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Computer Program for the Calculation of the Crystal Structure Invariants Based on Certain Conditional Distributions

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ABSTRACT

Effective techniques leading from the values of the crystal structure invariants to the values of individual phases have recently been obtained. In the present report a new formula expressing the structure invariants in terms of the observed crystal structure amplitudes is given, and a computer program is described which facilitates the computation of the invariants.

PROBLEM STATUS

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

AUTHORIZATION

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COMPUTER PROGRAM FOR THE CALCULATION OF THE CRYSTAL STRUCTURE INVARIANTS BASED ON CERTAIN CONDITIONAL DISTRIBUTIONS

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1. INTRODUCTION

It is assumed that the unit cell of a crystal consists of N identical atoms. Denote by $\vec{r}_j$ the position vector of the atom labeled j and by ϕ the phase of the normalized structure factor E. Then the equation

$$E_{\vec{h}} = |E_{\vec{h}}| \exp(i\phi_{\vec{h}}) = \frac{1}{N^{1/2}} \sum_{j=1}^{N} \exp(2\pi i \vec{h}\cdot\vec{r}_j) \tag{1.1}$$

leads directly to

$$\left\langle E_{\vec{h}} \exp(-2\pi i \vec{h}\cdot\vec{r}) \right\rangle_{\vec{h}}$$

$$= \frac{1}{N^{1/2}} \left\langle \sum_{j=1}^{N} \exp[2\pi i \vec{h}\cdot(\vec{r}_j - \vec{r})] \right\rangle_{\vec{h}} \left.\begin{aligned} &= \frac{1}{N^{1/2}} \text{ if } \vec{r} = \vec{r}_j \\ &= 0 \text{ if } \vec{r} \neq \vec{r}_j \end{aligned}\right\} \tag{1.2}$$

It is clear from (1.2) that the crystal structure is determined by the complex normalized structure factors $E_{\vec{h}}$. Since the position vectors $\vec{r}_j$ depend on the choice of origin as well as on the crystal structure, (1.1) does not imply that the normalized structure factors $E_{\vec{h}}$ are determined by the crystal structure alone. As it turns out, however, the magnitudes $|E_{\vec{h}}|$ of the normalized structure factors are in fact uniquely determined by the crystal structure and are independent of the choice of origin. The values of the phases $\phi_{\vec{h}}$, on the other hand, depend on the choice of origin as well as on the crystal structure [1, 2].

A finite number of magnitudes $|E_{\vec{h}}|$ are obtainable from experiment, while the phases $\phi_{\vec{h}}$ cannot be measured. Nevertheless, (1.2) is still useful in the determination of crystal structures since the prior knowledge that the unit cell is composed of N identical point atoms severely restricts the possible values of the phases $\phi_{\vec{h}}$. In fact, once the origin and the enantiomorph have been specified, the magnitudes $|E_{\vec{h}}|$ are sufficient to determine uniquely those phases $\phi_{\vec{h}}$ with the property that the left side of (1.2), as a function of $\vec{r}$, is then zero everywhere except at N points where it has the value $1/N^{1/2}$. Owing to the finite number of data available from experiment, (1.2) is actually nonvanishing in N discrete regions, not points, and is only approximately zero elsewhere. In practice, therefore, it is the maxima of (1.2) which yield the atomic positions.

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The problem of actually determining the values of the phases $\phi_{\vec{h}}$ when only the magnitudes $|E_{\vec{h}}|$ are given is the so-called phase problem. The solution of this problem is facilitated by the introduction of certain linear combinations of the phases, the structure invariants

$$\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}, \tag{1.3}$$

where

$$\vec{h}_1 + \vec{h}_2 + \vec{h}_3 = 0. \tag{1.4}$$

The structure invariants are important because they serve as the connecting link between the magnitudes $|E|$ and the phases ϕ. On the one hand, the magnitudes of the structure invariants, or, equivalently, the values of

$$\cos\left(\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}\right), \tag{1.5}$$

where (1.4) holds, are uniquely determined by the magnitudes $|E_{\vec{h}}|$. On the other hand, once the origin and the enantiomorph have been specified, the values of the structure invariants (1.5) determine uniquely the values of the individual phases $\phi_{\vec{h}}$. The problem is to calculate the values of the structure invariants (1.5) from the observed magnitudes of the structure factors and then, assuming the values of the former to have been found, to determine the values of the individual phases. An effective technique for solving the latter problem based on the Principle of Least Squares is now available [3]. The present report, addressing itself to the former problem, is devoted to a description of a computer program for calculating the values of the structure invariants (1.5) employing a formula based on certain conditional probability distributions of several structure factors [4]. The program listing is given in Appendix A.

Only the case that the space group is $P2_1$ and

$$\vec{h}_i = h_i 0 \ell_i, \quad i = 1, 2, 3 \tag{1.6}$$

is considered in this report. In this case the values of the invariants (1.3) are 0 or π, and the values of the cosines (1.5) are ±1. The more general problem presents no additional essential difficulties, and the corresponding computer programs will be written at a future date.

2. THE MAIN FORMULA

Assuming that (1.4) holds, the formula to be programmed is

$$\cos\left(\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}\right) = M(D - KS). \tag{2.1}$$

In (2.1) D is given by

$$D = \frac{\sum_{i=1}^{3} m_i D_i}{\sum_{i=1}^{3} m_i} \tag{2.2}$$

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where

$$D_i = \left\langle \left(\left| E_{-\vec{h}_j + \vec{k}} \right|^2 - 1 \right) \middle| \left| E_{\vec{k}} \right| > t, \left| E_{\vec{h}_j + \vec{k}} \right| > t \right\rangle_{\vec{k}}, \tag{2.3}$$

$i = 1, 2, 3$ when $j = 2, 3, 1$ respectively, m_i is the number of contributors to the average D_i, and t is a fixed real number greater than one, e.g., $t = 1.5$. Each of the three averages (2.3) is extended over all vectors $\vec{k}$ in reciprocal space such that $|E_{\vec{k}}| > t$ and $\left|E_{\vec{h}_j + \vec{k}}\right| > t$.

