTION ACCEPTANCE BASED ON INDEX VALUES
      IF( IABS(JH).GT.LIMITH ) GO TO 256
      IF( IABS(JK).GT.LIMITK ) GO TO 256
      IF( IABS(JL).GT.LIMITL ) GO TO 256
      GO TO 260
  240 IDEC=IDEC-1
  245 CONTINUE
      GO TO 300
C                                PROCESS REJECTIONS
  250 CONTINUE
C                                REJECT FOR SMALL E
      IF(CE.LT.ERJ) GO TO 256
C                                REJECT FOR LOW ACTIVITY
      IF(BN.LT.FLOAT(KCOUNT)) GO TO 256
C                                REJECT FOR DISPARATE PHASES
  251 CONTINUE
      IF (INEC.GT.INSC1) GO TO 252
      TPP= ABS(RI-BR)
      IF (TPP.GT.PI) TPP=2.0*PI-TPP
      IF (TPP.GE.CHANGE) GO TO 256
  252 CONTINUE
C                                REJECT IF LISTED REJECTION
      IF(NREJ.LE.0) GO TO 260
      DO 255 J=1,NREJ
      IF(JH.NE.HREJ(J)) GO TO 255
      IF(JK.NE.KREJ(J)) GO TO 255
      IF(JL.EQ.LREJ(J)) GO TO 256
  255 CONTINUE
      GO TO 260
C
C                                LIST REJECTS AND RETRIEVE NEXT RECORD
  256 NBRJ=NBRJ+1
      IF (NBRJ.EQ.1) WRITE (MW,258)
  258 FORMAT (////33X,*H     K     L        EI          R          CE          BR
     1          NN    * //)
      WRITE (MW,257) JH,JK,JL,EI,BR,CE,RI,BN
  257 FORMAT (*                        REJECTED *,3I5,5F10.4)
      CE=EI
      BR=RI
      BN=0.0
      RA=0.0
      RB=0.0
      XTRA1=0.0
      XTRA2=0.0
      WRITE(ISK  ) JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
      GO TO (160,210,201),INBR
  260 CONTINUE
C
  262 CONTINUE
C                                        WRITE DISK FOR SEARCH
      WRITE(IDISK) JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
C                                        EXPAND OR PASS
      GO TO (265,265,201),INBR
```

```
  265 CONTINUE
C
C                                                EXPAND
            CALL TXPAND
C
      IF( NC+ME .GE. IDIMS )  GO TO 280
      NBASIC=NBASIC+1
      DO 270 J=1,ME
      NC=NC+1
      H(NC)=HE(J)
      K(NC)=KE(J)
      L(NC)=LE(J)
      E(NC)=EE(J)
      R(NC)=RE(J)
      EC(NC)=EX(J)
      AP(NC)=AX(J)
      BP(NC)=BX(J)
      CNTRB(NC)=BN
C                    RESET FOR *EZW*
  270 CONTINUE
      NCSAVE=NC
      IF(LISTX.LT.1) GO TO 280
      LISTX=LISTX-1
      WRITE(MW,275) (HE(J),KE(J),LE(J),EE(J),RE(J),
     1 J=1,ME)
  275 FORMAT (10H0 EXPAND  /*0    H     K     L        E       PHASE */
     1          (3I5,2F10.4) )
  280 GO TO (160,210),INBR
  300 CONTINUE
      LISTX=0
C                                                INITIALIZE SEARCH
C
      WRITE(IDISK) HLT,JK,JL,B,B,B,B,B,B,B,B,B
      IF (NBRJ.LE.0) GO TO 310
      REWIND ISK
      IBRJ=0
  305 IBRJ=IBRJ+1
      READ (ISK ) JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
      WRITE(IDISK)JH,JK,JL,EI,RI,CE,BR,BN,RA,RB,XTRA1,XTRA2
      IF (IBRJ.LT.NBRJ) GO TO 305
      REWIND ISK
  310 CONTINUE
      IF(IRMTR.EQ.0) REWIND MTR
      REWIND IDISK
C                                                PRINT PARAMETERS
      WRITE(MW,315) (TITLE(I),I=1,ITLWD),NC,INEC,IDEC,LSQ,NBRJ,NBASIC,
     1IRMTR,IFLMTR,MTD,NTD,MTR,MTW,ERJ,PRJ,KCOUNT
  315 FORMAT (1H1,5A8//*   NC    INEC  IDEC   LSQ  NBRJ NBASIC IRMTR IFLM
     1TR MTD    NTD  MTR   MTW       ERJ      CHANGE  KCOUNT */12I6,2F10.4
     2,I6///)
  317 CONTINUE
  316 FORMAT (40X,3I6)
      IF(NC.NE.0) GO TO 325
      NC=NCSAVE
      GO TO 350
  325 CONTINUE
C                                                SORT
      CALL SRTSAB(NC,9,1,3,H,K,L,E,R,EC,AP,BP,CNTRB)
C                                                SEARCH TABLE PREPARATION
         CALL MKTBL (IT,150,H,NC,K,L)
C                                                INITIALIZE BASIC SET
  350 CONTINUE
      IH=0
      INSN=0
      IB=1
```

```
      CALL ACTION(HKL,INE,IDE,IB)
C                                          PASS SEARCH BINARY
      IF(INSP.EQ.0)  GO TO 400
      IB=6
      INM=IDIMS
      IF(INSP.LT.0)  INM=IABS(INSP)
  451 INSN=INSN+1
      IF(INSN.GT.INM)  GO TO 459
  452 READ (IDISK) IH,IK,IL,FE,FR,BE,BR,BN,PA,PB,XTRA1,XTRA2
      IF(IH.GE.HLT) GO TO 459
      CALL ACTION (HKL,ME,ME,IB)
      GO TO 451
  459 INSN=INSN-1
C                                          BINARY(DISK) SEARCH INPUT
  400 IF(INS.EQ.0  .OR.  IH.GE.HLT)  GO TO 450
      INBR=1
      INM=IDIMS
      IF(INS.LT.0) INM=IABS(INS)
  410 INSC=INSC+1
      IF(INSC.GT.INM) GO TO 440
      READ (IDISK) IH,IK,IL,FE,FR,BE,BR,BN,PA,PB,XTRA1,XTRA2
      IF(IH.LT.HLT) GO TO 500
  440 INSC=INSC-1
  450 CONTINUE
      INSC=INSC + INSN
      INSC1=INSC
      IF(IDS.EQ.0) GO TO 495
C                                          BCD  SEARCH INPUT
      INBR=2
      INM=IDIMS
      IF(IDS.LT.0) INM=IABS(IDS)
  460 IDSC=IDSC+1
      IF(IDSC.GT.INM) GO TO 490
      READ(NTD,FMT) IH,IK,IL,FE,FR
C                                     VARIABLE FORMAT
      IF( ABS(FR) .GT. CNVRT) FR=FR*RADNS
      BE=FE
      BR=FR
      BN=0.0
      PA=0.0
      PB=0.0
  470 CONTINUE
      IF(IH.LT.HLT) GO TO 500
  490 IDSC=IDSC-1
  495 CONTINUE
      IF (NBRJ.LE.0) GO TO 600
      INBR=3
      IBRJ=0
  497 IBRJ=IBRJ+1
      IF (IBRJ.GT.NBRJ) GO TO 600
      READ (IDISK) IH,IK,IL,FE,FR,BE,BR,BN,PA,PB,XTRA1,XTRA2
      GO TO 500
C                                          INITIALIZE BASIC VECTORS
  500 IB=2
C
C                        EXCEPTIONAL CONDITION DISCONTINUE
      IF (SENSE SWITCH 3) 570,565
C
  565 CALL ACTION(HKL,ME,ME,IB)
C                                          SEARCH
      CALL SEARCH(HKL,H,K,L,NC,IT)
C                                          FUNCTIONS FOR EACH BASIC VECTOR
      IB=4
      CALL ACTION(HKL,ME,ME,IB)
      GO TO 575
```

```
  570 IB=6
      CALL ACTION (HKL,ME,ME,IB)
  575 CONTINUE
C         ON-LINE MONITORING
C     IF(BINSW(1)) CALL DSPLAY(INSC,5,IDSC,5)
C                                          LOOP THRU VECTORS OF BASIC SET
      GO TO (410,460,497),INBR
C
  600 CONTINUE
C                                          FUNCTIONS OVER BASIC SET
C                                              (CORRELATIONS)
      IB=5
      CALL ACTION(HKL,INS,IDS,IB)
C                                          SUMMARY
      CYCLE=.FALSE.
      GO TO (75,25),IFMTB
      END


              SUBROUTINE  ACTION  ( H,KACTN,LACTN,IB )
C ACTION TANGENT PHASE ADJUSTMENTS
C
C
C             H*BASIC VECTOR,K*POINTER,L*POINTER (H-V(K)=V(L))
C
C        ***********************************************
      COMMON /REFLCT/MH(4650),MK(4650),ML(4650),E(4650),R(4650),EC(4650)
      COMMON /1/        AP(4650),BP(4650),CNTRB(4650)
      COMMON ISPARE(25),F(50)
C
      COMMON/ATOMS/SIG2,SIG4
C
      DIMENSION H(3),M(3)
      INTEGER H,HLT
C
      EQUIVALENCE (F(1),FE),(F(2),FR),(F(3),BE),(F(4),BR),(F(5),BN)
      EQUIVALENCE (F(6),PA),(F(7),PB)
      EQUIVALENCE (ISPARE(3),LSC),(ISPARE(1),MTW),(ISPARE(4),I1403)
      EQUIVALENCE (F(50),SCLALL),(F(49),CHANGE),(ISPARE(5),LISTK)
C
C
      EQUIVALENCE(F(9),CREAL),(F(10),CIMAG)
      EQUIVALENCE (F(11),A),(F(12),B),(F(13),SCL)
      EQUIVALENCE (F(20),BASIC),(F(21),PASS)
      EQUIVALENCE (F(22),SFE),(F(23),SBE),(F(24),SFR),(F(25),SDR)
C
C       VARIABLE        F( )        STORAGE ASSIGNMENT DESCRIPTION
C
C        FE              1          OBSERVED E
C        FR              2          OBSERVED (PREVIOUS) PHASE
C        BE              3          CALCULATED E
C        BR              4          CALCULATED (CURRENT) PHASE
C        BN              5          NUMBER OF INTERACTIONS
C        PA              6          REAL       PHASE COMPONENT
C        PB              7          IMAGINARY PHASE COMPONENT
C
C             LSQ=1 TANGENT FORMULA
C                   LSQ=3  TANGENT FOR E ONLY, NO NEW PHASE
C        ***********************************************
C
      XTRA1=0.0
      XTRA2=0.0
      MW=61
      ISK=3
      HLT=200
```

```
      PI=3.1415926535898
      CIRCLE=3.142
      TUPI=6.2831853071796
              K=KACTN
              L=LACTN
C
C
C                     ENTER PROPER PROGRAM SEGMENT
      GO TO (100,200,300,400,500,600),IB
C
  100 CONTINUE
C                     INITIALIZE OVER BASIC SET          AND FOR THIS ROUT.
      REWIND ISK
      DO 105 J=20,35
  105 F(J)=0.
      ABN=0.
      RETURN
  200 CONTINUE
C                     INITIALIZE FOR EACH BASIC VECTOR
      BN=0.
      A=0.
      B=0.
      CREAL=0.0
      CIMAG=0.0
      IF (LISTK.LT.1) GO TO 250
      WRITE (MW,245) H(1),H(2),H(3),(F(J),J=1,2)
  245 FORMAT (1H0, * BASIC REFLECTION=* 3I5,2F8.3)
      WRITE (MW,246)
  246 FORMAT(            *0         H    K    L        E        R      H    K
     1  L       E        R * /)
  250 CONTINUE
      RETURN
  300 CONTINUE
C                     COMPUTE FUNCTIONS AND SUMS FOR EACH INTERACTION
C                          THIS SECTION ENTERED BY SEARCH IB=3
      BN=BN+1.
      C=ABS(E(K)*E(L))
      D=R(K)+R(L)
      A=A+C* COS(D)
      B=B+C* SIN(D)
C
  375 CONTINUE
      IF(LISTK.LT.1) GO TO 385
      WRITE(MW,380)MH(K),MK(K),ML(K),E(K),R(K),MH(L),MK(L),ML(L),E(L)
     1,R(L)
  380 FORMAT (5X,3I5,2F8.3,3I5,2F8.3)
  385 CONTINUE
C
      RETURN
C                     PROCESS PASSED VECTORS
  600 CONTINUE
      DO 605 I=15,16
  605 F(I)=0.
      BR=FR
      PASS=PASS+1.
      CREAL=0.0
      IMAG=0.0
      SCL=3.5
      GO TO 450
C                                FUNCTIONS
  400 CONTINUE
C                     RESULTS FOR EACH BASIC VECTOR
C
      A = A*SIG2/(SIG4*BN)
      B = B*SIG2/(SIG4*BN)
```

```
C
      IF (A.EQ.0.0.AND.B.EQ.0.0) GO TO 401
      RAWP=ATAN2 (B,A)
      GO TO 402
  401 CONTINUE
      RAWP=0.0
  402 CONTINUE
      BR=FR
      IF(LSQ.EQ.1) BR=RESET(H,RAWP)
      BE =SQRT(A*A+B*B)
      SFE=SFE+FE
      SBE=SBE+BE
      SCL=2.5
      ABN=ABN + BN
      IF(LISTK.GT.0) LISTK=LISTK-1
  450 CONTINUE
C                                 SUMS
      BASIC=BASIC+1.
C                                 SAVE FOR SCALING
      WRITE (ISK) (M(J),J=1,3), (F(I),I=1,14)
      RETURN
  500 CONTINUE
C                     RESULTS OVER BASIC SET
C                                 SCALES AND COUNTS
      AFE=SFE/(BASIC-PASS)
      ABE=SBE/ (BASIC-PASS)
      ABN=ABN/ (BASIC-PASS)
      SCALE=AFE/ABE
C        DONT SCALE IF USING CORRECTION TERM
      N=BASIC
      REWIND ISK
      SDE=0.
      SFEA=0.
      SBEA=0.
C
C                     HEADING
      WRITE(MW,505)
  505 FORMAT(1H1,40X,41H* * *    TANGENT FORMULA RESULTS    * * * ///
     188H     H     K     L    OBS R  CALC R   OBS E  CALC E     A        B
     2      N                        /// )
C
C                     RE-SCALE,PRINT,AND SAVE
      DO 550 J=1,N
      READ (ISK) (M(I),I=1,3), (F(II),II=1,14)
      IF(SCL.GT.3.0) GO TO 515
      BE=BE*SCALE
      PA=A*SCALE
      PB=B*SCALE
      SDE=SDE + ABS( FE-BE)
  515 SFEA=SFEA+FE
      SBEA=SBEA+BE
C                                 PRINT
      WRITE(MW,525)(M(I),I=1,3),FR,BR,FE,EE,PA,PB,BN
C
  525 FORMAT(1H ,3I5,7F8.3,2F8.3)
C                                 SAVE BINARY FOR NEXT CYCLE
      WRITE(MTW) (M(I),I=1,3),FE,BR,BE,FR,BN,PA,PB,XTRA1,XTRA2
  550 CONTINUE
      REWIND ISK
      WRITE(MTW) HLT,HLT,HLT,(F(I),I=1,9)
C                     CORRELATION RESULTS ON-AND OFF-LINE
      RE=SDE/SFE
      SCLALL=SFEA/SBEA
      AFEA=SFEA/BASIC
      WRITE (MW,570)RE,SCALE,SCLALL,BASIC,PASS
```

```
  570 FORMAT(37H0 R-FACTORS FOR CALCULATED VALUES- E,F8.4
     1,/24H0 SCALE FACTORS- CALC E,F8.4, 8H OVERALL,F8.4/24H0 VECTOR  CO
     2UNTS-  TOTAL,F8.1,7H PASSED,F8.1/)
      RETURN
C
      END