Again S in (2.1) is given by

$$S = \frac{\sum_{i=1}^{3} n_i S_i}{\sum_{i=1}^{3} n_i}, \tag{2.4}$$

where

$$S_i = 2 \left\langle \left(\left| E_{-\vec{h}_i + \vec{k}} \right|^2 - 1 \right) \middle| \left| E_{\vec{k}} \right| > t \right\rangle_{\vec{k}}, \tag{2.5}$$

$i = 1, 2, 3$, n_i is the number of contributors to the average (2.5), and t has already been defined in (2.3) to be an arbitrary fixed number exceeding unity. Each of the three averages (2.5) is extended over all vectors in reciprocal space such that $|E_{\vec{k}}| > t$.

The parameters K and M of (2.1) are determined as a function of

$$A = \frac{2}{N^{1/2}} \left| E_{\vec{h}_1} E_{\vec{h}_2} E_{\vec{h}_3} \right| = \frac{2}{N^{1/2}} \left| E_1 E_2 E_3 \right| \tag{2.6}$$

in such a way that the resulting empirical distribution of computed cosines (1.5) agrees with the theoretical conditional distribution, given A. The method for doing this is described in the following sections.

3. DETERMINATION OF K

It is known that, in the case under consideration, the probability that

$$\cos\left(\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}\right) = -1 \tag{3.1}$$

is given by

$$P_- = \frac{1}{1 + e^A} \tag{3.2}$$

where A is defined by (2.6). In short, for each fixed A, the fraction P_- of cosines (1.5) which is negative is known and given by (3.2). The computed D's and S's from (2.2) and (2.4) are arranged in decreasing order of A and grouped into sets of some 100 to 300 members. In each such set the value of A is essentially constant. In the set defined by A, K is determined in such a way that that fraction of the quantities

$$D - KS \tag{3.3}$$

which is negative agrees with the theoretical fraction as given by (3.2). It is to be noted that in the three or four groups corresponding to the very largest values of A, there may be only 20 to 50 members since in this range the values of A change rapidly.

4. DETERMINATION OF M

Once K is determined as a function of A, the value of M in (2.1) is readily determined for each fixed A by observing that

$$\left\langle \left| \cos\left(\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}\right) \right| \right\rangle = M \left\langle |D-KS| \right\rangle = 1, \tag{4.1}$$

so that

$$M = 1 / \left\langle |D-KS| \right\rangle \tag{4.2}$$

where the average in (4.2) is taken over all members of the group belonging to the given value of A.

5. DETERMINATION OF $\cos\left(\phi_{\vec{h}_1} + \phi_{\vec{h}_2} + \phi_{\vec{h}_3}\right)$

In each group corresponding to a fixed value of A, the computed values of (2.1) are arranged in decreasing order. It is to be anticipated that the very largest computed values of (2.1) should in fact be +1, and that the very smallest computed values of (2.1) should be -1. Hence a certain fraction, ranging from about 0.5 for the largest values of A to about 0.1 for the smallest values of A, is specified. It is assumed that, for each A, this fraction of the most positive computed values of (2.1) is in fact equal to +1, and that this same fraction of the most negative computed values of (2.1) is in fact equal to -1. For each A the cosines corresponding to the middle range of computed values of (2.1) are assumed not to be definitely determined. For the smallest value of A (around 0.5) it is presumed that cosines cannot be reliably computed. Hence, for these values of A, only the most extreme positive or negative computed values of (2.1) (approximately one-tenth of all computed values) are assumed to correspond to correct values of the cosine.

6. INPUT DATA

The following is a list of input data cards arranged in the order required by the program:

(1) (4I5)

HMAX, KMAX, LMIN, LMAX

HMAX, KMAX, and LMAX contain the maximum values attained by h, k, and ℓ, respectively. Similarly, LMIN contains the minimum ℓ value.

(2) (2I5)

LIST, NBL

LIST is the number of reflections in each logical record, and NBL is the number of logical records on the input data tape containing

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h, k, ℓ, and $|E|$ for each observable reflection. The program handles a maximum of 1500 reflections in each logical record.

(3) (I5)

NPD

NPD is the number of reflections for which $|E| > t$.

(4) (F5.2)

T

T = t is defined in Section 2 above.

(5) (I5)

KG

KG is the number of groups obtained when the invariants are partitioned in such a way as to make the A value essentially constant within each group.

(6) (20I5)

NG

NG is an array in which the number of invariants contained in group I is stored in NG(I), $1 \leq I \leq 16$.

(7) (20F5.2)

PCT

PCT(I) contains the fraction of cosines accepted as correctly determined in group I as described in Section 5.

(8) (3I5, 5X, F5.3)

h, k, ℓ, $|E|$

This deck contains one data card for each reflection for which $|E| > t$.

(9) (I5)

LPL

LPL is the number of logical records on the input data tape containing the structure invariants.