                SUBROUTINE TXPAND
CTXPAND          GENERATES SYMMETRY MATES FOR MOST SPACE GROUPS
C               FOR XTAN
C
C
C                SYMMETRY GENERATOR STORAGES
      COMMON/GENRTR/KTUBE,JSYM,JGEN,KK,JDESIG,CENTER,TJ,I3,ME
     1              ,MSYM(3,4,48),JGENER(146),IDENT(48),JHP(3,48)
     2              ,IBLONG(48),ID(96),INDXP(3)
      DIMENSION KKK(48),JSIGN(48)
      EQUIVALENCE (ID(1),KKK(1)),(ID(49),JSIGN(1)),(I3,I4)
C                 CALLING PROGRAM DEPENDENT
      COMMON/EXPAND/HE(96),KE(96),LE(96),EE(96),RE(96),EX(96),AX(96),
     1BX(96)
     2              ,JH,JK,JL,EI,RI,CE,RA,RB
      INTEGER HE
      DIMENSION CMNT(8)
      DATA (ISTART=1)
C               FIRST CALL READS AND CHECKS MATRICES
                GO TO (5,50),ISTART
    5 ISTART=2
      I3=61
C               CENTER=0 $ CENTERED SPACE GROUP
C
      READ 15,JSYM,CENTER,(CMNT(L),L=1,8),
     1 ((( MSYM(I,J,K),J=1,4),I=1,3),K=1,JSYM)
   15 FORMAT(I5,F5.0,7A8,A6/(4I5))
C
      CALL GENCHK
C
      WRITE (I3,20)(CMNT(L),L=1,8)
   20 FORMAT(34H0SYMMETRY MATRICES FOR SPACE GROUP,7A8,A6)
      GO TO (550,600),KTUBE
C
C               SUBSEQUENT CALLS EXPAND UNIQUE VECTORS
   50 CONTINUE
C               INITIALIZE
      T=0.
      PHASE=RI
      J=1
      K=2
      N=0
      INDXP(1)=      JH
      INDXP(2)=      JK
      INDXP(3)=      JL
C               FILL GENERATION BAND
   70 CALL GEN
C               DISCONTINUE ON ERROR
      GO TO (75,600),KTUBE
C               INTERROGATE FIRST MATRIX
   75 CALL FLSFUN(K)
C               INSIST ON IDENTITY MATRIX FIRST
      IF(KK.NE.1) GO TO 600
      GO TO (300,600,600),K
  100 CONTINUE
C               GENERATE NEXT SYMMETRY MATE
      CALL FLSFUN(K)
```

```
      GO TO (125,500,600),K
C                    SO THAT A AND B ADJUSTMENT WILL WORK
  125 IF(KK.NE.1 .AND. KK.NE.7 ) GO TO 600
      T=TJ*6.283185307179 6
      J=1
      PHASE=RI
C              DO NOT ADD CURRENT REFLECTION IF DUPLICATE
  200 DO 250 I=1,N
      IF(INDXP(1) .NE. HE(I) ) GO TO 250
      IF( INDXP(2) .NE. KE(I) ) GO TO 250
      IF( INDXP(3) .EQ. LE(I) ) GO TO 400
  250 CONTINUE
C              ADD NEWLY GENERATED SYMMETRY MATE
  300 N=N+1
      HE(N)=      INDXP(1)
      KE(N)=      INDXP(2)
      LE(N)=      INDXP(3)
      RE(N)=HEMIR (PHASE + T)
      S= COS(RE(N) )
      AX(N)=RA*SIGN(1.,S)
      S=SIN(RE(N) )
      BX(N)=RB*SIGN(1.,S)
  400 CONTINUE
C              GENERATE NEGATIVE OF PREVIOUS REFLECTION
      GO TO (410,100),J
  410 J=2
      DO 425 I=1,3
      INDXP(I)=-INDXP(I)
  425 CONTINUE
      PHASE=-RI
      GO TO 200
C              GENERATION COMPLETE
  500 ME=N
C                          FILL E SLOTS
      DO 510 I=1,N
      FE(I)=EI
  510 EX(I)=CE
  550 CONTINUE
      RETURN
C              ERROR CONDITION DETECTED
  600 CONTINUE
      PRINT 605,KTUBE,K,KK,JDESIG
  605 FORMAT(25H0 ERROR DURING GENERATION  ,4I4)
      STOP
      END
         SUBROUTINE MKTBL (T,N,D,L,DK,DL)
CMKTBL     PREPARATION OF PSEUDO-ADDRESS TABLE. PRESUMES (L) SORTED
C INCREASING ORDER INTEGER DATA(D) OF LIMITED NUMBER OF SPECIES. TABLE
C (T) ENTRIES ARE CUMULATIVE COUNT FOR EACH POSSIBLE SPECIE(N). FOR
C GIVEN H, (H= T(1)=I) IS INDEX LOC. IN T SUCH T(I)-T(I-1) IS NUMBER OF
C H DATA, T(I-1)+1 IS LOC. RELATIVE TO D(1) OF FIRST SUCH H.
C
      DIMENSION T(N),D(L)
      DIMENSION DK(L),DL(L)
      INTEGER T,D,CMPR,SZ
      INTEGER DK,DL
      INTEGER PARMTR
C          SZ=SIZE TABLE T REQUIRED, N=SIZE AVAILABLE
      PARMTR=7
      SZ=D(L)-D(1) + PARMTR
      IF(SZ.LE.N) GO TO 20
      PRINT 15,SZ,N
   15 FORMAT(12H TABLE SMALL2I5)
      STOP
```

```
 20    T(1)=D(1)-PARMTR
 25    T(PARMTR-1)=0
       ITEMP=L
       T(2)= 1000
       T(3)=-1000
       T(4)= 1000
       T(5)=-1000
C
C
       DO 125 IJ=1,ITEMP
C              MINIMUM K
       T(2)= MIN0 ( DK(IJ),T(2) )
C              MAXIMUM K
       T(3)= MAX0 ( DK(IJ),T(3) )
C              MINIMUM L
       T(4)= MIN0 ( DL(IJ),T(4) )
C              MAXIMUM L
       T(5)= MAX0 ( DL(IJ),T(5) )
  125 CONTINUE
C          CMPR IS CURRENT SPECIE TYPE COMPARAND
 30    CMPR=PARMTR
C          M IS CUMULATIVE COUNT AND LOCATION IN D
   35 M=1
C          KND IS SPECIE NOW AVAILABLE
   40 KND=D(M)-T(1)
 45    IF(KND-CMPR) 85,50,70
   50 M=M+1
   55 IF(M.LE.L) GO TO 40
   60 T(CMPR)=M-1
   65 RETURN
   70 T(CMPR)=M-1
   75 CMPR=CMPR+1
   80 IF(CMPR.LE.(D(L)-T(1))) GO TO 45
   85 PRINT 90,CMPR
 90    FORMAT(1H0,20X,32H*MKTBL* DATA NOT PROPERLY SORTED,I5)
       STOP
       END


       SUBROUTINE SEARCH(HKL,H,K,L,N,IT)
CSEARCH         SIGMA-2 TYPE INTERACTION SEARCH,  ASSUMES LEXICOGRAPHICAL
C LY INCREASING ORDERED VECTORS(H,K,L) COMPRISING EXPANDED DECK, FOR
C HKL,FINDS (L) WHERE H-K=L USING TABLE OF RELATIVE LOCATION AND NUMBER
C OF VARIOUS SPECIES OF(L),(H,K,L),
C
       INTEGER H,HA,HD,HKL
       EQUIVALENCE (J(1),HA),(J(2),KA),(J(3),LA)
       DIMENSION HKL(3),IT(150),H(N),K(N),L(N),J(3)
C
C  HA/H, H/K, HD/L ,IN H-K=L NO,  HD=HA-H
C
       ISRCH=10
       IRANGE=2
   35 IBRNCH=3
    5 HA=HKL(1)
   10 KA=HKL(2)
   15 LA=HKL(3)
   20 MH=H(N)
   40 DO 135  I=1,N
   45 HD=HA-H(I)
   50 IF(HD.LT.H(I).OR.HD.GT.MH) GO TO 135
   55 KD=KA-K(I)
      IF( KD.LT.IT(2) .OR. KD.GT.IT(3) ) GO TO 135
   65 LD=LA-L(I)
      IF( LD.LT.IT(4) .OR. LD.GT.IT(5) ) GO TO 135
```

```
C
   75          M1=HD-IT(1)
   80          M2=IT(M1-1)+1
   85          M3=IT(M1)
   90       IF(M2.GT.M3) GO TO 135
C                          RANGING
C         SUB-SET BETWEEN M2 AND M3 REDUCED SUCCESSIVELY BY IRANGE
C          UNTIL SEARCH SET OF SIZE ISRCH DETERMINED.
C
  210          M4=M3-M2+1
  215          IF(M4.LE.ISRCH) GO TO 95
               M5=M2 + M4/IRANGE
  230          IF(KD-K(M5)) 255,240,245
  240          IF(LD-L(M5)) 255,265,245
  245          M2=M5
  250          GO TO 210
  255          M3=M5
  260          GO TO 210
C                        PROCESS EQUALITY (INFREQUENTLY)
  265          II=I
  270          IF(M5.LT.II) GO TO 135
  275          CALL ACTION (J,II,M5,IBRNCH)
  280          GO TO 135
C
C              SEQUENTIAL DIRECT COMPARISONS
C
   95    DO 130 M=M2,M3
  100 IF(KD.LT.K(M)) GO TO 135
  105 IF(KD.NE.K(M).OR.LD.NE.L(M)) GO TO 130
  110 MM=M
  115 II=I
  116 IF(MM.LT.II) GO TO 135
C              *ACTION* ROUTINE ENTERED EACH TIME INTERACTION IS FOUND
  120      CALL ACTION (J,II,MM,IBRNCH)
  125 GO TO 135
  130    CONTINUE
  135 CONTINUE
      RETURN
      END


      SUBROUTINE GENCHK                                                 GENC0020
C     VERSION OF NOV 62                                                 GENC0030
CGENCHK- ARRANGES AND CHECKS SYMMETRY OPERATIONS FOR GEN.               GENC0010
C                        LIFTED FROM  =  X-RAY 63  =
C                        JAMES STEWART   DARREL HIGH
C                        ADAPTED ON CDC 3800 BY STEPHEN BRENNER,NRL
C     A FORTRAN SUBROUTINE TO CHECK SYMMETRY OPERATIONS SUPPLIED TO DATAGENC0040
C     REDUCTION PROGRAM AND PUT THEM IN PROPER FORM FOR GEN THE         GENC0050
C     FOURIER CODE GENERATOR. THE ROTATION MATRICES ARE SEARCHED FOR    GENC0060
C     DUPLICATES, THE PRESENCE OF THE IDENTITY MATRIX IS ESTABLISHED,   GENC0070
C     THE SYMOP MATRICES ARE CHECKED FOR ROWS OR COLUMNS OF ZEROS. IF   GENC0080
C     THERE ARE MORE THAN ONE SET OF ROTATION MATRICES(I.E. TETRAGONAL  GENC0090
C     OR HIGHER SYMMETRY(HKL,-HKL,H-KL,-H-KL))A CHECK IS MADE TO MAKE   GENC0100
C     SURE ALL SETS HAVE EQUAL NUMBERS OF ENTRIES.                      GENC0110
C     THE SUBROUTINE IS CALLED BY CALL GENCHK                           GENC0120
C     ALL NECESSARY QUANTITIES ARE IN COMMON STORAGE.                   GENC0130
C                                                                       GENC0190
C              SYMMETRY GENERATOR STORAGES
      COMMON/GENRTR/KTURE,JSYM,JGEN,KK,JDESIG,CENTER,TJ,I3,ME
     1              ,MSYM(3,4,48),JGENER(146),IDENT(48),JHP(3,48)
     2              ,IBLONG(48),ID(96),INDXP(3)
      DIMENSION KKK(48),JSIGN(48)
      EQUIVALENCE (ID(1),KKK(1)),(ID(49),JSIGN(1)),(I3,I4)
C        /GENRTR/ OCCUPIES $ 1070 $ LOCATIONS.
```

```
C                                                                       GENC0300
C     MAKE A CONSTANT FOR DO LOOP UPPER LIMITS.                         GENC0310
      N3=3                                                              GENC0320
C     CLEAR ORDERING CODE BAND TO ZERO                                  GENC0330
      DO 901 J=1,96                                                     GENC0340
  901 ID(J)=0                                                           GENC0360
      DO 902 J=1,48
  902 IDENT(J)=0
C     SET SIGNAL TO NO MISHAPS                                          GENC0370
      KBAD=1                                                            GENC0380
C     CHECK ROTATION MATRICES FOR DUPLICATION.                          GENC0390
      KTUBE=0                                                           GENC0400
 1001 KGEN=1                                                            GENC0410
 1002 KGEN1=KGEN+1                                                      GENC0420
       IF(JSYM - 1) 8990,1101,1003                                      GENC0430
 1003  DO 1010 J = KGEN1,JSYM                                           GENC0440
      DO 1004 LGEN =1,N3                                                GENC0450
      DO 1004 LGEN1=1,N3                                                GENC0460
      IF(MSYM(LGEN,LGEN1,KGEN)-MSYM(LGEN,LGEN1,J ))1005,1004,1005       GENC0470
 1004 CONTINUE                                                          GENC0480
      GO TO 1090                                                        GENC0490
 1005 DO 1006 LGEN = 1,N3                                               GENC0500
      DO 1006 LGEN1=1,N3                                                GENC0510
      IF(MSYM(LGEN,LGEN1,KGEN)+MSYM(LGEN,LGEN1,J))1010,1006,1010        GENC0520
 1006 CONTINUE                                                          GENC0530
 1007 KBAD=2                                                            GENC0540
 1010 CONTINUE                                                          GENC0550
      KGEN=KGEN+1                                                       GENC0560
      IF(KGEN-JSYM)1002,1101,1101                                       GENC0570
C     ERROR DETECTED DUPLICATE ROTATION AMONG SYMOPS.                   GENC0580
 1090 WRITE (I4,1091)K,JGEN                                             GENC0590
 1091 FORMAT(50H ROTATIONAL PART OF TH SYMMETRY OPERATION OF CARD I4,19HGENC0600
     1 IDENTICAL TO CARD I4,1H.)                                        GENC0610
      KTUBE=KTUBE+1                                                     GENC0620
      GO TO 9001
C     MAKE SURE IDENTITY ROTATION MATRIX PRESENT AND NO COLUMN OR ROW   GENC0640
C    1IS ALL ZEROS.                                                     GENC0650
 1101 CONTINUE                                                          GENC0660
      DO 1120 J=1,JSYM                                                  GENC0670
      NOT=0                                                             GENC0680
      DO 1105 LGEN=1,N3                                                 GENC0690
      NKTUBE=0                                                          GENC0700
      DO 1104 LGEN1=1,N3                                                GENC0710
      IF(MSYM(LGEN,LGEN1,J))1103,1104,1102                              GENC0720
 1102 IF(LGEN-LGEN1)1103,11031,1103                                     GENC0730
 1103 NOT=1                                                             GENC0740
      GO TO 1105                                                        GENC0750
11031 NKTUBE=1                                                          GENC0760
 1104 CONTINUE                                                          GENC0770
      IF(NKTUBE)11041,11041,1105                                        GENC0780
11041 KTUBE=KTUBE+1                                                     GENC0790
 1190 WRITE (I4,1191)J,LGEN1                                            GENC0800
 1191 FORMAT(15H SYMMETRY CARD I4,5H ROW I4,29H OF ROTATION MATRIX ALL ZGENC0810
     1ERO.)                                                             GENC0820
      NOT=1                                                             GENC0830
 1105 CONTINUE                                                          GENC0840
      DO 1107 LGEN1=1,N3                                                GENC0850
      DO 1106 LGEN=1,N3                                                 GENC0860
      IF(MSYM(LGEN,LGEN1,J))1107,1106,1107                              GENC0870
 1106 CONTINUE                                                          GENC0880
 1192 WRITE (I4,1193)J,LGEN                                             GENC0890
 1193 FORMAT(15H SYMMETRY CARD I4,8H COLUMN I4,29H OF ROTATION MATRIX ALGENC0900
     1L ZERO.)                                                          GENC0910
      KTUBE=KTUBE+1                                                     GENC0920
 1107 CONTINUE                                                          GENC0930
```

```
C       CHECK TO SEE IF IDENTITY MATRIX FOUND.                          GENC0940
        IF(NOT)1120,1110,1120                                           GENC0950
C       IF IDENTITY MATRIX SEEMS FOUND MAKE SURE TRANSLATION VECTOR ZERO. GENC0960
 1110   DO 1111 LGEN=1,N3                                               GENC0970
        IF(MSYM(LGEN,4,J))1120,1111,1120                                GENC0980
 1111   CONTINUE                                                        GENC0990
        IDENT(1)=J                                                      GENC1000
        ID(J)=1                                                         GENC1010
        NID=2                                                           GENC1020
 1120   CONTINUE                                                        GENC1030
        IF(IDENT(1))1194,1194,1201                                      GENC1040
C       IF NO IDENTITY MATRIX GIVE UP DATA REDUCTION.                   GENC1050
 1194   WRITE (I4,1195)                                                 GENC1060
 1195   FORMAT(26H NO IDENTITY MATRIX FOUND.)                           GENC1070
        KTUBE=KTUBE+1                                                   GENC1080
        GO TO 1601                                                      GENC1090
C       HAVING FOUND THE IDENTITY MATRIX FIND HOW MANY ROTATION MATRICES GENC1100
C       BELONG TO ONE SYMMETRY CLASS HEREINAFTER-WHOOPS-AND SORT THESE  GENC1110
C       TOGETHER BY MEANS OF AN INDEX IDENT(J). CHECK TO MAKE SURE EACH GENC1120
C       GROUP OF ROTATION MATRICES HAS THE SAME NUMBER OF MATRICES.     GENC1130
C       RETURN ERROR IF THIS CONDITION NOT MET.                         GENC1140
 1201   ASSIGN 1211 TO ISWMTP                                           GENC1150
        NO=1                                                            GENC1160
        K=IDENT(1)                                                      GENC1170
C       SEARCH FOR NON-ASSIGNED SIMILAR MATRICES.                       GENC1180
 1205   DO 1210 J=NO,JSYM                                               GENC1190
C       SKIP TESTS IF ENTRY ALREADY ASSIGNED.                           GENC1200
        IF(ID(J))1210,1206,1210                                         GENC1210
 1206   DO 1209 IP=1,N3                                                 GENC1220
        DO 1209 IS=1,N3                                                 GENC1230
        IF(MSYM(IP,IS,K))1207,1208,1207                                 GENC1240
 1207   IF(MSYM(IP,IS,J))1209,1210,1209                                 GENC1250
 1208   IF(MSYM(IP,IS,J))1210,1209,1210                                 GENC1260
 1209   CONTINUE                                                        GENC1270
C       MATRICES ARE SIMILAR IF HERE.                                   GENC1280
        GO TO (1710,1701),KBAD                                          GENC1290
 1701   DO 1705 IP=1,N3                                                 GENC1300
        DO 1705 IS=1,N3                                                 GENC1310
        IF(MSYM(IP,IS,K) +MSYM(IP,IS,J)) 1210,1705,1210                 GENC1320
 1705   CONTINUE                                                        GENC1330
C       MATRICIES ARE ENANTIOMORPHOUS IF HERE.                          GENC1340
        ID(J) = 1                                                       GENC1350
        GO TO 1210                                                      GENC1360
 1710   CONTINUE                                                        GENC1370
        ID(J)=1                                                         GENC1380
        IDENT(NID)=J                                                    GENC1390
        NROTP=NROTP+1                                                   GENC1400
        NID=NID+1                                                       GENC1410
 1210   CONTINUE                                                        GENC1420
C       SWITCH TO CHANGE PATH AFTER FIRST TIME.                         GENC1430
        GO TO ISWMTP,(1211,1212)                                        GENC1440
 1211   NROT=NID-1                                                      GENC1450
        ASSIGN 1212 TO ISWMTP                                           GENC1460
        GO TO 1213                                                      GENC1470
C       CHECK THAT ALL GROUPS HAVE SAME NUMBER AS FIRST.                GENC1480
 1212   IF(NROT-NROTP)1290,1213,1290                                    GENC1490
 1213   NROTP=1                                                         GENC1500
C       SEARCH FOR NEXT UNASSIGNED(FIRST LEFT IN TABLE)                 GENC1510
        DO 1214 J=1,JSYM                                                GENC1520
        IF(ID(J))1214,1215,1214                                         GENC1530
 1214   CONTINUE                                                        GENC1540
        GO TO 1301                                                      GENC1550
C       MARK IT AND GO ON.                                              GENC1560
 1215   K=J                                                             GENC1570
        IDENT(NID)=J                                                    GENC1580
```

```
      NO=K+1                                                            GENC1590
      NID=NID+1                                                         GENC1600
      ID(J)=1                                                           GENC1610
      IF(NO-JSYM)1205,1205,1301                                         GENC1620
C     ERROR BLOCK-UNEVEN GROUPS.                                        GENC1630
 1290 KTUBE=KTUBE+1                                                     GENC1640
      WRITE (I4,1291)                                                   GENC1650
 1291 FORMAT(86H THERE IS EITHER A SYMMETRY OPERATION CARD MISSING OR INGENC1660
     1 EXCESS OF THE CORRECT NUMBER.)                                   GENC1670
      GO TO 1601                                                        GENC1680
 1301 CONTINUE                                                          GENC1690
C     CHECK IF NROT IS 8(INDICATES A NON-CENTRO SPACE GROUP WHICH       GENC1700
C     COULD BE CENTRIC).                                                GENC1710
 1401 IF(NROT-8)1402,1402,1490                                          GENC1720
 1402 GO TO(1501,1501,1490,1501,1490,1490,1490,1403),NROT               GENC1730
 1403 IF(CENTER)1404,1490,1404
 1404 WRITE (I3,1405)                                                   GENC1750
 1405 FORMAT(55H SPACE GROUP COULD BE MADE CENTRIC BY CHANGE IN ORIGIN,)GENC1760
      GO TO 1601                                                        GENC1770
 1490 WRITE (I4,1491)NROT                                               GENC1780
 1491 FORMAT(1H I4,32H ROTATION MATRICES FOUND, WHY...)                 GENC1790
      KTUBE=KTUBE+1                                                     GENC1800
      GO TO 1601                                                        GENC1810
C     CHECK THAT NO-H,-K,-L ROTATION POSSIBLE.                          GENC1820
 1501 GO TO(1601,1590),KBAD                                             GENC1830
 1590 WRITE (I4,1591)                                                   GENC1840
 1591 FORMAT(62H SYMMETRY OPERATION TABLE CONTAINS OPERATION THROUGH A CGENC1850
     1ENTER.)                                                           GENC1860
      GO TO 1601                                                        GENC1870
C     CHANGE THE TRANSLATION VECTOR COMPONENTS TO MODULO TWELVE.        GENC1880
 1601 DO 1609 J=1,JSYM                                                  GENC1890
      DO 1609 I=1,N3                                                    GENC1900
C1603 CALL XMODTW(MSYM(I,4,J))                                          GENC1910
 1603 IF(MSYM(I,4,J)) 1604,1609,1609                                    GENC1920
 1604 MSYM(I,4,J) = MSYM(I,4,J) + 12                                    GENC1930
 1609 CONTINUE                                                          GENC1940
C     TEST THAT ROTATION MATRICES HAVE DETERMINANT + OR - ONE.          GENC1950
 1801 DO 1804 J = 1,JSYM                                                GENC1960
      ICKEY = MSYM(1,1,J)*(MSYM(2,2,J)*MSYM(3,3,J)-MSYM(2,3,J)*MSYM(3,2,GENC1970
     1J))-MSYM(2,1,J)*(MSYM(1,2,J)*MSYM(3,3,J)-MSYM(1,3,J)*MSYM(3,2,J))+GENC1980
     2MSYM(3,1,J)*(MSYM(1,2,J)*MSYM(2,3,J)-MSYM(1,3,J)*MSYM(2,2,J))     GENC1990
      IF(ICKEY) 1802,1890,1802                                          GENC2000
 1802 IF(ICKEY - 1) 1803,1804,1803                                      GENC2010
 1803 IF(ICKEY + 1) 1890,1804,1890                                      GENC2020
 1890 WRITE (I3,1891)J                                                  GENC2030
 1891 FORMAT(35H THE DETERMINANT OF ROTATION MATRIX  I3, 19H IS NOT + ORGENC2040
     1 - ONE,    )                                                      GENC2050
      KTUBE = KTUBE + 1                                                 GENC2060
      GO TO 1804                                                        GENC2070
 1804  CONTINUE                                                         GENC2080
C     CHECK FOR GROUP PROPERTIES.                                       GENC2090
C     ALL CHECKING COMPLETED                                            GENC2100
 8901 IF(KTUBE)8902,8902,8990                                           GENC2110
 8902 CONTINUE                                                          GENC2120
      WRITE (I3,8903)                                                   GENC2130
 8903 FORMAT(38H1SYMMETRY OPERATION CHECKING COMPLETE.)                 GENC2140
C     WRITE OUT FOURIER SYMOP MATRICES AND VECTORS                      GENC2150
      WRITE (I3,8904)                                                   GENC2160
 8904 FORMAT(1H0,10X,15HROTATION MATRIX ,6X,32HTRANSLATION VECTOR (IN TWGENC2170
     1ELFTHS)/1H0)                                                      GENC2180
        DO 8955 IJK = 1,JSYM                                            GENC2190
       J  =  IDENT(IJK)                                                 GENC2200
 8954 WRITE (I3,8905)J,((MSYM(I,IP,J),IP=1,4),I=1,3)                    GENC2210
 8905 FORMAT(1H ,I4,8X,3I4,9X,I4/13X,3I4,9X,I4/13X,3I4,9X,I4/1H )       GENC2220
 8955 CONTINUE                                                          GENC2230
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```
      GO TO 9001                                                        GENC2240
 8990 WRITE (I3,8991)KTUBE                                              GENC2250
 8991 FORMAT(1H I4,24H ERRORS FOUND IN SYMOPS.)                         GENC2260
      GO TO 8902                                                        GENC2270
 9001 CONTINUE                                                          GENC2280
C                 KTUBE     =1 $ OK          =2 $ ERROR
      KTUBE=MIN0(KTUBE,1)+1
      RETURN                                                            GENC2300
      END                                                               GENC2310


      SUBROUTINE GEN
CGEN   - DEVELOPS FOURIER DIRECTING CODES FOR EACH REFLECTION.          GEN 0010
C     VERSION OF 4 AUGUST 1963                                          GEN 0030
C                        LIFTED FROM  =  X-RAY 63  =
C                       JAMES STEWART   DARREL HIGH
C                        ADAPTED ON CDC 3800 BY STEPHEN BRENNER,NRL
C     H,K,AND L ARE OPERATED UPON BY THE ROTATION MATRICES STORED       GEN 0040
C     FROM THE SYMMETRY CARDS. THESE WERE PLACED IN PROPER FORM BY      GEN 0050
C     SUBROUTINE GENCHK. THIS SUBROUTINE GENERATES A CODE(JDESIG)FOR    GEN 0060
C     EACH TRICLINIC REFLECTION (1=+++,2=-++,3=+-+,4=++-,5=---,6=+--,   GEN 0070
C     7=-+-,8=--+) AS WELL AS A CODE (KK) WHICH TELLS THE TYPE OF       GEN 0080
C     FRINGE FUNCTION TO BE APPLIED TO CHANGE THE PHASE OF THE UNIQUE   GEN 0090
C     REFLECTION TO THAT OF THE GENERATED REFLECTION DESIGNATED BY THE  GEN 0100
C     JDESIG.THE ROTATIONS ARE GROUPED BY THE ABSOLUTE VALUES OF THE    GEN 0110
C     GENERATED MILLER INDICES.                                         GEN 0120
C                                                                       GEN 0160
C               SYMMETRY GENERATOR STORAGES
      COMMON/GENRTR/KTUBE,JSYM,JGEN,KK,JDESIG,CENTER,TJ,I3,ME
     1              ,MSYM(3,4,48),JGENER(146),IDENT(48),JHP(3,48)
     2              ,IBLONG(48),ID(96),INDXP(3)
      DIMENSION KKK(48),JSIGN(48)
      EQUIVALENCE (ID(1),KKK(1)),(ID(49),JSIGN(1)),(I3,I4)
C        /GENRTR/ OCCUPIES $ 1070 $ LOCATIONS.
C        THE ORIGINAL * ISIGN * HAS BEEN ALTERED TO * JSIGN *
      KTUBE=0
      JSYM = JSYM                                                       GEN 0300
      DO 901 I = 1,JSYM                                                 GEN 0310
      JSIGN(I)=0
      KKK(I) = 0                                                        GEN 0330
      JHP(1,I) = 0                                                      GEN 0340
      JHP(2,I) = 0                                                      GEN 0350
      JHP(3,I) = 0                                                      GEN 0360
      IBLONG(I) = 0                                                     GEN 0370
 901  CONTINUE                                                          GEN 0380
C     GENERATE A SET OF EQUIV. REFS. FROM THE UNIQUE ONE.               GEN 0390
      DO 1701 K = 1,JSYM                                                GEN 0400
      IDO = IDENT(K)                                                    GEN 0410
      DO 1301 I = 1,3                                                   GEN 0420
 1301 JHP(I,K) = INDXP(1)*MSYM(1,I,IDO)+INDXP(2)*MSYM(2,I,IDO)+         GEN 0430
     1          INDXP(3)*MSYM(3,I,IDO)                                  GEN 0440
C     FIND THE VALUE OF JDESIG WHICH TELLS THE REFLECTION CLASS         GEN 0450
      IF(JHP(1,K)) 1401,1405,1409                                       GEN 0460
 1401 IF(JHP(2,K)) 1402,1403,1404                                       GEN 0470
 1402 IF(JHP(3,K)) 1505,1505,1508                                       GEN 0480
 1403 IF(JHP(3,K)) 1505,1505,1502                                       GEN 0490
 1404 IF(JHP(3,K)) 1507,1502,1502                                       GEN 0500
 1405 IF(JHP(2,K)) 1406,1407,1408                                       GEN 0510
 1406 IF(JHP(3,K)) 1505,1505,1503                                       GEN 0520
 1407 IF(JHP(3,K)) 1505,1425,1501                                       GEN 0530
 1408 IF(JHP(3,K)) 1507,1501,1501                                       GEN 0540
 1409 IF(JHP(2,K)) 1410,1411,1412                                       GEN 0550
 1410 IF(JHP(3,K)) 1506,1506,1503                                       GEN 0560
 1411 IF(JHP(3,K)) 1506,1501,1501                                       GEN 0570
 1412 IF(JHP(3,K)) 1504,1501,1501                                       GEN 0580
```

```
 1425  CONTINUE                                                          GEN 0590
       WRITE (I3,1426)(INDXP(I),I=1,3)                                   GEN 0600
 1426 FORMAT(60H0HOW CAN A 0,0,0 REFLECTION RESULT FROM GENERATION FROM GEN 0610
     1THE  I4,1H,I4,1H,I4)                                               GEN 0620
       KTURE=3
       GO TO 1901
C      SET CORRECT VALUE OF JDESIG FOR THIS REFLECTION                   GEN 0640
C      CORRESPONDS TO +++                                                GEN 0650
 1501 JSIGN(K)=1
       GO TO 1555                                                        GEN 0670
C      CORRESPONDS TO -++                                                GEN 0680
 1502 JSIGN(K)=2
       GO TO 1555                                                        GEN 0700
C      CORRESPONDS TO +-+                                                GEN 0710
 1503 JSIGN(K)=3
       GO TO 1555                                                        GEN 0730
C      CORRESPONDS TO ++-                                                GEN 0740
 1504 JSIGN(K)=4
       GO TO 1555                                                        GEN 0760
C      CORRESPONDS TO --+                                                GEN 0770
 1505 JSIGN(K)=5
       GO TO 1551                                                        GEN 0790
C      CORRESPONDS TO +--                                                GEN 0800
 1506 JSIGN(K)=6
       GO TO 1551                                                        GEN 0820
C      CORRESPONDS TO -+-                                                GEN 0830
 1507 JSIGN(K)=7
       GO TO 1551                                                        GEN 0850
C      CORRESPONDS TO --+                                                GEN 0860
 1508 JSIGN(K)=8
C      FOR CENTRIC SPACE GROUPS, 5-8 ARE IDENTICAL WITH 1-4, RESP.       GEN 0880
 1551 IF(CENTER) 1555,1554,1555
 1554 JSIGN(K)=JSIGN(K)-4
 1555  CONTINUE                                                          GEN 0910
C      FIND H*T AND SET PHASE CODE(KK).                                  GEN 0920
C      PHASE CODE INDICATORS. 1 CORRESPONDS TO TRANSLATION OF ZERO       GEN 0930
C      TWELFTHS, 2 TO ONE TWELFTH, ,,,,,, 12 TO 11/12.  THESE CODES      GEN 0940
C      GIVE THE TRANSLATION SYMOPS FOR LEAST SQUARES =ATOM GENERATION=   GEN 0950
C      AND THE PROPER FRINGE FUNCTION RELATION FOR THE FOURRIER          GEN 0960
C      =REFLECTION GENERATION=.                                          GEN 0970
 1601 KK      =        INDXP(1)*MSYM(1,4,IDO)+INDXP(2)*MSYM(2,4,IDO)*    GEN 0980
     1                 INDXP(3)*MSYM(3,4,IDO)
 1602 IF(KK) 1603,1607,1605                                              GEN 1000
 1603 KK=KK+12                                                           GEN 1010
       GO TO 1602                                                        GEN 1020
 1605 KK=MOD(KK,12)                                                      GEN 1030
 1607 KK=KK+1                                                            GEN 1040
C      PRINT  1608, (INDXP(I), I=1,3), KK,JSYM                           ******
C1608 FORMAT (1X, 3HGEN,5I5)                                             ******
       KKK(K)=KK                                                         GEN 1050
       GO TO (1701,1690,1701,1701,1701,1690,1701,1690,                   GEN 1060
     1        1701,1701,1701,1690),KK                                    GEN 1070
C      SET JGENER TO CORRECT KK                                          GEN 1080
 1690 WRITE (I4,1691)KK                                                  GEN 1090
 1691 FORMAT(51H IMPOSSIBLE TRANSLATION FOR CRYSTALLOGRAPHIC SYMOP,5H  KGEN 1100
     1K=,I4,1H,)                                                         GEN 1110
       KTURE = 3'                                                        GEN 1120
 1701 CONTINUE                                                           GEN 1130
C      AT THIS POINT THE TABLES OF GENERATED REFL. ARE STORED ALONG      GEN 1140
C      WITH TABLES OF SIGN AND PHASE INFORMATION.                        GEN 1150
C      SEARCH THE WHOLE TABLE OF GENERATED HKLS FOR DUPLICATES           GEN 1160
C      AND WHEN ONE OF SIMILAR MAGNITUDE HKL IS FOUND, ASSIGN AN INDEX   GEN 1170
C      CALLED IBLONG (I)                                                 GEN 1180
       ISTART = 1                                                        GEN 1190
       IAM = 1                                                           GEN 1200
```