Samples of the input data card formats are given in Appendix B in the same order as the above listing. In addition to the above input data cards, two input data tapes are required:

(1) Tape number 04

This tape contains h, k, ℓ, and $|E|$ for each observable reflection, recorded in odd parity (binary mode). NBL and LIST (read from a punched card) give respectively the number of logical records on tape 4 and the number of reflections in each logical record. Tape 4 should contain a maximum of 1500 reflections in each logical record. The maximum number of logical records depends on LIST according to the following inequality:

$$\mathrm{NBL} \leq 7000/\mathrm{LIST}.$$

(2) Tape number 01

This tape contains the following information, also recorded in binary mode, for each structure invariant:

$$\vec{h}_1,\ \vec{h}_2,\ \vec{h}_3,\ |E_{\vec{h}_1}|,\ |E_{\vec{h}_2}|,\ |E_{\vec{h}_3}|,\ |E_{\vec{h}_1} E_{\vec{h}_2} E_{\vec{h}_3}|,\ A.$$

The structure invariants must be arranged in decreasing order on A. LPL (read from a punched card) gives the number of logical records on tape 1. Each logical record contains a maximum of 240 structure invariants, with the exact number NE stored before the given record.

7. OUTPUT DATA

The following describes information stored on two output tapes and printed on-line. Both tapes record data in binary mode. On tape number 02 the invariants in each group are arranged in decreasing order of M(D–KS). Tape number 03 contains the same information as tape 2 except that the structure invariants within each group are arranged in decreasing order on A. Two listings are printed on-line by the program; one corresponds to information as arranged on tape 2, and the other corresponds to tape 3. For each group the following information is recorded:

(1) number of invariants,

(2) average A value,

(3) K,

(4) M,

(5) T,

(6) number of negative cosines expected,

(7) number of positive cosines expected,

(8) percent of cosines to be accepted as correctly determined,

(9) number of positive cosines accepted,

(10) number of negative cosines accepted,

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(11) one line for each invariant arranged in decreasing order of either M(D−KS) or A, giving the following information:

index number of the invariant, $\vec{h}_1$, $\vec{h}_2$, $\vec{h}_3$, $|E_{\vec{h}_1}|$, $|E_{\vec{h}_2}|$, $|E_{\vec{h}_3}|$, A, number of contributors to D, number of contributors to S, D, S, M(D−KS), and cosine (if accepted as correctly determined, cosine will be listed as ±1, otherwise 0 will be listed).

A sample of the output data is given in Appendix C.