```
      MULT = 1                                                          GEN 1210
      IBLONG(1) = 1                                                     GEN 1220
C    IF THERE IS ONLY ONE SYMOP  WHY BOTHER, . . . . .                  GEN 1230
      IF (JSYM-1) 2225,2225,2205                                        GEN 1240
C                                                                       GEN 1250
 2205 IGODE = ISTART + 1                                                GEN 1260
      IF (IGODE-JSYM) 2206,2206,2225                                    GEN 1270
C     GO OVER THE LIST OF GENERATED REFLECTIONS LABELING THOSE WHICH    GEN 1280
C     HAVE THE SAME MAGNITUDE OF H,K,L                                  GEN 1290
 2206 DO 2214 I=IGODE,JSYM                                              GEN 1300
C    ON FIRST PASS COUNT UP THE NUMBER OF NON DUPLICATED REFLECTIONS    GEN 1310
C       INCLUDING THE POSSIBILITY OF CENTRO RELATED ONES,               GEN 1320
      IF (ISTART-1) 2209,2207,2209                                      GEN 1330
 2207 DO 2208 IG=1,3                                                    GEN 1340
      IF (JHP(IG,I)-JHP(IG,1)) 12209,2208,12209                         GEN 1350
 2208 CONTINUE                                                          GEN 1360
      MULT = MULT + 1                                                   GEN 1370
      GO TO 2209                                                        GEN 1380
12209 DO 12210 IG = 1,3                                                 GEN 1390
      IF(JHP(IG,I) + JHP(IG,1)) 2209,12210,2209                         GEN 1400
12210  CONTINUE                                                         GEN 1410
      MULT = MULT + 1                                                   GEN 1420
 2209 CONTINUE                                                          GEN 1430
C     SEE IF THERE IS ANOTHER REFLECTION WITH EXACTLY SAME MAGNITUDE HKLGEN 1440
      DO 2210 IG=1,3                                                    GEN 1450
      IF(IABS(JHP(IG,I)) - IABS(JHP(IG,ISTART))) 2214,2210,2214         GEN 1460
 2210 CONTINUE                                                          GEN 1470
C     THIS REFLECTION BELONGS TO THE SAME GROUP OF MAGNITUDE HKL        GEN 1480
      IBLONG(I) = IAM                                                   GEN 1490
 2214 CONTINUE                                                          GEN 1500
C     SEE IF EVERY ONE HAS BEEN ASSIGNED A GROUP ID (IBLONG)            GEN 1510
 2215 DO 2217 I=1,JSYM                                                  GEN 1520
      IF (IBLONG(I)) 2217,2218,2217                                     GEN 1530
C     SOME STILL UNASSIGNED,GO BACK AND KEEP SEARCHING                  GEN 1540
 2218 IAM = IAM + 1                                                     GEN 1550
      IBLONG(I) = IAM                                                   GEN 1560
      ISTART = I                                                        GEN 1570
      GO TO 2205                                                        GEN 1580
 2217 CONTINUE                                                          GEN 1590
C     SEE IF NEXT H,K,L WAS THE SAME AND HAS BEEN IDENTIFIED,           GEN 1600
 2225 CONTINUE                                                          GEN 1610
      IMAT = 1                                                          GEN 1620
      JGEN = 1                                                          GEN 1630
      IMON = 1                                                          GEN 1640
C     COPY THE TABLES INTO  THE JGENER BAND SEPARATING EACH SET OF      GEN 1650
C     H, K, L BY -1 AND ENDING WITH -2 AND THE REFLECTION MULTIPLICITY  GEN 1660
      DO 2525 I=1,IAM                                                   GEN 1670
 2501 JGENER(JGEN) = -1                                                 GEN 1680
      JGENER(JGEN+1) = IABS(JHP(1,IMAT))                                GEN 1690
      JGENER(JGEN+2) = IABS(JHP(2,IMAT))                                GEN 1700
      JGENER(JGEN+3) = IABS(JHP(3,IMAT))                                GEN 1710
      JGEN = JGEN + 4                                                   GEN 1720
      DO 2511 J=1,JSYM                                                  GEN 1730
      IF (IMON-IBLONG(J)) 2511,2510,2511                                GEN 1740
 2510 JGENER(JGEN)=JSIGN(J)
      JGENER(JGEN+1) = KKK(J)                                           GEN 1760
      JGEN = JGEN+2                                                     GEN 1770
 2511 CONTINUE                                                          GEN 1780
      IMON = IMON+1                                                     GEN 1790
      DO 2520 J=1,JSYM                                                  GEN 1800
      IF (IMON-IBLONG(J)) 2520,2521,2520                                GEN 1810
 2521 IMAT = J                                                          GEN 1820
      GO TO 2525                                                        GEN 1830
 2520 CONTINUE                                                          GEN 1840
      GO TO 1801                                                        GEN 1850
```

```
 2525 CONTINUE                                                          GEN 1860
 1801 JGENER(JGEN)=-2                                                   GEN 1870
C     SET MULTIPLICITY OF CURRENT REFLECTION AT THE END OF THE          GEN 1880
C     GENERATION TABLE.                                                 GEN 1890
      JGEN=JGEN+1                                                       GEN 1900
C      THE LAST JGENER(JEN) IS ACTUALLY THE MULTIPLICITY OF THE REFL.   GEN 1910
      JGENER(JGEN) = JSYM/MULT                                          GEN 1920
 1901 CONTINUE
C                    KTURE    =1 $ OK         =2 $ ERROR
      KTURE=MIN0(KTURE,1)+1
      RETURN
      END                                                               GEN 1960


      SUBROUTINE FLSFUN(ICONTR)
CORFUN    REFLECTION GENERATOR FOR ORFLS MODIFIED VERSION FOR X-RAY
C     VERSION 1 JUNE 1963
C                         LIFTED FROM  =  X-RAY 63  =
C                         JAMES STEWART   DARREL HIGH
C                         ADAPTED ON CDC 3800 BY STEPHEN BRENNER,NRL
C
C                SYMMETRY GENERATOR STORAGES
      COMMON/GENRTR/KTURE,JSYM,JGEN,KK,JDESIG,CENTER,TJ,I3,ME
     1              ,MSYM(3,4,48),JGENER(146),IDENT(48),JHP(3,48)
     2              ,IBLONG(48),ID(96),INDXP(3)
      DIMENSION KKK(48),JSIGN(48)
      EQUIVALENCE (ID(1),KKK(1)),(ID(49),JSIGN(1)),(I3,I4)
C        /GENRTR/ OCCUPIES $ 1070 $ LOCATIONS.
      INTEGER HJ
      DIMENSION HJ(3)
      EQUIVALENCE (INDXP,HJ)
C
C               ENTER WITH ICONTR=2
C                 FLSFUN SETS ICONTR=1
C                 FLSFUN SETS ICONTR=2 AT COMPLETION OF GENERATION
C              ICONTR=3  FOR ERROR
      GO TO (102,101), ICONTR
 101  ICONTR = 1
      J = 1
      JGEN = JGEN
 102  IF(JGENER(J) + 1) 601,103,201
 103  J = J+ 6
C     GET OUT THE ABSOLUTE VALUE OF THE INDICES
      IATCH = JGENER(J - 5)
      IKAY = JGENER(J - 4)
      IELL = JGENER(J - 3)
      GO TO 202
 201  J = J + 2
C     SET UP THE SIGN ASSIGNER
 202  JDESIG = JGENER(J - 2)
C     SET TRANSLATION GENERATOR
      KK = JGENER(J - 1)
C     PUT OUT CORRECT TRANSLATION FOR THIS GENERATION.,
C
      GO TO(301,9975,302,303,304,9975,305,9975,306,307,308,9975),KK
C
 301  TJ = 0.0
      GO TO 401
 302  TJ = 0.16666667
      GO TO 401
 303  TJ = 0.25000000
      GO TO 401
 304  TJ = 0.333333333
      GO TO 401
 305  TJ = 0.5000000000
```

```
      GO TO 401
 306  TJ = 0.66666667
      GO TO 401
 307  TJ = 0.7500000000
      GO TO 401
 308  TJ = 0.833333333
      GO TO 401
C     PLACE THE CORRECT COMBINATION OF SIGNS ON H,K,L
 401  GO TO(402,403,402,402,403,402,403,403),JDESIG
C
 402  HJ(1) = IATCH
      GO TO 405
 403  HJ(1) = -IATCH
 405  GO TO (406,406,407,406,407,407,406,407),JDESIG
 406  HJ(2) = IKAY
      GO TO 411
 407  HJ(2) = -IKAY
C
C
 411  GO TO(412,412,412,413,413,413,413,412),JDESIG
 412  HJ(3) = IELL
      GO TO 501
 413  HJ(3) = -IELL
C
501   RETURN
 9975 PRINT 9980,KK,JGEN,J
 9980 FORMAT(40HOFLSFUN ERROR ,,, IMPOSSIBLE TRANSLATION ,3I5)
      ICONTR=3
      GO TO 501
 601  ICONTR = 2
      GO TO 501
      END


      SUBROUTINE SRTSAB (LS,INDE,NA,NK,H,K,L,E,R,A1,A2,A3,A4)
      INTEGER H
      DIMENSION H(LS),K(LS),L(LS),E(LS),R(LS)
      DIMENSION A1(LS),A2(LS),A3(LS),A4(LS)
C
C          7030  SORTING ROUTINE BY STEVE A. BRENNER,NRL
C
C
C
      N=LS
      N2=N/2
      KK=N2+1
      DO 50 I=2,N2
      KK=KK-1
      II=KK
      GO TO (5,15,25),NK
    5 CALL SIFTUP (II,N,L,K,H,E,R,A1,A2,A3,A4,LS)
      GO TO 45
C
   15 CALL SIFTUP (II,N,K,H,L,E,R,A1,A2,A3,A4,LS)
      GO TO 45
C
   25 CALL SIFTUP (II,N,H,K,L,E,R,A1,A2,A3,A4,LS)
   45 CONTINUE
   50 CONTINUE
      J=N+1
      KCST=1
      DO 150 I=2,N
      J=J-1
      JJ=J
      GO TO (105,115,125),NK
```

```
  105 CALL SIFTUP (KCST,JJ,L,K,H,E,R, A1,A2,A3,A4,LS)
      GO TO 145
C
  115 CALL SIFTUP (KCST,JJ,K,H,L,E,R, A1,A2,A3,A4,LS)
      GO TO 145
  125 CALL SIFTUP (KCST,JJ,H,K,L,E,R, A1,A2,A3,A4,LS)
  145 CONTINUE
      CALL EXCHG  (KCST,J,H,K,L,E,R,A1,A2,A3,A4,LS)
  150 CONTINUE
      RETURN
      END


      SUBROUTINE SIFTUP (I,N,IH,IK,IL,ES,RS,A1,A2,A3,A4,LS)
      DIMENSION IH(LS),IK(LS),IL(LS)
      DIMENSION ES(LS),RS(LS)
      DIMENSION A1(LS),A2(LS),A3(LS),A4(LS)
      ICOPY1=IK(I)
      ICOPY2=IL(I)
       COPY3= ES(I)
       COPY4=RS(I)
       COPY5=A1(I)
       COPY6=A2(I)
       COPY7=A3(I)
       COPY8=A4(I)
      ICOPY=IH(I)
 1000 J=2*I
      IF (J-N) 2000,2100,4000
 2000 IF (IH(J+1)-IH(J)) 2100,2010,2050
 2010 IF (IK(J+1)-IK(J)) 2100,2020,2050
 2020 IF (IL(J+1)-IL(J)) 2100,2100,2050
 2050 J=J+1
 2100 IF (IH(J)-ICOPY) 4000,2110,2200
 2110 IF (IK(J)-ICOPY1) 4000,2120,2200
 2120 IF (IL(J)-ICOPY2) 4000,4000,2200
 2200 CONTINUE
      IH(I)=IH(J)
      IK(I)=IK(J)
      IL(I)=IL(J)
      ES(I)=ES(J)
      RS(I)=RS(J)
      A1(I)=A1(J)
      A2(I)=A2(J)
      A3(I)=A3(J)
      A4(I)=A4(J)
      I=J
      GO TO 1000
 4000 IH(I)=ICOPY
      IK(I)=ICOPY1
      IL(I)=ICOPY2
      ES(I)= COPY3
      RS(I)= COPY4
      A1(I)= COPY5
      A2(I)= COPY6
      A3(I)= COPY7
      A4(I)= COPY8
      I=1
      RETURN
      END


      SUBROUTINE EXCHG (KCST,J,H,K,L,E,R,A1,A2,A3,A4,LS)
      INTEGER H
      DIMENSION H(LS), K(LS),L(LS)
      DIMENSION E(LS),R(LS)
```

```
      DIMENSION A1(LS),A2(LS),A3(LS),A4(LS)
      IT1= H(KCST)
      IT2= K(KCST)
      IT3= L(KCST)
       T4=E(KCST)
       T5=R(KCST)
       T6=A1(KCST)
       T7=A2(KCST)
       T8=A3(KCST)
       T9=A4(KCST)
      H(KCST)=H(J)
      K(KCST)=K(J)
      L(KCST)=L(J)
      E(KCST)=E(J)
      R(KCST)=R(J)
      A1(KCST)=A1(J)
      A2(KCST)=A2(J)
      A3(KCST)=A3(J)
      A4(KCST)=A4(J)
      H(J)=    IT1
      K(J)=    IT2
      L(J)=    IT3
      E(J)    = T4
      R(J)    = T5
      A1(J)= T6
      A2(J)= T7
      A3(J)= T8
      A4(J)= T9
      RETURN
      END
         FUNCTION RESET (H,A)
C RESET        FUNCTION ADJUSTS PHASES ACCORDING TO VECTOR TYPE.
C
C
      DIMENSION H(3),TYPE(3),KIND(27),ALPH(9)
      INTEGER H,TYPE
      DATA (ISTART=1)
C
C              INITIAL ENTRY READS CONTROL FUNCTIONS CARD.
      I61=61
      PI2=1.57079632679
      PI=3.14159265359
      GO TO (5,50),ISTART
    5 ISTART=2
      READ 10,(KIND(I),I=1,27),(ALPH(J),J=1,6)
   10 FORMAT(27I1,5A8,A5)
C        LOAD ZEROS WITH STANDARD
      DO 15 I=1,27
      IF (KIND(I).LE.0) KIND(I)=8
   15 CONTINUE
C        PRINT FOR REFERENCE
      WRITE (I61,20),(KIND(I),I=1,27),(ALPH(J),J=1,6)
   20 FORMAT(24H0PHASE ADJUSTMENT SPECS.,2X,27I2,2X,6A8)
      C=99.9
      GO TO 300
   50 CONTINUE
C                                                ADJUSTMENT OPTIONS
C        INDEX TYPES     1=O  2=G  3=U
C              VECTOR CLASSIFICATION (TYPE)
C  H    000 000 000 GGG GGG GGG UUU UUU UUU     SIGNIFICANCE OF
C  K    000 GGG UUU 000 GGG UUU 000 GGG UUU      POSITIONS IN TABLE.
C  L    OGU OGU OGU OGU OGU OGU OGU OGU OGU
C
C       1   4   7  10  13  16  19  22  25     *** POSITION
C
```

```
C         A VECTOR IS CLASSIFIED ACCORDING TYPE.
C          THE ENTRY IN THE CORRESPONDING POSITION CAUSES PHASE
C          ADJUSTMENT AS FOLLOWS...
C              ENTRY      FUNCTION  (PHASE ADJUSTED TO...)
C                1         REAL     0 OR PI                          210
C                2         IMAGINARY  -PI/2 OR +PI/2                 220
C                3         * NO CHANGE *                             230
C                4         0                                         240
C                5         PI                                        250
C                6         +PI/2                                     260
C                7         -PI/2                                     270
C                8         BETWEEN   -PI AND +PI                     280
C                9         BETWEEN    0  AND 2PI                     290
C              TYPE DETERMINATION
      DO 75 I=1,3
      TYPE(I)=1
      IF( H(I).EQ.0 ) GO TO 75
      TYPE(I)=MOD( IABS( H(I) ),2 ) + 2
   75 CONTINUE
C         * KIND * ADDRESS (REVERSE FORTRAN NORMAL)
      LOC= TYPE(3) + 3*TYPE(2) + 9*TYPE(1) - 12
      KADJ=KIND(LOC)
      B=A
C                        ADJUST INITIALLY TO -PI,+PI
      B=HEMIR(B)
C                        DO ADJUSTMENT
          GO TO (210,220,230,240,250,260,270,280,290),KADJ
  210 CONTINUE
      C=0.0
      IF( ABS(B).GT.PI2 ) C=PI
      GO TO 300
  220 CONTINUE
      C=PI2
      IF( B.LT.0.0 ) C=-C
      GO TO 300
  230 CONTINUE
      C=A
      GO TO 300
  240 CONTINUE
      C=0.0
      GO TO 300
  250 CONTINUE
      C=PI
      GO TO 300
  260 CONTINUE
      C=PI2
      GO TO 300
  270 CONTINUE
      C=-PI2
      GO TO 300
  280 CONTINUE
      C=B
      GO TO 300
  290 CONTINUE
      C=B
      IF( B.LT.0.0 ) C=B+PI+PI
      GO TO 300
C
  300 CONTINUE
      RESET=C
      RETURN
      END
```

```
      FUNCTION HEMIR (B)
CHEMIR    REDUCES RADIAN ANGLE TO THE RANGE +3.14(180) TO -3.14(-180)
C
C
      PI=3.14159265359
      TUPI=6.2831853071796
    5 A=B
      A=AMOD(A,TUPI)
      IF( ABS(A) .GT. PI ) A=A - SIGN(TUPI,A)
   25 HEMIR=A
      RETURN
      END
```

Appendix C

SAMPLE INPUT CONTROL CARDS

This is a typical example of the refinement of the phases from the basic deck in the first two cycles. In subsequent cycles, additional phases are generated from the set already refined.