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APPENDIX A

PROGRAM LISTING

```
      PROGRAM M DMKS
      EQUIVALENCE  (E(1), J1(1)),  (E(244), J2(1)),  (E(487), J3(1)),
     1  (E(730), J4(1)),  (E(973), J5(1)),  (E(1216), J6(1)),
     2  (E(1459), J7(1)),  (E(1702), J8(1)),  (E(1945), J9(1)),
     3  (E(2188), E1J(1)),  (E(2431), E2J(1)),  (E(2674), E3J(1)),
     4  (E(2917), AJ(1)),  (E(3160),EPJ(1)),  (E(3403), A2J(1)),
     5  (E(4375),C1J(1)),  (E(5347), C2J(1)),  (E(6319), A1J(1))

      DIMENSION J1(243),J2(243),J3(243),J4(243),J5(243),J6(243),J7(243),
     1  J8(243),J9(243),E1J(243),E2J(243),E3J(243),AJ(243),EPJ(243),
     2          C1J(243),C2J(243),A1J(243),A2J(243),IO(243)
      DIMENSION CO(243),DMKS(243),NG(16),PCT(16)
      DIMENSION KH(1300),KK(1300),KL(1300),EI(1300),E(29,13,35),
     1  H1(200),K1(200),L1(200),H2(200),K2(200),L2(200),
     2  H3(200),K3(200),L3(200),AX(200),EP(200),E1(200),E2(200),E3(200)
      TYPE INTEGER H1,H2,H3,H4,HA,HM,H,HMAX,HAM

   90 FORMAT(3I5,5X,F5.3)
   93 FORMAT(78X,13HNO. OF CONTR.,/,46X,2HE1,5X,2HE2,5X,2HE3,8X,1HA,7X,
     1  4HTO D,5X,4HTO S,6X,1HD,9X,1HS,6X,7HM(D-KS),4X,6HCOSINE,/)
   94 FORMAT(1H1)
   96 FORMAT(20I5)
   97 FORMAT(20F5.2)
  850 FORMAT(  * NUMBER IN GROUP =  * , I5,  /,* AVERAGE A = *, F6.2, /,
     1   * K = *,  F9.2,   /,  * M =  *, F10.4 /, * T = * , F6.1, / )
  851 FORMAT(  * NO NEGATIVES = *, I5, /, * NO POSITIVES = *, I5,  /,
     1  * PERCENT ACCEPTED = *, F6.2, /,  * NUMBER POSITIVE ACCEPTED = *
     2  , I5, /,* NUMBER NEGATIVES ACCEPTED = *, I5, /)
  852 FORMAT(I8,2X,3(3I3,2X),3F7.3,F9.3,2F9.0,4F10.4,/)

      READ 96, HMAX,KMAX,LMIN,LMAX
      LLIM = IABS(LMIN) + 1
      IHKL = (LMAX + LLIM) * (HMAX + 1) * (KMAX + 1)
      NTOT = 0
      DO 5 I = 1,IHKL
    5 E(I) = -2.0

C     THE FOLLOWING ROUTINE READS A DATA TAPE CONTAINING
C                                H, K, L, E
C     FOR EACH REFLECTION WITH A MAXIMUM OF 1300 REFLECTIONS IN  EACH
C     LOGICAL RECORD.  LIST GIVES THE NUMBER OF REFLECTIONS IN EACH
C     LOGICAL RECORD AND NBL GIVES THE NUMBER OF LOGICAL RECORDS ON
C     THE TAPE.

      READ 96, LIST,NBL
   10 DO 30 J = 1,NBL
      READ (4) (KH(M),KK(M),KL(M),EI(M), M = 1,LIST)
      DO 20 N = 1,LIST
      L1 = KH(N) + 1
      L2 = KK(N) + 1
      L3 = KL(N) + LLIM
      E(L1,L2,L3) = EI(N)
   20 CONTINUE
   30 CONTINUE
      READ 96, NPD
      READ 97, T
      READ 96, KG
      READ 96, (NG(I),I = 1,KG)
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      READ 97, (PCT(I), I = 1,KG)
C          READ ONE DATA CARD CONTAINING H,K,L,E FOR EACH REFLECTION
C              FOR WHICH E IS GREATER THAN T.
      READ 90,(KH(I),KK(I),KL(I),EI(I),I = 1,NPD)
      KG = NG(1)
      NKG = 1
      KTT = 0
C     THE DATA TAPE FOR TRIPLES HAS THE NUMBER OF TRIPLES IN A
C     GIVEN LOGICAL RECORD STORED IMMEDIATELY BEFORE THAT RECORD.  THE
C     FOLLOWING INFORMATION IS STORED FOR EACH TRIPLE
C     H1, K1, L1, H2, K2, L2, H3, K3, L3, E1, E2, E3, E1*E2*E3, A.
C     THERE IS A MAXIMUM OF 200 TRIPLES IN EACH LOGICAL RECORD.  LPL
C     CONTAINS THE NUMBER OF LOGICAL RECORDS ON THE TAPE.
      READ 96, LPL
      DO 550 LP = 1,LPL
      READ(1) NE
      READ (1)(H1(N),K1(N),L1(N),H2(N),K2(N),L2(N),H3(N),K3(N),L3(N),
     1  E1(N),E2(N),E3(N),EP(N),AX(N),N = 1,NE)
      DO 500 I = 1,NE
      CT1 = CT2 = AV1 = AV2 = 0
      DO 4999 MD = 1,3
      E1S = E1(I) * E1(I)
      E2S = E2(I) * E2(I)
      E3S = E3(I) * E3(I)
      DO 350 LL = 1,NPD
      H4 = KH(LL)
      K4 = KK(LL)
      L4 = KL(LL)
      EKH = EI(LL)
      DO 300 IH = 1,2
      DO 200 IK = 1,2
      HM = H4 - H3(I)
      KM = K4 - K3(I)
      LM = L4 - L3(I)
      KAM = KM
      IF(KM .LT. 0) KAM = -KM
      IF(HM - 0) 75,74,80
   74 IF(LM - 0) 75,75,80
   75 HAM = -HM
      LAM = -LM
      GO TO 81
   80 HAM = HM
      LAM = LM
   81 IF(HAM .GT. HMAX .OR. KAM .GT. KMAX .OR. IABS(LAM) .GT. LMAX)
     1  GO TO 101
      EKMH3 = E(HAM + 1,KAM + 1,LAM + LLIM)
      IF(EKMH3 .LT. -1.) GO TO 101
      EKMH3 = EKMH3 * EKMH3 - 1.0
      AV2 = AV2 + EKMH3
      CT2 = CT2 + 1.0
      H = H1(I) + H4
      K = K1(I) + K4
      L = L1(I) + L4
      KA = K
      IF(K .LT. 0) KA = -K
```

```
      IF(H - 0) 71,70,72
   70 IF(L - 0) 71,71,72
   71 HA = -H
      LA = -L
      GO TO 73
   72 HA = H
      LA = L