```
    4     5                                  NO. 19 P.385    P212121  D4/2
    1     0     0     0          1            X          Y          Z
    0     1     0     0          1
    0     0     1     0          1
   -1     0     0     6          2            1/2-X     -Y      1/2+Z
    0    -1     0     0          2
    0     0     1     6          2
    1     0     0     6          3            1/2+X 1/2-Y          -Z
    0    -1     0     6          3
    0     0    -1     0          3
   -1     0     0     0          4            -X     1/2+Y      1/2-Z
    0     1     0     6          4
    0     0    -1     6          4                  LAST P212121 D4/2
11 111 221121   1    122   2    P212121 D4/2    RESET CARD
 3176.          153032.
                     4   4   3 .3   2.2 (3I5,F10.3,24X,F10.3)
      1    1                     5    CYCLE ON ORIGINAL DECK
    8     1     0     4.651                0.00       0.00
   11     5     0     4.444                1.57       1.57
    0     4     1     3.924                0.00       0.00
    0     9     2     3.662                1.57       1.57
    4    14     2     3.318                0.00       3.14
    5     7     0     3.242               -1.57      -1.57
    8    17     0     3.085                3.14       3.14
    4    18     1     3.012                3.14       0.0
   11     7     0     2.988               -1.57      -1.57
    5    16     2     2.865                0.00       0.00
    8     5     1     2.795                0.00       0.00
    0    13     1     2.763               -1.57      -1.57
    8     3     1     2.758                3.14       3.14
   11     9     1     2.536                1.57       1.57
    8     7     2     2.514                3.14       3.14
    0     6     2     2.499                3.14       3.14
    1     6     1     2.457                3.14       0.0
   10     5     3     2.400               -1.57      -1.57
    8     4     1     2.390               -1.57       -1.57
    4    22     1     2.324                0.00       3.14
    4    21     0     2.262                3.14       0.0
    8     7     0     2.230                0.00       0.00
    1    17     3     2.157                1.57      -1.57
    4    23     1     2.156                0.00       3.14
    7    19     2     2.120                1.57      -1.57
    3    10     1     2.114               -1.57      -1.57
    0     8     2     2.113                0.00       0.00
    0    21     1     2.103               -1.57      -1.57
```

```
  4   20    0     2.101              3.14      0.0
  1   10    2     2.075              3.14      0.0
 10    9    2     2.059             -1.57     -1.57
  3   21    0     2.019             -1.57     -1.57
  4   22    0     2.008              0.0      3.14
  4    3    2     2.005              3.14      0.0
  0    1    4     1.990              0.00      0.0
  1   15    3     1.982             -1.57      1.57
  5    3    1     1.965              1.57      1.57
  3   17    2     1.964              0.00      0.00
  4   11    3     1.956              3.14      0.00
  6   10    3     1.948              0.00      0.00
  7   16    3     1.943              1.57     -1.57
  4   15    2     1.941              0.00      3.14
 11   11    1     1.935             -1.57     -1.57


  5   25    0     1.927             -1.57     -1.57
  4   13    2     1.917              3.14      0.0
  7    7    2     1.874             -1.57      1.57
  4   10    3     1.845              3.14      0.0
 12    1    1     1.822             -1.57      1.57
  5   13    2     1.821              1.57      1.57
  1    8    2     1.791              1.57     -1.57
  4   14    0     1.726              0.00      3.14
  0    2    1     1.724              3.14      3.14
  5   12    3     1.716              3.14      3.14
  3   14    0     1.712              1.57      1.57
  8    1    2     1.637              3.14      3.14
  4   19    1     1.632              3.14      0.00
  4   22    2     1.628              3.14      0.0
  8    5    2     1.554              0.00      0.00
  7   13    1     1.544             -1.57      1.57
  4   17    1     1.466              0.00      3.14
  6   21    2     1.414             -1.57     -1.57
200
                          3 .3  2.2 (3I5,F10.3,24X,F10.3)
 1        1
 1        1   1            1      1ST ADDITION.ONE CYCLE
  0   11    4     2.778
  0    5    2     2.287
  9    3    0     2.060
  3    8    0     1.972
  0   25    2     1.971
  8   12    0     1.959
  1   19    0     1.953
  9    1    0     1.939
  4    7    3     1.920
  8    0    1     1.900
  0   21    4     1.899
  0   17    2     1.864
  8   11    2     1.846
  7    9    3     1.844
  7    9    0     1.842
  1   27    0     1.839
  5    5    0     1.818
  9   11    2     1.816
  1   15    0     1.816
  0   21    3     1.814
  0   15    3     1.807
  5    8    3     1.806
  7   14    4     1.800
  8    8    1     1.799
```

```
  1   13    4     1.793
  0    4    0     1.787
  5    4    4     1.775
  4   18    2     1.775
  1    2    1     1.772
  5   23    0     1.761
  8    9    4     1.752
  0   10    3     1.746
  0    5    3     1.737
  2   16    2     1.733
  5   12    2     1.727
  1    6    2     1.727
  2   12    2     1.725
  2    7    0     1.719
  2   22    4     1.703
  0   19    2     1.701


  9    9    2     1.697
  3    6    0     1.693
 11    2    1     1.680
 11    1    1     1.680
 11    0    1     1.680
  7   13    0     1.679
  6    0    0     1.676
  7   13    4     1.671
 10    0    2     1.668
  7    8    2     1.647
  4   14    3     1.642
  0   16    2     1.639
  0   21    2     1.634
  7   12    4     1.631
 10    0    0     1.622
  8    1    1     1.611
  7    4    2     1.610
  1    3    3     1.608
  1   26    1     1.601
  7   17    2     1.583
  5   21    1     1.574
  1   19    2     1.570
  7   10    0     1.556
 10   13    2     1.550
  0   19    1     1.547
  8   14    0     1.539
  4    6    4     1.537
  7   15    3     1.536
  8   16    3     1.535
  2    5    0     1.533
  8   12    4     1.532
  3   16    2     1.532
  6   19    3     1.522
  7   11    2     1.509
200
 1        1   1            1      2ND ADDITION,ONE CYCLE
  8   18    0     1.508
 11    2    0     1.503
  7    5    3     1.495
  0   20    1     1.495
  0   18    0     1.483
  9    6    0     1.482
 11    7    1     1.476
  1    5    2     1.474
  0   15    5     1.473
```

7	10	2	1.470
4	1	1	1.468
11	4	0	1.463
4	25	1	1.461
1	17	2	1.461
9	5	1	1.459
7	17	3	1.452
8	10	1	1.448
9	14	0	1.445
2	9	2	1.443
10	1	2	1.439
10	4	1	1.436
0	22	1	1.432
9	1	4	1.431
8	13	3	1.431
9	11	1	1.430
10	3	3	1.429
3	12	1	1.425
4	23	2	1.422
9	2	2	1.421
10	7	2	1.418
1	21	2	1.418
8	4	0	1.412
3	9	3	1.411
3	12	3	1.407
10	11	1	1.402
2	26	2	1.398
5	0	4	1.396
0	17	1	1.396
5	11	1	1.389
1	10	3	1.388
0	12	3	1.387
8	3	3	1.385
6	13	1	1.385
8	9	1	1.383
8	18	2	1.375
2	17	0	1.374
9	10	0	1.371
4	7	4	1.370
6	8	3	1.368
1	19	4	1.364
7	2	0	1.360
1	16	2	1.357
1	11	1	1.356
0	1	3	1.355
2	12	3	1.353
5	9	1	1.346
3	11	4	1.337
4	19	2	1.335
5	9	0	1.334
2	14	2	1.334
3	7	4	1.328
1	23	1	1.326
8	14	3	1.325
7	6	2	1.324
6	15	2	1.323
6	9	2	1.323
4	25	0	1.318
6	17	3	1.311
12	3	0	1.307
9	1	2	1.307

8	17	3	1.307
1	4	1	1.307
1	25	2	1.306
0	5	1	1.306
7	20	1	1.298
4	24	1	1.298
8	14	1	1.297
2	25	1	1.297
4	9	3	1.296
8	6	3	1.286
2	20	0	1.282

200

Appendix D

PROGRAM OUTPUT AFTER PROCESSING THE SAMPLE INPUT CONTROL CARDS IN APPENDIX C

When printing on any output source (off-line or on-line), the first character of each line is a carriage control character for spacing on the printer. For example, the character 0 is a double space before printing; the character 1 ejects the page before printing; and a blank character causes a single space after printing.

```
1SYMMETRY OPERATION CHECKING COMPLETE.
0          ROTATION MATRIX       TRANSLATION VECTOR (IN TWELFTHS)
0
    1            1   0   0              0
                 0   1   0              0
                 0   0   1              0

    2           -1   0   0              6
                 0  -1   0              0
                 0   0   1              6

    3            1   0   0              6
                 0  -1   0              6
                 0   0  -1              0

    4           -1   0   0              0
                 0   1   0              6
                 0   0  -1              6
0SYMMETRY MATRICES FOR SPACE GROUP                          NO. 19 P.385   P212121  D4/2
0PHASE ADJUSTMENT SPECS.   1 1 8 1 1 1 8 2 2 1 1 2 1 8 8 1 8 8 8 1 2 2 8 8 2 8 8    P212121 D4/2   RESET CARD
 SIG2=       3176.000 SIG4=     153032.000
1ELAPSED MINUTES=    0.401*.
   INEC   IDEC   NBKJ NCSAVE   INSC   IDSC   INSN NBASIC
      0      0      0      0      0      0      0      0


  CYCLE ON ORIGINAL DECK

    INE    IDF   INS    IDS    INER   IDER   INSP   IFMTB   LSQ
     -0      1     1     -0     -0     -0     -0      2      1
0 EXPAND
0   H    K    L        E       PHASE
    8    1    0     4.6510     0.0000
   -8   -1   -0     4.6510     0.0000
    8   -1   -0     4.6510     3.1416
   -8    1    0     4.6510     3.1416
0 EXPAND
0   H    K    L        E       PHASE
   11    5    0     4.4440     1.5700
  -11   -5   -0     4.4440    -1.5700
   11   -5   -0     4.4440     1.5700
```

```
  -11     5     0     4.4440   -1.5700
0 EXPAND
0   H     K     L        E       PHASE
    0     4     1     3.9240    0.0000
   -0    -4    -1     3.9240    0.0000
    0    -4     1     3.9240    3.1416
   -0     4    -1     3.9240    3.1416
0 EXPAND
0   H     K     L        E       PHASE
    0     9     2     3.6620    1.5700
   -0    -9    -2     3.6620   -1.5700
    0    -9     2     3.6620    1.5700
   -0     9    -2     3.6620   -1.5700
1 CYCLE ON ORIGINAL DECK
```

NC	INEC	IDEC	LSQ	NBRJ	NBASIC	IRMTR	IFLMTR	MTD	NTD	MTR	MTW	ERJ	CHANGE	KCOUNT
404	0	61	1	0	61	-0	-0	60	60	25	25	0.3000	3.1416	3

```
0 BASIC REFLECTION=     8     1     0   4.651    0.000
0          H     K     L        E        R      H     K     L        E        R

          -3   -10    -1    2.114    1.570     11    11     1    1.935   -1.570
          -3   -10     1    2.114   -1.570     11    11    -1    1.935    1.570
          -3    10    -1    2.114    1.572     11    -9     1    2.536   -1.570
          -3    10     1    2.114   -1.572     11    -9    -1    2.536    1.570
          -0    -6    -2    2.499   -3.140      8     7     2    2.514    3.140
           0    -6     2    2.499    3.140      8     7    -2    2.514   -3.140
          -0    -4    -1    3.924    0.000      8     5     1    2.795    0.000
           0    -4     1    3.924    3.142      8     5    -1    2.795    3.142
          -0    -2    -1    1.724   -3.140      8     3     1    2.758    3.140
           0    -2     1    1.724   -0.002      8     3    -1    2.758    0.002
          -0     4    -1    3.924    3.142      8    -3     1    2.758   -3.140
           0     4     1    3.924    0.000      8    -3    -1    2.758   -0.002
          -0     6    -2    2.499   -3.140      8    -5     2    1.554    3.142
           0     6     2    2.499    3.140      8    -5    -2    1.554    3.142
          -0     8    -2    2.113    0.000      8    -7     2    2.514    0.002
           0     8     2    2.113    0.000      8    -7    -2    2.514   -0.002
           1   -15    -3    1.982    1.570      7    16     3    1.943   -1.570
           1   -15     3    1.982   -1.570      7    16    -3    1.943    1.570
```

1	8	-2	1.791	-1.572	7	-7	2	1.874	1.572
1	8	2	1.791	-1.570	7	-7	-2	1.874	1.570
1	17	-3	2.157	1.570	7	-16	3	1.943	-1.572
1	17	3	2.157	-1.570	7	-16	-3	1.943	1.572
3	17	-2	1.964	3.142	5	-16	2	2.865	0.000
3	17	2	1.964	0.000	5	-16	-2	2.865	3.142
4	-22	-1	2.324	3.140	4	23	1	2.156	3.140
4	-22	1	2.324	0.002	4	23	-1	2.156	0.002
4	-21	-0	2.262	3.142	4	22	0	2.008	3.140
4	-20	-0	2.101	0.000	4	21	0	2.262	0.000
4	-18	-1	3.012	0.000	4	19	1	1.632	0.000
4	-18	1	3.012	3.142	4	19	-1	1.632	3.142
4	-17	-1	1.466	-0.002	4	18	1	3.012	0.000
4	-17	1	1.466	-3.140	4	18	-1	3.012	3.142
4	-14	-2	3.318	3.140	4	15	2	1.941	3.140
4	-14	2	3.318	-3.140	4	15	-2	1.941	-3.140
4	-13	-2	1.917	3.142	4	14	2	3.318	3.140
4	-13	2	1.917	3.142	4	14	-2	3.318	-3.140
4	-10	-3	1.845	0.000	4	11	3	1.956	0.000
4	-10	3	1.845	3.142	4	11	-3	1.956	3.142

0 BASIC REFLECTION= 11 5 0 4.444 1.570

0 H	K	L	E	R	H	K	L	E	R
-1	6	-1	2.457	3.142	12	-1	1	1.822	-1.570
-1	6	1	2.457	3.142	12	-1	-1	1.822	-1.572
-0	-4	-1	3.924	0.000	11	9	1	2.536	1.570
0	-4	1	3.924	3.142	11	9	-1	2.536	-1.570
3	10	-1	2.114	1.570	8	-5	1	2.795	0.000
3	10	1	2.114	-1.570	8	-5	-1	2.795	3.142
4	-14	-2	3.318	3.140	7	19	2	2.120	-1.570
4	-14	2	3.318	-3.140	7	19	-2	2.120	-1.572
4	-11	-3	1.956	3.142	7	16	3	1.943	-1.570
4	-11	3	1.956	0.000	7	16	-3	1.943	1.570
4	18	-1	3.012	3.142	7	-13	1	1.544	-1.570
4	18	1	3.012	0.000	7	-13	-1	1.544	1.570
5	-16	-2	2.865	3.142	6	21	2	1.414	-1.570
5	-16	2	2.865	0.000	6	21	-2	1.414	1.570

0 BASIC REFLECTION= 0 4 1 3.924 0.000

0 H	K	L	E	R	H	K	L	E	R
-11	-7	-0	2.988	1.570	11	11	1	1.935	-1.570

-11	-5	-0	4.444	-1.570	11	9	1	2.536	1.570
-11	9	1	2.536	-1.570	11	-5	-0	4.444	1.570
-11	11	1	1.935	1.570	11	-7	-0	2.988	-1.570
-10	-5	3	2.410	1.572	10	9	-2	2.059	1.570
-10	9	-2	2.059	1.572	10	-5	3	2.400	1.570
-8	-3	-1	2.758	-3.140	8	7	2	2.514	3.140
-8	-3	1	2.758	-0.002	8	7	0	2.230	0.000
-8	-1	-0	4.651	0.000	8	5	1	2.795	0.000
-8	-1	2	1.637	3.140	8	5	-1	2.795	3.142
-8	1	0	4.651	3.142	8	3	1	2.758	3.140
-8	1	2	1.637	0.002	8	3	-1	2.758	0.002
-8	3	-1	2.758	3.140	8	1	2	1.637	3.140
-8	3	1	2.758	0.002	8	1	0	4.651	0.000
-8	5	-1	2.795	0.000	8	-1	2	1.637	0.002
-8	5	1	2.795	3.142	8	-1	-0	4.651	3.142
-8	7	0	2.230	3.142	8	-3	1	2.758	-3.140
-8	7	2	2.514	0.002	8	-3	-1	2.758	-0.002
-5	-12	3	1.716	3.140	5	16	-2	2.865	3.142
-5	-3	1	1.965	1.570	5	7	0	3.242	-1.570
-5	7	0	3.242	1.570	5	-3	1	1.965	-1.570
-5	16	-2	2.865	0.000	5	-12	3	1.716	0.002
-4	-18	-1	3.012	0.000	4	22	2	1.628	0.000
-4	-18	1	3.012	3.142	4	22	0	2.008	3.140
-4	-17	1	1.466	-0.002	4	21	0	2.262	0.000
-4	-15	2	1.941	3.140	4	19	-1	1.632	3.142
-4	-14	-0	1.726	-3.140	4	18	1	3.012	0.000
-4	-14	2	3.318	3.140	4	18	-1	3.012	3.142
-4	-13	2	1.917	0.000	4	17	-1	1.466	0.002
-4	-11	3	1.956	3.142	4	15	-2	1.941	-3.140
-4	-10	3	1.845	3.142	4	14	-2	3.318	-3.140
-4	14	-2	3.318	3.140	4	-10	3	1.845	3.142
-4	15	-2	1.941	-0.002	4	-11	3	1.956	0.000
-4	17	-1	1.466	3.140	4	-13	2	1.917	3.142
-4	18	-1	3.012	3.142	4	-14	2	3.318	-3.140
-4	18	1	3.012	0.000	4	-14	-0	1.726	3.140
-4	19	-1	1.632	0.000	4	-15	2	1.941	0.002
-4	21	0	2.262	3.142	4	-17	1	1.466	-3.140
-4	22	0	2.008	-3.140	4	-18	1	3.012	3.142
-4	22	2	1.628	0.000	4	-18	-1	3.012	0.000
-3	-10	1	2.114	-1.570	3	14	0	1.712	1.570
-3	14	0	1.712	1.572	3	-10	1	2.114	-1.572
-1	-6	-1	2.457	0.000	1	10	2	2.075	0.000
-1	10	2	2.075	3.142	1	-6	-1	2.457	3.142
0	-9	2	3.662	1.570	-0	13	-1	2.763	-1.572
-0	-4	-1	3.924	0.000	0	8	2	2.113	0.000

```
        -0   -2   -1   1.724  -3.140    0    6    2   2.499   3.140
0 BASIC REFLECTION=    0    9    2   3.662   1.570
0        H    K    L       F       R    H    K    L       F       R

        -8    4    1   2.390   1.570    8    5    1   2.795   0.000

        -8    5    1   2.795   3.142    8    4    1   2.390  -1.570
        -5  -16    2   2.865   3.142    5   25    0   1.927  -1.570
        -5   -7   -0   3.242   1.570    5   16    2   2.865   0.000
        -5   -3   -1   1.965  -1.570    5   12    3   1.716   3.140
        -5   12    3   1.716   0.002    5   -3   -1   1.965   1.570
        -5   16    2   2.865   3.142    5   -7   -0   3.242  -1.570
        -5   25    0   1.927   1.570    5  -16    2   2.865   0.000



        -4  -13    2   1.917   0.000    4   22    0   2.008   3.140
        -4  -10    3   1.845   3.142    4   19   -1   1.632   3.142
        -4   19   -1   1.632   0.000    4  -10    3   1.845   3.142
        -4   22    0   2.008  -3.140    4  -13    2   1.917   3.142
        -1   -6   -1   2.457   0.000    1   15    3   1.982   1.570
        -1   15    3   1.982  -1.570    1   -6   -1   2.457   3.142
         0   -4    1   3.924   3.142    0   13    1   2.763  -1.570
         0    1    4   1.990   0.000   -0    8   -2   2.113   0.000
1                                        * * *    TANGENT FORMULA RESULTS     * * *


     H    K    L   OBS R  CALC R   OBS E  CALC E     A       B       N


     8    1    0   0.000   0.000   4.651   2.408   2.408  -0.000  38.000
    11    5    0   1.570   1.571   4.444   2.813   0.000   2.813  14.000
     0    4    1   0.000   0.000   3.924   2.657   2.657  -0.000  47.000
     0    9    2   1.570   1.571   3.662   2.174   0.130   2.170  16.000
     4   14    2   3.140  -3.020   3.318   2.500  -2.481  -0.302  19.000
     5    7    0  -1.570  -1.571   3.242   1.671   0.000  -1.671  21.000
     8   17    0   3.140   3.142   3.085   1.806  -1.806   0.000  10.000
     4   18    1   0.000   0.256   3.012   1.850   1.790   0.469  24.000
    11    7    0  -1.570  -1.571   2.968   2.729  -0.000  -2.729  11.000
     5   16    2   0.000  -0.071   2.865   1.829   1.825  -0.131  12.000
     8    5    1   0.000  -0.000   2.795   2.403   2.403  -0.001  16.000
     0   13    1  -1.570  -1.571   2.763   2.767  -0.001  -2.767   8.000
     8    3    1   3.140  -3.117   2.758   2.645  -2.644  -0.066  24.000
    11    9    1   1.570   1.513   2.536   2.536   0.147   2.532  11.000
```

8	7	2	3.140	-3.084	2.514	2.935	-2.930	-0.169	11.000
0	6	2	3.140	3.142	2.499	2.657	-2.657	0.000	19.000
1	6	1	0.000	0.645	2.457	1.121	0.896	0.673	15.000
10	5	3	-1.570	1.851	2.400	2.337	-0.646	2.246	3.000
8	4	1	-1.570	-1.437	2.390	1.128	0.150	-1.118	15.000
4	22	1	3.140	-3.142	2.324	2.474	-2.474	-0.000	6.000
4	21	0	0.000	0.000	2.262	2.207	2.207	0.000	23.000
8	7	0	0.000	0.000	2.230	1.968	1.968	0.000	17.000
1	17	3	-1.570	-1.570	2.157	1.879	0.001	-1.879	4.000
4	23	1	3.140	3.141	2.156	1.963	-1.963	0.001	7.000
7	19	2	-1.570	-1.809	2.120	3.290	-0.777	-3.197	3.000
3	10	1	-1.570	-1.571	2.114	3.175	-0.001	-3.175	14.000
0	8	2	0.000	0.000	2.113	2.646	2.640	-0.180	20.000
0	21	1	-1.570	-1.571	2.103	2.033	-0.000	-2.033	5.000
4	20	0	0.000	0.000	2.101	2.672	2.672	-0.000	15.000
1	10	2	0.000	0.750	2.075	1.837	1.344	1.252	8.000
10	9	2	-1.570	-1.223	2.059	0.921	0.314	-0.866	5.000
3	21	0	-1.570	-1.571	2.019	1.191	-0.000	-1.191	8.000
4	22	0	3.140	3.142	2.008	2.410	-2.410	0.000	17.000
4	3	2	0.000	0.910	2.005	2.051	1.259	1.619	7.000
0	1	4	0.000	1.571	1.990	0.762	0.001	0.762	5.000
1	15	3	1.570	1.293	1.982	1.831	0.501	1.761	5.000
5	3	1	1.570	1.677	1.965	2.296	-0.245	2.283	10.000
3	17	2	0.000	3.142	1.964	3.484	-3.484	0.000	4.000
4	11	3	0.000	-0.091	1.956	2.284	2.275	-0.209	11.000
6	10	3	0.000	2.956	1.948	2.242	-2.204	0.413	4.000
7	16	3	-1.570	-1.743	1.943	3.500	-0.599	-3.449	4.000
4	15	2	3.140	2.971	1.941	2.276	-2.243	0.387	16.000
11	11	1	-1.570	-1.570	1.935	3.223	0.002	-3.223	6.000
5	25	0	-1.570	-1.571	1.927	1.333	-0.000	-1.333	12.000
4	13	2	0.000	-0.251	1.917	1.797	1.741	-0.446	12.000
7	7	2	1.570	1.385	1.874	2.836	0.525	2.787	6.000
4	10	3	0.000	0.286	1.845	2.617	2.511	0.739	13.000
12	1	1	1.570	1.166	1.822	2.480	0.977	2.280	7.000
5	13	2	1.570	1.761	1.821	2.090	-0.394	2.053	5.000
1	8	2	-1.570	-1.786	1.791	2.038	-0.436	-1.991	10.000
4	14	0	3.140	0.000	1.726	2.153	2.153	-0.000	15.000
0	2	1	3.140	3.142	1.724	2.697	-2.697	0.000	27.000
5	12	3	3.140	3.141	1.716	1.243	-1.243	0.001	7.000
3	14	0	1.570	1.571	1.712	2.762	0.000	2.762	12.000
8	1	2	3.140	-3.141	1.637	2.143	-2.143	-0.001	14.000

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     4   19    1   0.000  -0.326   1.632   1.827   1.731  -0.386  14.000
     4   22    2   0.000  -0.223   1.628   1.788   1.744  -0.395   9.000
     8    5    2   0.000  -0.189   1.554   2.544   2.499  -0.479   6.000
     7   13    1   1.570   1.727   1.544   1.989  -0.310   1.965   8.000
     4   17    1   3.140   3.020   1.466   2.385  -2.368   0.288  17.000
     6   21    2  -1.570  -1.571   1.414   4.218   0.000  -4.218   2.000
0 R-FACTORS FOR CALCULATED VALUES- F,  0.3111
0 SCALE FACTORS- CALC F,  0.0606 OVERALL  1.0000
0 VECTOR  COUNTS-  TOTAL    61.0 PASSED     0.0

1ELAPSED MINUTES=    0.168*,

   INEC   IDEC   NRHJ NCSAVE   INSC   IDSC   INSN NRASIC
      0     61      0    414     61      0      0     61



    INE    IDE    INS    IDS   INER   IDER   INSP  IFMTR    LSQ
      1     -0      1     -0     -0     -0     -0      1      1


                                  H    K    L      EI         R        CE        BR        NN

                        REJECTED  10    5    3  2.4000   -1.5700    2.3367    1.8509    3.0000
                        REJECTED   3   17    2  1.9640    0.0000    3.4844    3.1416    4.0000
                        REJECTED   6   10    3  1.9480    0.0000    2.2418    2.9564    4.0000
                        REJECTED   4   14    0  1.7260    3.1400    2.1535    0.0000   15.0000
                        REJECTED   6   21    2  1.4140   -1.5700    4.2181   -1.5708    2.0000
1

   NC   INEC   IDEC    LSQ   NESJ NBASIC IRMTR IFLMTR MTD    NTD   MTR   MTW      ERJ     CHANGE  KCOUNT
  368     61      0      1      5     56    -0     -0   60     60    25    25   0.3000    3.1416       3


1                                        * * *    TANGENT FORMULA RESULTS    * * *

     H     K     L   OBS F  CALC F   OBS F  CALC F      A        B        N
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8	1	0	0.000	0.000	4.651	2.269	2.269	-0.000	36.000
11	5	0	1.571	1.571	4.444	2.308	0.000	2.308	12.000
0	4	1	0.000	0.000	3.924	2.645	2.645	-0.000	43.000
0	9	2	1.571	1.571	3.662	1.989	-0.000	1.989	16.000
4	14	2	-3.020	-2.832	3.318	2.228	-2.122	-0.680	19.000
5	7	0	-1.571	-1.571	3.242	2.317	-0.000	-2.317	17.000
8	17	0	3.142	3.142	3.085	1.907	-1.907	-0.000	10.000
4	18	1	0.256	0.208	3.012	1.985	1.942	0.409	22.000
11	7	0	-1.571	-1.571	2.988	2.309	-0.000	-2.309	11.000
5	16	2	-0.071	-0.130	2.865	2.374	2.354	-0.308	9.000
8	5	1	-0.000	0.026	2.795	2.509	2.508	0.066	14.000
0	13	1	-1.571	-1.571	2.763	2.697	-0.000	-2.697	8.000
8	3	1	-3.117	-3.138	2.758	2.420	-2.420	-0.008	23.000
11	9	1	1.513	1.442	2.536	2.268	0.292	2.249	10.000
8	7	2	-3.084	-3.104	2.514	2.546	-2.544	-0.096	11.000
0	6	2	3.142	3.142	2.499	2.242	-2.242	0.000	19.000
1	6	1	0.645	0.481	2.457	1.721	1.526	0.796	12.000
8	4	1	-1.437	-1.391	2.390	1.430	0.256	-1.407	14.000
4	22	1	-3.142	-2.945	2.324	1.988	-1.950	-0.388	6.000
4	21	0	0.000	0.000	2.262	1.998	1.998	-0.000	22.000
8	7	0	0.000	0.000	2.230	2.010	2.010	-0.000	16.000
1	17	3	-1.570	-1.582	2.157	2.961	-0.033	-2.961	3.000
4	23	1	3.141	-3.114	2.156	2.283	-2.282	-0.063	6.000
7	19	2	-1.869	-1.933	2.120	2.974	-1.053	-2.781	3.000
3	10	1	-1.571	-1.583	2.114	2.651	-0.032	-2.651	14.000
0	8	2	0.000	0.000	2.113	2.780	2.780	0.000	18.000
0	21	1	-1.571	-1.571	2.103	2.650	-0.000	-2.650	5.000
4	20	0	0.000	0.000	2.101	2.241	2.241	-0.000	15.000
1	10	2	0.750	0.711	2.075	1.862	1.411	1.215	8.000
10	9	2	-1.223	-1.566	2.059	2.536	0.012	-2.536	3.000
3	21	0	-1.571	-1.571	2.019	1.458	-0.000	-1.458	6.000
4	22	0	3.142	3.142	2.008	2.235	-2.235	0.000	17.000
4	3	2	0.910	0.666	2.005	2.174	1.710	1.342	7.000
0	1	4	1.571	1.571	1.990	0.734	0.000	0.734	5.000
1	15	3	1.293	1.715	1.982	2.125	-0.306	2.103	4.000
5	3	1	1.677	1.565	1.965	2.130	0.013	2.130	10.000
4	11	3	-0.091	-0.215	1.956	2.325	2.272	-0.495	10.000
7	16	3	-1.743	-1.451	1.943	3.884	0.464	-3.856	3.000
4	15	2	2.971	2.987	1.941	2.030	-2.005	0.313	15.000
11	11	1	-1.570	-1.617	1.935	2.727	-0.125	-2.724	6.000
5	25	0	-1.571	-1.571	1.927	2.162	0.000	-2.162	10.000

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     4    13     2  -0.251  -0.438   1.917   2.113   1.913  -0.897  11.000
     7     7     2   1.385   1.393   1.874   2.680   0.473   2.638   6.000
     4    10     3   0.266   0.363   1.845   2.498   2.336   0.886  13.000
    12     1     1   1.166   1.080   1.822   1.875   0.884   1.654   7.000
     5    13     2   1.761   1.707   1.821   2.034  -0.275   2.015   5.000
     1     8     2  -1.766  -1.652   1.791   1.857  -0.150  -1.851  10.000
     0     2     1   3.142   3.142   1.724   2.379  -2.379   0.000  27.000
     5    12     3   3.141   3.051   1.716   2.722  -2.711   0.247   4.000
     3    14     0   1.571   1.571   1.712   2.344  -0.000   2.344  12.000
     8     1     2  -3.141   3.107   1.637   2.315  -2.314   0.081  12.000
     4    19     1  -0.326  -0.346   1.632   2.275   2.140  -0.771  12.000
     4    22     2  -0.223  -0.085   1.628   1.771   1.765  -0.150   8.000
     8     5     2  -0.189  -0.201   1.554   2.176   2.132  -0.434   6.000
     7    13     1   1.727   1.711   1.544   2.166  -0.302   2.145   8.000
     4    17     1   3.020   2.941   1.466   2.264  -2.219   0.451  16.000
    10     5     3   1.851   2.058   2.400   1.977  -0.925   1.748   3.000
     3    17     2   3.142  -2.894   1.964   2.859  -2.772  -0.699   4.000
     6    10     3   2.956   2.731   1.948   1.821  -1.669   0.727   4.000
     4    14     0   0.000   0.000   1.726   1.731   1.731  -0.000  15.000
     6    21     2  -1.571  -1.503   1.414   3.586   0.245  -3.578   2.000
0 R-FACTORS FOR CALCULATED VALUES- F,  0.2768
0 SCALE FACTORS- CALC F,  0.0517 OVERALL  1.0000
0 VECTOR  COUNTS-  TOTAL    61.0 PASSED     0.0

1ELAPSED MINUTES=    0.125*,

   INEC   IDEC   NBRJ NCSAVE   INSC   IDSC   INSN NBASIC
     61      0      5    368     56      0      0     56



 1ST ADDITION,ONE CYCLE

   INE    IDF    INS    IDS   INER   IDER   INSP   IFMTB    LSQ
     1     -0      1      1     -0     -0      1      1      1


                                   H     K     L      EI          R          CE         BR         NN
```