  73  IF(HA .GT. HMAX .OR. KA .GT. KMAX .OR. IABS(LA) .GT. LMAX) 750,740
  740 EH1PK = E(HA + 1,KA + 1,LA + LLIM)
      IF(EH1PK .LT.-1.0) GO TO 760
      EH1PKS = EH1PK * EH1PK
      EH1PKSM1 = EH1PKS - 1.0
      GO TO 760
  750 EH1PK = -2
  760 CONTINUE
      IF(EH1PK .GE. T) 900,902
  900 AV1 = AV1 + EKMH3
      CT1 = CT1 + 1.0
  902 CONTINUE
  101 IF(K4 .EQ. 0) GO TO 201
      K4 = -K4
  200 CONTINUE
  201 IF(H4 .EQ. 0 .AND. L4 .EQ. 0) GO TO 301
      H4 = -H4
      L4 = -L4
  300 CONTINUE
  301 CONTINUE
  350 CONTINUE
      IT = H1(I) $ H1(I) = H2(I) $ H2(I) = H3(I) $ H3(I) = IT
      IT = K1(I) $ K1(I) = K2(I) $ K2(I) = K3(I) $ K3(I) = IT
      IT = L1(I) $ L1(I) = L2(I) $ L2(I) = L3(I) $ L3(I) = IT
      TI = E1(I) $ E1(I) = E2(I) $ E2(I) = E3(I) $ E3(I) = TI
 4998 CONTINUE
 4999 CONTINUE
      AV1 = AV1 / CT1
      AV2 = 2.0 * AV2 / CT2
      WRITE(20) H1(I),K1(I),L1(I),H2(I),K2(I),L2(I),H3(I),K3(I),L3(I),
     1  E1(I),E2(I),E3(I),AX(I),EP(I),  CT1,CT2,AV1,AV2
      KTT = KTT + 1
      IF(KTT .EQ. KG) 601,500
  601 CONTINUE
      KTT = 0
      REWIND 20
      WRITE (30) E
      DO 6015 N = 1,KG
      READ (20)  J1(N),J2(N),J3(N),J4(N),J5(N),J6(N),J7(N),J8(N),J9(N),
     1  E1J(N),E2J(N),E3J(N),AJ(N),EPJ(N),       C1J(N),C2J(N),
     2  A1J(N),A2J(N)
 6015 CONTINUE
      REWIND 20
      REWIND 30
      CO = 0
      CM = 0.5
      CT = 1.0
      MA = KG / 2
      IF(KG .EQ. MA * 2) 602,603
  602 AA = (AJ(MA) + AJ(MA + 1) ) / 2
      GO TO 604
  603 AA = AJ(MA + 1)
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604 PCTNEG = 1.0 / (1.0 + EXPF(AA))
    PCTPOS = 1.0 - PCTNEG
    NNEG = PCTNEG * KG + 0.5
    NPOG = PCTPOS * KG + 0.5
    NNAC = NNEG * PCT(NKG) + 0.50
    NPAC = NPOG * PCT(NKG) + 0.50
    SDMKS = 0
    DO 625 LN = 1,10
    KTNEG = 0
    DO 620 LQ = 1,KG
    XDMKS = A1J(LQ) - CM * A2J(LQ)
    IF(XDMKS .LT. 0) 610,620
610 KTNEG = KTNEG + 1
620 CONTINUE
    IF(NNEG - KTNEG) 623,626,621
621 CO = CM
    CM = 0.5 * (CM + CT)
    GO TO 625
623 CT = CM
    CM = 0.5 * (CO + CM)
625 CONTINUE
626 CONTINUE
    SDMKS = 0
    DO 630 LQ = 1,KG
    DMKS(LQ) = A1J(LQ) - CM * A2J(LQ)
    SDMKS = SDMKS + ABSF(DMKS(LQ))
630 CONTINUE
    XM = KG / SDMKS
    DO 635 LQ = 1,KG
    DMKS(LQ) = DMKS(LQ) * XM
635 CONTINUE
    DO 636 LQ = 1,KG
    IO(LQ) = LQ
636 CONTINUE
    DO 640 LI = 1,KG
    LP1 = LI + 1
    DO 640 LJ = LP1,KG
    II = IO(LI)
    JJ = IO(LJ)
    IF(DMKS(II) - DMKS(JJ)) 637,640,640
637 ITEMP = IO(LI)
    IO(LI) = IO(LJ)
    IO(LJ) = ITEMP
640 CONTINUE
    DO 645 JJ = 1,NPAC
    J = IO(JJ)
    CO(J) = 1.0
645 CONTINUE
    NPA = NPAC + 1
    LU = KG - NNAC
    DO 646 JJ = NPA,LU
    J = IO(JJ)
    CO(J) = 0
646 CONTINUE
    LU = LU + 1
    DO 647 JJ = LU,KG
    J = IO(JJ)
    CO(J) = -1.0
647 CONTINUE
```

```
      PRINT 850, KG,AA,CM,XM,T
      PRINT 851, NNEG,NPOG,PCT(NKG),NPAC, NNAC
      PRINT 93
      WRITE (2)  KG,AA,CM,XM,T
      WRITE (2) NNEG,NPOG,PCT(NKG),NPAC,NNAC
      WRITE (3)  KG,AA,CM,XM,T
      WRITE (3) NNEG,NPOG,PCT(NKG),NPAC,NNAC
      DO 650 JJ = 1,KG
      J = IO(JJ)
      KTR = J + NTOT
      PRINT 852, KTR,J1(J),J2(J),J3(J),J4(J),J5(J),J6(J),J7(J),J8(J),
     1  J9(J),E1J(J),E2J(J),E3J(J),AJ(J),C1J(J),C2J(J),A1J(J),A2J(J),
     2  DMKS(J),CO(J)
      WRITE (2)  KTR,J1(J),J2(J),J3(J),J4(J),J5(J),J6(J),J7(J),J8(J),
     1  J9(J),E1J(J),E2J(J),E3J(J),AJ(J),EPJ(J),C1J(J),C2J(J),
     2  A1J(J),A2J(J),DMKS(J),CO(J)
      J = JJ
      KTR = J + NTOT
      WRITE (3)  KTR,J1(J),J2(J),J3(J),J4(J),J5(J),J6(J),J7(J),J8(J),
     1  J9(J),E1J(J),E2J(J),E3J(J),AJ(J),EPJ(J),C1J(J),C2J(J),
     2  A1J(J),A2J(J),DMKS(J),CO(J)
  650 CONTINUE
      NTOT = NTOT + KG
      NKG = NKG + 1
      KG = NG(NKG)
      REWIND 20
      READ (30) E
      REWIND 30
  500 CONTINUE
  550 CONTINUE
      REWIND 3
      PRINT 94
      DO 800 I = 1,16
      READ (3)   KG,AA,CM,XM,T
      READ (3) NNEG,NPOG,PCTNKG,NPAC,NNAC
      PRINT 850, KG,AA,CM,XM,T
      PRINT 851, NNEG,NPOG,PCTNKG,NPAC,NNAC
      PRINT 93
      DO 700 J = 1,KG
      READ (3)   KTR,J1(J),J2(J),J3(J),J4(J),J5(J),J6(J),J7(J),J8(J),
     1  J9(J),E1J(J),E2J(J),E3J(J),AJ(J),EPJ(J),C1J(J),C2J(J),
     2  A1J(J),A2J(J),DMKS(J),CO(J)
      PRINT 852, KTR,J1(J),J2(J),J3(J),J4(J),J5(J),J6(J),J7(J),J8(J),
     1  J9(J),E1J(J),E2J(J),E3J(J),AJ(J),C1J(J),C2J(J),A1J(J),A2J(J),
     2  DMKS(J),CO(J)
  700 CONTINUE
  800 CONTINUE
      END
```

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APPENDIX B

SAMPLE INPUT DATA

(1) HMAX, KMAX, LMIN, LMAX

28 12 -17 17

(2) LIST, NBL

500 15

(3) NPD

825

(4) T

1.5

(5) KG

16

(6) NG(I), $1 \le I \le 16$

10 20 30 40 100 100 100 200 200 200 200 200 200 200 200 243

(7) PCT(I), $1 \le I \le 16$

50 50 50 50 50 45 45 40 35 30 25 25 20 20 15 10

(8) h, k, ℓ, |E|

3	1	2	3781
3	0	2	3732
24	4	4	3627
5	0	2	3574
21	0	4	3453

(9) LPL

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APPENDIX C

SAMPLE PROGRAM OUTPUT

NUMBER IN GROUP = 10
AVERAGE A = 3,84
K = 0,25
M = 3,2750
T = 1,5

NO NEGATIVES = 0
NO POSITIVES = 10
PERCENT ACCEPTED = 0,50
NUMBER POSITIVE ACCEPTED = 5
NUMBER NEGATIVES ACCEPTED = 0

															NO. OF CONTR. TO D	NO. OF CONTR. TO S	D	S	M(D-KS)	COSINE
										E1	E2	E3	A							
4	3	0	2	-5	-0	-2	2	0	0	3,732	3,574	1,838	3,888		1340	8075	0,7349	0,6688	1,8592	1,0000
5	5	0	2	4	0	-7	-9	-0	5	3,574	2,836	2,401	3,860		786	6562	0,6475	0,4072	1,7872	1,0000
3	5	0	2	-7	-0	5	2	0	-7	3,574	2,866	2,579	4,190		948	6743	0,6237	0,4889	1,6424	1,0000
2	3	0	2	-7	-0	5	4	0	-7	3,732	2,866	2,836	4,811		909	6858	0,5927	0,4240	1,5939	1,0000
10	3	0	2	24	0	-5	-27	-0	3	3,732	2,617	2,166	3,355		444	4970	0,4008	0,3757	1,0050	1,0000
8	5	0	2	5	0	-1	-10	-0	-1	3,574	3,448	1,779	3,477		949	7233	0,3837	0,3566	0,9646	0,0000
1	3	0	2	-5	-0	1	2	0	-3	3,732	3,448	3,170	6,470		1073	7938	0,2431	0,3197	0,5343	0,0000
7	3	0	2	3	0	2	-6	-0	-4	3,732	3,732	1,692	3,738		1003	7488	0,1627	0,3674	0,2319	0,0000
6	2	0	-3	-7	-0	5	5	0	-2	3,170	2,866	2,645	3,811		931	7441	0,1177	0,2315	0,1959	0,0000
9	21	0	4	-5	-0	1	-16	0	-5	3,453	3,448	1,787	3,374		572	5608	0,1072	0,2018	0,1857	0,0000

NUMBER IN GROUP = 20
AVERAGE A = 2,55
K = 0,25
M = 4,0202
T = 1,5

NO NEGATIVES = 1
NO POSITIVES = 19
PERCENT ACCEPTED = 0,50
NUMBER POSITIVE ACCEPTED = 10
NUMBER NEGATIVES ACCEPTED = 1

										E1	E2	F3	A	NO. OF CONTR. TO D	TO S	D	S	M(D-KS)	COSINE
13	5	0	-1	-5	-0	-16	0	0	17	3,448	3,131	1,778	3,044	445	4803	0,5822	0,3072	2,0319	1,0000
27	5	0	2	-4	-0	-1	-1	0	-1	3,574	2,451	1,730	2,404	1265	8060	0,5511	0,5251	1,6878	1,0000
20	3	0	2	-2	-0	7	-1	0	-9	3,732	2,579	1,674	2,555	824	6616	0,5052	0,3637	1,6655	1,0000
18	5	0	2	-4	-0	7	-1	0	-9	3,574	2,836	1,674	2,691	765	6365	0,5054	0,4049	1,6249	1,0000
29	5	0	2	4	0	1	-9	-0	-3	3,574	2,451	1,697	2,358	899	7206	0,4716	0,3444	1,5499	1,0000
14	5	0	2	20	0	-9	-25	-0	7	3,574	2,341	2,291	3,040	492	4991	0,4943	0,4954	1,4891	1,0000
19	3	0	2	-20	-0	9	17	0	-11	3,732	2,341	1,907	2,642	601	5394	0,4606	0,4115	1,4382	1,0000
21	5	0	2	-21	-0	-4	16	0	2	3,574	3,453	1,298	2,541	634	5559	0,4209	0,4411	1,2486	1,0000
16	21	0	4	-2	-0	3	-19	0	-7	3,453	3,170	1,556	2,701	530	5336	0,2956	0,2431	0,9439	1,0000
11	21	0	4	2	0	-7	-23	-0	3	3,453	2,579	2,331	3,292	553	4796	0,3059	0,3046	0,9236	1,0000
22	21	0	4	5	0	-1	-26	-0	-3	3,453	3,448	1,329	2,510	506	5041	0,3154	0,3465	0,9198	0,0000
17	3	0	2	7	0	-5	-10	-0	3	3,732	2,866	1,588	2,694	858	6959	0,2867	0,3229	0,8278	0,0000
26	5	0	-1	-4	-0	7	-1	0	-6	3,448	2,836	1,588	2,463	758	6855	0,2512	0,1879	0,8212	0,0000
25	5	0	2	-5	-0	1	0	0	-3	3,574	3,448	1,253	2,449	1081	7718	0,3003	0,3984	0,8070	0,0000
30	2	0	-3	24	0	-5	-26	-0	8	3,170	2,617	1,753	2,306	429	4991	0,2058	0,1814	0,6451	0,0000
26	3	0	2	-28	-0	-0	25	0	-2	3,732	2,861	1,440	2,439	430	4845	0,1931	0,3311	0,4433	0,0000
28	21	0	4	2	0	-3	-23	-0	-1	3,453	3,170	1,361	2,363	505	5332	0,1170	0,1773	0,2922	0,0000
12	3	0	2	-27	-0	6	24	0	-8	3,732	2,450	2,213	3,209	468	4877	0,1366	0,3997	0,1476	0,0000
15	5	0	16	9	0	-15	-14	-0	-1	3,131	2,967	2,048	3,017	326	4165	0,0526	0,1318	0,0788	0,0000
24	3	0	2	-27	-0	-1	24	0	-1	3,732	2,495	1,661	2,453	372	4956	-0,0399	0,2520	-0,4138	-1,0000