REJECTED 6 21 2 1.4140 -1.5708 3.5860 -1.5025 2.0000

1 1ST ADDITION,ONE CYCLE

NC	INEC	IDEC	LSQ	NERJ	NBASIC	IRMTR	IFLMTR	MTD	NTD	MTR	MTW	ERJ	CHANGE	KCOUNT
396	61	0	1	1	60	-0	-0	60	60	25	25	0.3000	3.1416	3

1 * * * TANGENT FORMULA RESULTS * * *

H	K	L	OBS R	CALC R	OBS E	CALC E	A	B	N
8	1	0	0.000	0.000	4.651	2.269	2.269	-0.000	36.000
11	5	0	1.571	1.571	4.444	2.308	0.000	2.308	12.000
0	4	1	0.000	0.000	3.924	2.645	2.645	-0.000	43.000
0	9	2	1.571	1.571	3.662	1.989	-0.000	1.989	16.000
4	14	2	-2.832	-2.832	3.318	2.228	-2.122	-0.680	19.000
5	7	0	-1.571	-1.571	3.242	2.317	-0.000	-2.317	17.000
8	17	0	3.142	3.142	3.085	1.907	-1.907	-0.000	10.000
4	18	1	0.208	0.208	3.012	1.985	1.942	0.409	22.000
11	7	0	-1.571	-1.571	2.988	2.309	-0.000	-2.309	11.000
5	16	2	-0.130	-0.130	2.865	2.374	2.354	-0.308	9.000
8	5	1	0.026	0.026	2.795	2.509	2.508	0.066	14.000
0	13	1	-1.571	-1.571	2.763	2.697	-0.000	-2.697	8.000
8	3	1	-3.138	-3.138	2.758	2.420	-2.420	-0.008	23.000
11	9	1	1.442	1.442	2.536	2.268	0.292	2.249	10.000
8	7	2	-3.104	-3.104	2.514	2.546	-2.544	-0.096	11.000
0	6	2	3.142	3.142	2.499	2.242	-2.242	0.000	19.000
1	6	1	0.481	0.481	2.457	1.721	1.526	0.796	12.000
8	4	1	-1.391	-1.391	2.390	1.430	0.256	-1.407	14.000
4	22	1	-2.945	-2.945	2.324	1.988	-1.950	-0.388	6.000
4	21	0	0.000	0.000	2.262	1.998	1.998	-0.000	22.000
8	7	0	0.000	0.000	2.230	2.010	2.010	-0.000	16.000
1	17	3	-1.582	-1.582	2.157	2.961	-0.033	-2.961	3.000
4	23	1	-3.114	-3.114	2.156	2.283	-2.282	-0.063	6.000
7	19	2	-1.933	-1.933	2.120	2.974	-1.053	-2.781	3.000
3	10	1	-1.583	-1.583	2.114	2.651	-0.032	-2.651	14.000
0	8	2	0.000	0.000	2.113	2.780	2.780	0.000	18.000
0	21	1	-1.571	-1.571	2.103	2.650	-0.000	-2.650	5.000
4	20	0	0.000	0.000	2.101	2.241	2.241	-0.000	15.000
1	10	2	0.711	0.711	2.075	1.862	1.411	1.215	8.000
10	9	2	-1.566	-1.566	2.059	2.536	0.012	-2.536	3.000
3	21	0	-1.571	-1.571	2.019	1.458	-0.000	-1.458	6.000

4	22	0	3.142	3.142	2.008	2.235	-2.235	0.000	17.000
4	3	2	0.666	0.666	2.005	2.174	1.710	1.342	7.000
0	1	4	1.571	1.571	1.990	0.734	0.000	0.734	5.000
1	15	3	1.715	1.715	1.982	2.125	-0.306	2.103	4.000
5	3	1	1.565	1.565	1.965	2.130	0.013	2.130	10.000
4	11	3	-0.215	-0.215	1.956	2.325	2.272	-0.495	10.000
7	16	3	-1.451	-1.451	1.943	3.884	0.464	-3.856	3.000
4	15	2	2.987	2.987	1.941	2.030	-2.005	0.313	15.000
11	11	1	-1.617	-1.617	1.935	2.727	-0.125	-2.724	6.000
5	25	0	-1.571	-1.571	1.927	2.162	0.000	-2.162	10.000
4	13	2	-0.438	-0.438	1.917	2.113	1.913	-0.897	11.000
7	7	2	1.393	1.393	1.874	2.680	0.473	2.538	6.000
4	10	3	0.363	0.363	1.845	2.498	2.336	0.886	13.000
12	1	1	1.080	1.080	1.822	1.875	0.884	1.654	7.000
5	13	2	1.707	1.707	1.821	2.034	-0.275	2.015	5.000
1	8	2	-1.652	-1.652	1.791	1.857	-0.150	-1.851	10.000
0	2	1	3.142	3.142	1.724	2.379	-2.379	0.000	27.000
5	12	3	3.051	3.051	1.716	2.722	-2.711	0.247	4.000
3	14	0	1.571	1.571	1.712	2.344	-0.000	2.344	12.000
8	1	2	3.107	3.107	1.637	2.315	-2.314	0.081	12.000
4	19	1	-0.346	-0.346	1.632	2.275	2.140	-0.771	12.000
4	22	2	-0.085	-0.085	1.628	1.771	1.765	-0.150	8.000
8	5	2	-0.201	-0.201	1.554	2.176	2.132	-0.434	6.000
7	13	1	1.711	1.711	1.544	2.166	-0.302	2.145	8.000
4	17	1	2.941	2.941	1.466	2.264	-2.219	0.451	16.000
10	5	3	2.058	2.058	2.400	1.977	-0.925	1.748	3.000
3	17	2	-2.894	-2.894	1.964	2.859	-2.772	-0.699	4.000
6	10	3	2.731	2.731	1.948	1.821	-1.669	0.727	4.000
4	14	0	0.000	0.000	1.726	1.731	1.731	-0.000	15.000
0	11	4	0.000	-1.571	2.778	1.616	-0.000	-1.616	6.000
0	5	2	0.000	-1.571	2.287	0.044	0.000	-0.044	7.000
9	3	0	0.000	1.571	2.060	1.490	0.000	1.490	9.000
3	8	0	0.000	1.571	1.972	2.832	0.000	2.832	15.000
0	25	2	0.000	-1.571	1.971	2.071	0.000	-2.071	3.000
8	12	0	0.000	0.000	1.959	1.595	1.595	0.000	2.000
1	19	0	0.000	-1.571	1.953	2.253	-0.000	-2.253	8.000
9	1	0	0.000	-1.571	1.939	1.261	-0.000	-1.261	14.000
4	7	3	0.000	0.995	1.920	2.289	1.247	1.920	6.000
8	0	1	0.000	1.571	1.900	0.115	-0.000	0.115	4.000
0	21	4	0.000	-1.571	1.899	2.160	0.000	-2.160	2.000
0	17	2	0.000	1.571	1.864	0.539	0.000	0.539	6.000

8	11	2	0.000	0.548	1.846	1.252	1.069	0.552	4.000
7	9	3	0.000	-1.031	1.844	1.398	0.719	-1.199	2.000
7	9	0	0.000	1.571	1.842	2.071	-0.000	2.071	13.000
1	27	0	0.000	-1.571	1.839	2.210	-0.000	-2.210	7.000
5	5	0	0.000	1.571	1.818	1.626	0.000	1.626	16.000
9	11	2	0.000	0.371	1.816	2.285	2.129	0.829	7.000
1	15	0	0.000	1.571	1.816	2.559	-0.000	2.559	5.000
0	21	3	0.000	-1.571	1.814	0.078	0.000	-0.078	3.000
0	15	3	0.000	1.571	1.807	2.273	0.000	2.273	3.000
5	8	3	0.000	-0.283	1.806	2.514	2.414	-0.701	4.000
7	14	4	0.000	-1.215	1.800	1.817	0.633	-1.703	3.000
8	8	1	0.000	3.018	1.799	0.768	-0.762	0.095	8.000
1	13	4	0.000	1.282	1.793	2.205	0.627	2.114	6.000
0	4	0	0.000	3.142	1.787	1.955	-1.955	0.000	13.000
5	4	4	0.000	-3.129	1.775	2.150	-2.150	-0.027	6.000
4	18	2	0.000	0.475	1.775	1.801	1.602	0.823	5.000
1	2	1	0.000	-2.572	1.772	1.106	-0.932	-0.596	10.000
5	23	0	0.000	1.571	1.761	1.467	0.000	1.467	6.000
8	9	4	0.000	-2.790	1.752	1.212	-1.138	-0.417	5.000
0	10	3	0.000	3.142	1.746	2.226	-2.226	0.000	14.000
0	5	3	0.000	-1.571	1.737	1.819	-0.000	-1.819	13.000
2	16	2	0.000	1.056	1.733	1.729	0.851	1.505	3.000
5	12	2	0.000	2.698	1.727	1.750	-1.580	0.751	5.000
1	6	2	0.000	2.263	1.727	1.636	-1.044	1.260	7.000
2	12	2	0.000	0.359	1.725	2.274	2.129	0.799	3.000
2	7	0	0.000	0.000	1.719	0.617	0.617	0.000	5.000
2	22	4	0.000	1.492	1.703	1.704	0.135	1.699	1.000
0	19	2	0.000	-1.571	1.701	1.346	0.000	-1.346	3.000
9	9	2	0.000	-2.115	1.697	2.631	-1.363	-2.250	6.000
3	6	0	0.000	-1.571	1.693	2.942	-0.000	-2.942	25.000
11	2	1	0.000	-3.134	1.680	1.347	-1.347	-0.011	4.000
11	1	1	0.000	-1.535	1.680	3.140	0.112	-3.138	6.000
11	0	1	0.000	1.571	1.680	1.042	-0.000	1.042	6.000
7	13	0	0.000	-1.571	1.679	1.333	-0.000	-1.333	11.000
6	0	0	0.000	0.000	1.676	1.994	1.994	-0.000	8.000
7	13	4	0.000	-0.058	1.671	0.660	0.659	-0.038	5.000
10	0	2	0.000	0.000	1.668	1.814	1.814	0.000	1.000
7	8	2	0.000	-1.752	1.647	1.556	-0.280	-1.531	10.000
4	14	3	0.000	-1.883	1.642	1.240	-0.381	-1.180	3.000
0	16	2	0.000	0.000	1.639	2.371	2.371	-0.000	2.000
0	21	2	0.000	-1.571	1.634	1.855	0.000	-1.855	2.000

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     7   12    4   0.000   1.572   1.631   2.976  -0.002   2.976   3.000
    10    0    0   0.000   3.142   1.622   2.467  -2.467   0.000  18.000
     8    1    1   0.000  -0.068   1.611   2.165   2.160  -0.147   9.000
     7    4    2   0.000  -0.420   1.610   2.052   1.873  -0.838   4.000
     1    3    3   0.000  -2.305   1.608   2.074  -1.389  -1.539   8.000
     1   26    1   0.000   2.505   1.601   1.643  -1.321   0.977   5.000
     7   17    2   0.000   1.929   1.583   2.374  -0.832   2.223   4.000
     5   21    1   0.000   1.758   1.574   2.331  -0.434   2.291   7.000
     1   19    2   0.000  -1.333   1.570   1.766   0.416  -1.716   5.000
     7   10    0   0.000   1.571   1.556   0.524  -0.000   0.524   6.000
    10   13    2   0.000   0.185   1.550   2.827   2.778   0.520   2.000
     0   19    1   0.000   1.571   1.547   2.093   0.000   2.093   5.000
     8   14    0   0.000   3.142   1.539   0.327  -0.327  -0.000   4.000
     4    6    4   0.000  -2.552   1.537   2.493  -2.073  -1.385  10.000
     7   15    3   0.000   1.642   1.536   2.751  -0.197   2.744   4.000
     8   16    3   0.000   1.701   1.535   1.471  -0.191   1.459   3.000
     2    5    0   0.000   0.000   1.533   0.000   0.000   0.000   0.000
     8   12    4   0.000  -1.347   1.532   0.963   0.213  -0.939   4.000
     3   16    2   0.000  -2.861   1.532   0.634  -0.609  -0.175   5.000
     6   19    3   0.000   2.644   1.522   0.723  -0.636   0.345   3.000
     7   11    2   0.000   3.064   1.509   1.521  -1.517   0.118   7.000
     6   21    2  -1.503  -1.418   1.414   4.010   0.611  -3.963   2.000
0 R-FACTORS FOR CALCULATED VALUES= E,  0.3702
0 SCALE FACTORS- CALC E,  0.0579 OVERALL  1.0082
0 VECTOR  COUNTS-  TOTAL   135.0 PASSED    60.0

1ELAPSED MINUTES=    0.178*,

   INEC   IDEC   NBRJ NCSAVE   INSC   IDSC   INSN NBASIC
     61      0      1    396     60     74     60     60


  2ND ADDITION,ONE CYCLE

    INE    IDE   INS.    IDS    INER   IDER   INSR   IFMTR    LSQ
      1     -0      1      1     -0     -0      1      1      1


                                   H     K     L      EI          R          CE         BR         NN
```

REJECTED	0	5	2	2.2870	0.0000	0.0441	-1.5708	7.0000
REJECTED	8	12	0	1.9590	0.0000	1.5951	0.0000	2.0000
REJECTED	8	0	1	1.9000	0.0000	0.1149	1.5708	4.0000
REJECTED	0	21	4	1.8990	0.0000	2.1596	-1.5708	2.0000
REJECTED	7	9	3	1.8440	0.0000	1.3977	-1.0306	2.0000
REJECTED	0	21	3	1.8140	0.0000	0.0783	-1.5708	3.0000
REJECTED	2	22	4	1.7030	0.0000	1.7042	1.4917	1.0000
REJECTED	10	0	2	1.6680	0.0000	1.8140	0.0000	1.0000
REJECTED	0	16	2	1.6390	0.0000	2.3711	0.0000	2.0000
REJECTED	0	21	2	1.6340	0.0000	1.8546	-1.5708	2.0000
REJECTED	10	13	2	1.5500	0.0000	2.8267	0.1850	2.0000
REJECTED	2	5	0	1.5330	0.0000	0.0000	0.0000	0.0000

1 2ND ADDITION,END

NC	INFC	ICEI
782	135	1

1 * * * TANGENT FORMULA RESULTS * * *

H	K	L				CALC E	A	B	N
8	1	0				2.269	2.269	-0.000	36.000
11	5	0				2.308	0.000	2.308	12.000
0	4	1				2.645	2.645	-0.000	43.000
0	9	2				1.989	-0.000	1.989	16.000
4	14	2				2.228	-2.122	-0.680	19.000
5	7	0	1.571	-1.571	3.242	2.317	-0.000	-2.317	17.000
8	17	0	3.142	3.142	3.085	1.907	-1.907	-0.000	10.000
4	18	1	0.208	0.208	3.012	1.985	1.942	0.409	22.000
11	7	0	1.571	-1.571	2.988	2.309	-0.000	-2.309	11.000
5	16	2	0.130	-0.130	2.865	2.374	2.354	-0.308	9.000
8	5	1	0.026	0.026	2.795	2.509	2.508	0.066	14.000
0	13	1	1.571	-1.571	2.763	2.697	-0.000	-2.697	8.000
8	3	1	3.138	-3.138	2.758	2.420	-2.420	-0.008	23.000
11	9	1	1.442	1.442	2.536	2.268	0.292	2.249	10.000
8	7	2	3.104	-3.104	2.514	2.546	-2.544	-0.096	11.000
0	6	2	3.142	3.142	2.499	2.242	-2.242	0.000	19.000
1	6	1	0.481	0.481	2.457	1.721	1.526	0.796	12.000
8	4	1	1.391	-1.391	2.390	1.430	0.256	-1.407	14.000

4	22	1	-2.945	-2.945	2.324	1.988	-1.950	-0.388	6.000
4	21	0	0.000	0.000	2.262	1.998	1.998	-0.000	22.000
8	7	0	0.000	0.000	2.230	2.010	2.010	-0.000	16.000
1	17	3	-1.582	-1.582	2.157	2.961	-0.033	-2.961	3.000
4	23	1	-3.114	-3.114	2.156	2.283	-2.282	-0.063	6.000
7	19	2	-1.933	-1.933	2.120	2.974	-1.053	-2.781	3.000
3	10	1	-1.563	-1.563	2.114	2.651	-0.032	-2.651	14.000
0	8	2	0.000	0.000	2.113	2.780	2.780	0.000	18.000
0	21	1	-1.571	-1.571	2.103	2.650	-0.000	-2.650	5.000
4	20	0	0.000	0.000	2.101	2.241	2.241	-0.000	15.000
1	10	2	0.711	0.711	2.075	1.862	1.411	1.215	8.000
10	9	2	-1.566	-1.566	2.059	2.536	0.012	-2.536	3.000
3	21	0	-1.571	-1.571	2.019	1.458	-0.000	-1.458	6.000
4	22	0	3.142	3.142	2.008	2.235	-2.235	0.000	17.000
4	3	2	0.666	0.666	2.005	2.174	1.710	1.342	7.000
0	1	4	1.571	1.571	1.990	0.734	0.000	0.734	5.000
1	15	3	1.715	1.715	1.982	2.125	-0.306	2.103	4.000
5	3	1	1.565	1.565	1.965	2.130	0.013	2.130	10.000
4	11	3	-0.215	-0.215	1.956	2.325	2.272	-0.495	10.000
7	16	3	-1.451	-1.451	1.943	3.884	0.464	-3.856	3.000
4	15	2	2.987	2.987	1.941	2.030	-2.005	0.313	15.000
11	11	1	-1.617	-1.617	1.935	2.727	-0.125	-2.724	6.000
5	25	0	-1.571	-1.571	1.927	2.162	0.000	-2.162	10.000
4	13	2	-0.438	-0.438	1.917	2.113	1.913	-0.897	11.000
7	7	2	1.393	1.393	1.874	2.680	0.473	2.638	6.000
4	10	3	0.363	0.363	1.845	2.498	2.336	0.886	13.000
12	1	1	1.080	1.080	1.822	1.875	0.884	1.654	7.000
5	13	2	1.707	1.707	1.821	2.034	-0.275	2.015	5.000
1	8	2	-1.652	-1.652	1.791	1.857	-0.150	-1.851	10.000
0	2	1	3.142	3.142	1.724	2.379	-2.379	0.000	27.000
5	12	3	3.051	3.051	1.716	2.722	-2.711	0.247	4.000
3	14	0	1.571	1.571	1.712	2.344	-0.000	2.344	12.000
8	1	2	3.107	3.107	1.637	2.315	-2.314	0.081	12.000
4	19	1	-0.346	-0.346	1.632	2.275	2.140	-0.771	12.000
4	22	2	-0.085	-0.085	1.628	1.771	1.765	-0.150	8.000
8	5	2	-0.201	-0.201	1.554	2.176	2.132	-0.434	6.000
7	13	1	1.711	1.711	1.544	2.166	-0.302	2.145	8.000
4	17	1	2.941	2.941	1.466	2.264	-2.219	0.451	16.000
10	5	3	2.058	2.058	2.400	1.977	-0.925	1.748	3.000
3	17	2	-2.894	-2.894	1.964	2.859	-2.772	-0.699	4.000
6	10	3	2.731	2.731	1.948	1.821	-1.669	0.727	4.000

4	14	0	0.000	0.000	1.726	1.731	1.731	-0.000	15.000
0	11	4	-1.571	-1.571	2.778	1.616	-0.000	-1.616	6.000
9	3	0	1.571	1.571	2.060	1.490	0.000	1.490	9.000
3	8	0	1.571	1.571	1.972	2.832	0.000	2.832	15.000
0	25	2	-1.571	-1.571	1.971	2.071	0.000	-2.071	3.000
1	19	0	-1.571	-1.571	1.953	2.253	-0.000	-2.253	8.000
9	1	0	-1.571	-1.571	1.939	1.261	-0.000	-1.261	14.000
4	7	3	0.995	0.995	1.920	2.289	1.247	1.920	6.000
0	17	2	1.571	1.571	1.864	0.539	0.000	0.539	6.000
8	11	2	0.548	0.548	1.846	1.252	1.069	0.652	4.000
7	9	0	1.571	1.571	1.842	2.071	-0.000	2.071	13.000
1	27	0	-1.571	-1.571	1.839	2.210	-0.000	-2.210	7.000
5	5	0	1.571	1.571	1.818	1.626	0.000	1.626	16.000
9	11	2	0.371	0.371	1.816	2.285	2.129	0.829	7.000
1	15	0	1.571	1.571	1.816	2.559	-0.000	2.559	5.000
0	15	3	1.571	1.571	1.807	2.273	0.000	2.273	3.000
5	8	3	-0.283	-0.283	1.806	2.514	2.414	-0.701	4.000
7	14	4	-1.215	-1.215	1.800	1.817	0.633	-1.703	3.000
8	8	1	3.018	3.018	1.799	0.768	-0.762	0.095	8.000
1	13	4	1.282	1.282	1.793	2.205	0.627	2.114	6.000
0	4	0	3.142	3.142	1.767	1.955	-1.955	0.000	13.000
5	4	4	-3.129	-3.129	1.775	2.150	-2.150	-0.027	6.000
4	18	2	0.475	0.475	1.775	1.801	1.602	0.823	5.000
1	2	1	-2.572	-2.572	1.772	1.106	-0.932	-0.596	10.000
5	23	0	1.571	1.571	1.761	1.467	0.000	1.467	6.000
8	9	4	-2.790	-2.790	1.752	1.212	-1.138	-0.417	5.000
0	10	3	3.142	3.142	1.746	2.226	-2.226	0.000	14.000
0	5	3	-1.571	-1.571	1.737	1.819	-0.000	-1.819	13.000
2	16	2	1.056	1.056	1.733	1.729	0.851	1.505	3.000
5	12	2	2.698	2.698	1.727	1.750	-1.580	0.751	5.000
1	6	2	2.263	2.263	1.727	1.636	-1.044	1.260	7.000
2	12	2	0.359	0.359	1.725	2.274	2.129	0.799	3.000
2	7	0	0.000	0.000	1.719	0.617	0.617	0.000	5.000
0	19	2	-1.571	-1.571	1.701	1.346	0.000	-1.346	3.000
9	9	2	-2.115	-2.115	1.697	2.631	-1.363	-2.250	6.000
3	6	0	-1.571	-1.571	1.693	2.942	-0.000	-2.942	25.000
11	2	1	-3.134	-3.134	1.680	1.347	-1.347	-0.011	4.000
11	1	1	-1.535	-1.535	1.680	3.140	0.112	-3.138	6.000
11	0	1	1.571	1.571	1.680	1.042	-0.000	1.042	6.000
7	13	0	-1.571	-1.571	1.679	1.333	-0.000	-1.333	11.000
6	0	0	0.000	0.000	1.676	1.994	1.994	-0.000	8.000

7	13	4	-0.058	-0.058	1.671	0.660	0.659	-0.038	5.000
7	8	2	-1.752	-1.752	1.647	1.556	-0.280	-1.531	10.000
4	14	3	-1.883	-1.883	1.642	1.240	-0.381	-1.180	3.000
7	12	4	1.572	1.572	1.631	2.976	-0.002	2.976	3.000
10	0	0	3.142	3.142	1.622	2.467	-2.467	0.000	18.000
8	1	1	-0.068	-0.068	1.611	2.165	2.160	-0.147	9.000
7	4	2	-0.420	-0.420	1.610	2.052	1.873	-0.838	4.000
1	3	3	-2.305	-2.305	1.608	2.074	-1.389	-1.539	8.000
1	26	1	2.505	2.505	1.601	1.643	-1.321	0.977	5.000
7	17	2	1.929	1.929	1.583	2.374	-0.832	2.223	4.000
5	21	1	1.758	1.758	1.574	2.331	-0.434	2.291	7.000
1	19	2	-1.333	-1.333	1.570	1.766	0.416	-1.716	5.000
7	10	0	1.571	1.571	1.556	0.524	-0.000	0.524	6.000
0	19	1	1.571	1.571	1.547	2.093	0.000	2.093	5.000
8	14	0	3.142	3.142	1.539	0.327	-0.327	-0.000	4.000
4	6	4	-2.552	-2.552	1.537	2.493	-2.073	-1.385	10.000
7	15	3	1.642	1.642	1.536	2.751	-0.197	2.744	4.000
8	16	3	1.701	1.701	1.535	1.471	-0.191	1.459	3.000
8	12	4	-1.347	-1.347	1.532	0.963	0.213	-0.939	4.000
3	16	2	-2.861	-2.861	1.532	0.634	-0.609	-0.175	5.000
6	19	3	2.644	2.644	1.522	0.723	-0.636	0.345	3.000
7	11	2	3.064	3.064	1.509	1.521	-1.517	0.118	7.000
8	18	0	0.000	0.000	1.508	0.128	0.128	-0.000	28.000
11	2	0	0.000	1.571	1.503	0.466	0.000	0.466	20.000
7	5	3	0.000	1.405	1.495	1.558	0.257	1.537	25.000
0	20	1	0.000	3.142	1.495	1.484	-1.484	0.000	21.000
0	18	0	0.000	0.000	1.483	1.947	1.947	-0.000	44.000
9	6	0	0.000	1.571	1.482	0.856	-0.000	0.856	14.000
11	7	1	0.000	-3.030	1.476	0.508	-0.505	-0.056	20.000
1	5	2	0.000	-2.553	1.474	0.892	-0.742	-0.495	23.000
0	15	5	0.000	-1.571	1.473	1.834	-0.000	-1.834	10.000
7	10	2	0.000	1.420	1.470	1.735	0.261	1.715	17.000
4	1	1	0.000	-1.168	1.468	1.800	0.672	-1.670	43.000
11	4	0	0.000	-1.571	1.463	1.603	-0.000	-1.603	21.000
4	25	1	0.000	0.314	1.461	2.206	2.098	0.682	15.000
1	17	2	0.000	1.842	1.461	0.698	-0.187	0.672	16.000
9	5	1	0.000	-2.089	1.459	2.257	-1.118	-1.961	23.000
7	17	3	0.000	-2.086	1.452	1.661	-0.819	-1.446	16.000
8	10	1	0.000	-0.940	1.448	0.821	0.484	-0.663	17.000
9	14	0	0.000	-1.571	1.445	0.549	-0.000	-0.549	12.000
2	9	2	0.000	-1.469	1.443	1.303	0.133	-1.296	14.000
10	1	2	0.000	2.608	1.439	2.518	-2.168	1.280	10.000
10	4	1	0.000	3.001	1.436	2.063	-2.043	0.289	20.000
0	22	1	0.000	0.000	1.432	2.305	2.305	-0.000	18.000
9	1	4	0.000	-0.016	1.431	1.229	1.229	-0.020	17.000

8	13	3	0.000	0.472	1.431	1.644	1.465	0.748	16.000
9	11	1	0.000	-1.284	1.430	2.135	0.603	-2.048	18.000
10	3	3	0.000	0.697	1.429	1.911	1.465	1.227	8.000
3	12	1	0.000	1.729	1.425	1.678	-0.264	1.657	31.000
4	23	2	0.000	0.473	1.422	1.452	1.292	0.662	18.000
9	2	2	0.000	-1.154	1.421	0.866	0.350	-0.792	17.000
10	7	2	0.000	1.989	1.418	0.515	-0.209	0.471	13.000
1	21	2	0.000	1.180	1.418	2.202	0.838	2.036	20.000
8	4	0	0.000	3.142	1.412	0.960	-0.960	0.000	23.000
3	9	3	0.000	-2.948	1.411	2.039	-2.001	-0.391	30.000
3	12	3	0.000	0.435	1.407	1.321	1.198	0.556	19.000
10	11	1	0.000	-1.838	1.402	2.305	-0.607	-2.223	9.000
2	26	2	0.000	-1.269	1.398	1.457	0.433	-1.391	9.000
5	0	4	0.000	0.000	1.396	0.147	0.147	0.000	6.000
0	17	1	0.000	1.571	1.396	1.426	-0.000	1.426	19.000
5	11	1	0.000	-1.712	1.389	2.317	-0.327	-2.293	24.000
1	10	3	0.000	2.351	1.388	1.256	-0.883	0.893	23.000
0	12	3	0.000	0.000	1.387	2.389	2.389	-0.000	22.000
8	3	3	0.000	0.050	1.385	2.296	2.293	0.115	18.000
6	13	1	0.000	-1.307	1.385	1.671	0.436	-1.613	20.000
8	9	1	0.000	-2.894	1.383	1.450	-1.405	-0.355	24.000
8	18	2	0.000	1.589	1.375	1.903	-0.035	1.902	22.000
2	17	0	0.000	3.142	1.374	1.989	-1.989	0.000	13.000
9	10	0	0.000	-1.571	1.371	1.162	-0.000	-1.162	17.000
4	7	4	0.000	2.620	1.370	2.102	-1.823	1.047	26.000
6	8	3	0.000	-0.782	1.368	1.343	0.954	-0.946	10.000
1	19	4	0.000	1.929	1.364	1.772	-0.622	1.659	12.000
7	2	0	0.000	1.571	1.360	1.739	-0.000	1.739	33.000
1	16	2	0.000	2.147	1.357	1.527	-0.831	1.281	17.000
1	11	1	0.000	-1.892	1.356	1.275	-0.403	-1.210	26.000
0	1	3	0.000	1.571	1.355	1.232	-0.000	1.232	24.000
2	12	3	0.000	-2.073	1.353	2.011	-0.967	-1.763	13.000
5	9	1	0.000	1.444	1.346	2.209	0.280	2.191	29.000
3	11	4	0.000	0.248	1.337	2.029	1.967	0.498	13.000
4	19	2	0.000	-0.657	1.335	1.734	1.373	-1.059	18.000
5	9	0	0.000	1.571	1.334	1.474	0.000	1.474	19.000
2	14	2	0.000	3.030	1.334	1.694	-1.684	0.189	11.000
3	7	4	0.000	-2.091	1.328	0.993	-0.493	-0.862	24.000
1	23	1	0.000	0.760	1.326	1.080	0.783	0.744	26.000
8	14	3	0.000	-1.526	1.325	1.169	0.052	-1.168	23.000
7	6	2	0.000	-2.159	1.324	0.262	-0.145	-0.218	22.000

6	15	2	0.000	2.772	1.323	1.572	-1.466	0.567	17.000
6	9	2	0.000	1.525	1.323	1.821	0.084	1.819	12.000
4	25	0	0.000	3.142	1.318	1.489	-1.489	0.000	22.000
6	17	3	0.000	0.912	1.311	1.567	0.959	1.240	8.000
12	3	0	0.000	0.000	1.307	0.815	0.815	0.000	22.000
9	1	2	0.000	1.374	1.307	1.063	0.208	1.043	16.000
8	17	3	0.000	-2.351	1.307	1.514	-1.065	-1.076	12.000
1	4	1	0.000	-2.026	1.307	1.415	-0.622	-1.271	30.000
1	25	2	0.000	-3.040	1.306	0.758	-0.755	-0.070	10.000
0	5	1	0.000	1.571	1.306	1.462	-0.000	1.462	40.000
7	20	1	0.000	-0.990	1.298	0.849	0.466	-0.710	13.000
4	24	1	0.000	-0.217	1.298	2.832	2.766	-0.610	17.000
8	14	1	0.000	-1.981	1.297	0.807	-0.322	-0.740	23.000
2	25	1	0.000	-2.038	1.297	0.979	-0.441	-0.874	17.000
4	9	3	0.000	2.536	1.296	2.473	-2.033	1.408	24.000
8	6	3	0.000	-1.864	1.286	2.023	-0.586	-1.936	19.000
2	20	0	0.000	0.000	1.282	1.313	1.313	-0.000	21.000
0	5	2	-1.571	-1.571	2.287	0.253	-0.000	-0.253	43.000
8	12	0	0.000	0.000	1.959	1.115	1.115	-0.000	20.000
8	0	1	1.571	1.571	1.900	1.320	-0.000	1.320	18.000
0	21	4	-1.571	-1.571	1.899	1.446	-0.000	-1.446	12.000
7	9	3	-1.031	-2.068	1.844	1.167	-0.557	-1.025	17.000
0	21	3	-1.571	1.571	1.814	1.044	-0.000	1.044	12.000
2	22	4	1.492	-2.573	1.703	1.389	-1.171	-0.747	5.000
10	0	2	0.000	0.000	1.668	1.066	1.066	-0.000	12.000
0	16	2	0.000	0.000	1.639	0.701	0.701	-0.000	17.000
0	21	2	-1.571	-1.571	1.634	0.695	0.000	-0.695	27.000
10	13	2	0.185	0.197	1.550	1.367	1.340	0.268	14.000
2	5	0	0.000	0.000	1.533	0.490	0.490	-0.000	18.000
6	21	2	-1.418	-1.883	1.414	1.873	-0.575	-1.783	10.000

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0 R-FACTORS FOR CALCULATED VALUES- E,  0.3662
0 SCALE FACTORS- CALC E,  0.0796 OVERALL  0.9982
0 VECTOR  COUNTS-  TOTAL   216.0 PASSED   122.0

1ELAPSED MINUTES=    0.374*,
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INEC	IDEC	NREJ	NCSAVE	INSC	IDSC	INSN	NBASIC
135	0	13	782	122	81	122	122

INE	IDE	INS	IDS	INER	IDER	INSP	IFMTB	LSQ
-0	-0	-0	-0	-0	-0	-0	1	1

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13. ABSTRACT

This report contains a description and operating instructions for the tangent-formula refinement program applicable to noncentrosymmetric crystals. This program is coded entirely in FORTRAN language for a large-sized memory computer and is completely listed in the Appendixes.

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