UNCLASSIFIED

NUMBER IN GROUP = 30
AVERAGE A = 1,99
K = 0,31
M = 5,7152
T = 1,5

NO NEGATIVES = 4
NO POSITIVES = 26
PERCENT ACCEPTED = 0,50
NUMBER POSITIVE ACCEPTED = 13
NUMBER NEGATIVES ACCEPTED = 2

										E1	E2	E3	A	NO. OF CONTR. TO D	TO S	D	S	M(D-KS)	COSINE
37	4	0	-7	-2	-0	7	-2	0	0	2,836	2,579	1,838	2,132	950	7104	0,5572	0.4470	2,3860	1,0000
44	7	0	-5	-9	-0	5	2	0	0	2,866	2,401	1,838	2,006	996	7219	0,5615	0.4971	2,3213	1,0000
33	9	0	-15	-12	-0	16	3	0	-1	2,967	2,262	2,043	2,175	378	4986	0,4662	0.2289	2,2558	1,0000
39	21	0	4	-18	-0	12	-3	0	-16	3,453	2,208	1,756	2,123	371	3739	0,4542	0.3140	2,0350	1,0000
43	4	0	1	20	0	-9	-24	-0	8	2,451	2,341	2,213	2,014	509	5173	0,4490	0.3053	2,0209	1,0000
60	21	0	4	2	0	0	-23	-0	-4	3,453	1,838	1,784	1,796	601	5546	0,4745	0.5464	1,7362	1,0000
45	2	0	-3	12	0	-12	-14	-0	15	3,170	2,103	1,882	1,990	448	5161	0,3352	0.1305	1,6825	1,0000
35	3	0	2	21	0	4	-24	-0	-6	3,732	3,453	1,052	2,150	524	5080	0,4143	0.4457	1,5720	1,0000
50	9	0	-15	-24	-0	5	15	0	10	2,967	2,617	1,575	1,940	265	3712	0,2918	0.0916	1,5039	1,0000
48	5	0	16	18	0	-12	-23	-0	-4	3,131	2,208	1,784	1,956	348	3581	0,3652	0.3309	1,4962	1,0000
46	5	0	2	-24	-0	5	19	0	-7	3,574	2,617	1,337	1,983	543	5240	0,3580	0.4276	1,2825	1,0000

49	5	0	2	-8	-0	5	3	0	-7	3,574	2,262	1,517	1,945	832	6665	0,3178	0,3429	1,2040	1,0000
47	3	0	2	12	0	-12	-15	-0	10	3,732	2,103	1,576	1,962	612	5563	0,2906	0,3550	1,0269	1,0000
38	5	0	-1	-28	-0	-0	23	0	1	3,448	2,861	1,361	2,129	402	4921	0,2466	0,2175	1,0209	0,0000
41	24	0	-5	-27	-0	6	3	0	-1	2,617	2,450	2,043	2,078	454	5147	0,1977	0,2864	0,6185	0,0000
54	4	0	-7	-25	-0	7	21	0	0	2,836	2,291	1,850	1,906	385	4640	0,1734	0,2175	0,6026	0,0000
55	5	0	-1	20	0	-9	-25	-0	10	3,448	2,341	1,455	1,863	429	5029	0,1871	0,3002	0,5332	0,0000
57	21	0	4	-8	-0	-14	-13	0	10	3,453	2,014	1,670	1,842	341	4188	0,1111	0,0596	0,5283	0,0000
31	5	0	-1	5	0	-2	-10	-0	3	3,448	2,645	1,588	2,297	826	7338	0,1364	0,1431	0,5238	0,0000
52	5	0	16	3	0	-1	-8	-0	-15	3,131	2,043	1,880	1,907	518	5135	0,1992	0,3546	0,5053	0,0000
42	5	0	-1	-3	-0	1	-2	0	0	3,448	2,043	1,838	2,053	1317	8422	0,2275	0,4632	0,4726	0,0000
32	3	0	2	5	0	-1	-8	-0	-1	3,732	3,448	1,107	2,259	963	7554	0,1582	0,2998	0,3686	0,0000
51	2	0	-3	-28	-0	-0	26	0	3	3,170	2,861	1,329	1,912	409	4742	0,1063	0,1810	0,2843	0,0000
36	4	0	-7	8	0	-5	-12	-0	12	2,836	2,262	2,103	2,140	594	5574	0,1230	0,2369	0,2800	0,0000
34	2	0	-3	-23	-0	3	21	0	0	3,170	2,331	1,850	2,168	518	5463	0,0555	0,1328	0,0803	0,0000
56	28	0	0	-4	-0	-1	-24	0	1	2,861	2,451	1,661	1,847	393	4891	0,0763	0,2139	0,0542	0,0000
53	2	0	-3	3	0	-1	-5	-0	4	3,170	2,043	1,856	1,906	949	7917	0,0470	0,1629	-0,0221	0,0000
40	7	0	-5	4	0	-7	-11	-0	12	2,866	2,836	1,644	2,119	551	5635	0,0785	0,2650	-0,0243	0,0000
58	4	0	1	23	0	-3	-27	-0	2	2,451	2,331	2,008	1,820	433	5047	0,0007	0,2004	-0,3539	-1,0000
59	5	0	-1	-8	-0	-15	3	0	16	3,448	1,880	1,756	1,805	420	4931	-0,1444	0,2119	-1,2039	-1,0000

UNCLASSIFIED

NUMBER IN GROUP = 40
AVERAGE A = 1,69
K = 0,06
M = 4,5181
T = 1,5

NO NEGATIVES = 6
NO POSITIVES = 34
PERCENT ACCEPTED = 0,50
NUMBER POSITIVE ACCEPTED = 17
NUMBER NEGATIVES ACCEPTED = 3

										E1	E2	E3	A	NO. OF CONTR. TO D	TO S	D	S	M(D-KS)	COSINE
89	3	0	2	-25	-0	7	22	0	-9	3,732	2,291	1,197	1,623	480	5039	0,6149	0,3956	2,6663	1,0000
65	5	0	2	5	0	2	-10	-0	-4	3,574	3,574	0,877	1,777	891	6917	0,5891	0,5179	2,5154	1,0000
62	21	0	4	-3	-0	1	-18	0	-5	3,453	2,043	1,603	1,794	615	5694	0,4834	0,3191	2,0940	1,0000
95	5	0	16	-2	-0	-0	-3	0	-16	3,131	1,838	1,756	1,603	551	5256	0,4788	0,5542	2,0069	1,0000
69	5	0	-1	-4	-0	-1	-1	0	2	3,448	2,451	1,302	1,745	1088	8116	0,4290	0,2815	1,8589	1,0000
68	5	0	2	-27	-0	2	22	0	-4	3,574	2,008	1,540	1,753	436	4913	0,4011	0,3865	1,7030	1,0000
72	5	0	16	17	0	-11	-22	-0	-5	3,131	1,907	1,836	1,739	339	3760	0,3766	0,2675	1,6260	1,0000
93	3	0	2	4	0	1	-7	-0	-3	3,732	2,451	1,111	1,612	971	7521	0,3396	0,2760	1,4563	1,0000
83	5	0	2	14	0	1	-19	-0	-3	3,574	2,048	1,437	1,668	560	5877	0,3103	0,2595	1,3285	1,0000
82	5	0	2	5	0	-2	-10	-0	0	3,574	2,645	1,120	1,679	899	7224	0,3136	0,3162	1,3277	1,0000
81	5	0	-1	4	0	-7	-9	-0	8	3,448	2,836	1,085	1,683	755	6519	0,3071	0,2162	1,3263	1,0000
78	5	0	-1	-5	-0	2	0	0	-1	3,448	2,645	1,183	1,711	1195	8250	0,3015	0,3521	1,2627	1,0000
94	21	0	4	-28	-0	-0	7	0	-4	3,453	2,861	1,023	1,603	464	4646	0,2799	0,2460	1,1953	1,0000
71	21	0	4	-22	-0	-5	1	0	1	3,453	1,836	1,730	1,739	580	5577	0,2878	0,4319	1,1783	1,0000
84	5	0	2	-27	-0	-1	22	0	-1	3,574	2,495	1,177	1,665	371	4909	0,2667	0,3226	1,1137	1,0000
100	5	0	-1	-23	-0	-4	18	0	5	3,448	1,784	1,603	1,564	461	5332	0,2572	0,1973	1,1063	1,0000
99	5	0	-2	8	0	-5	-13	-0	7	2,645	2,262	1,650	1,566	733	6514	0,2451	0,1952	1,0523	1,0000

97	5	0	-2	-27	-0	6	22	0	-4	2,645	2,450	1,540	1,583	391	5029	0,2380	0,1476	1,0335	0,0000
86	24	0	-5	-20	-0	9	-4	0	-4	2,617	2,341	1,710	1,662	476	4946	0,2092	0,1630	0,8991	0,0000
74	5	0	-1	5	0	-4	-10	-0	5	3,448	1,856	1,712	1,738	738	7056	0,2056	0,1120	0,8975	0,0000
88	21	0	4	-7	-0	5	-14	0	-9	3,453	2,866	1,047	1,643	508	5000	0,2129	0,3096	0,8744	0,0000
70	3	0	2	12	0	-16	-15	-0	14	3,732	2,262	1,302	1,743	409	4799	0,2130	0,3403	0,8663	0,0000
90	7	0	-5	8	0	-5	-15	-0	10	2,866	2,262	1,576	1,620	629	5817	0,2035	0,2931	0,8367	0,0000
66	28	0	0	-27	-0	6	-1	0	-6	2,861	2,450	1,588	1,765	376	4282	0,1784	0,1284	0,7698	0,0000
64	2	0	-7	19	0	10	-21	-0	-3	2,579	2,250	1,930	1,776	383	4605	0,1784	0,1301	0,7692	0,0000
72	21	0	4	4	0	1	-25	-0	-5	3,453	2,451	1,292	1,734	470	5047	0,1725	0,3129	0,6911	0,0000
91	5	0	-1	-24	-0	8	19	0	-7	3,448	2,213	1,337	1,618	472	5317	0,1530	0,2289	0,6267	0,0000
96	5	0	-1	4	0	4	-9	-0	-3	3,448	1,710	1,697	1,587	708	7056	0,1121	0,0971	0,4789	0,0000
82	2	0	-3	17	0	-11	-19	-0	14	3,170	1,907	1,733	1,662	387	5057	0,1081	0,1056	0,4587	0,0000
87	3	0	2	16	0	5	-19	-0	-7	3,732	1,787	1,556	1,646	478	5570	0,1075	0,2504	0,4149	0,0000
76	5	0	16	7	0	-5	-12	-0	-11	3,131	2,866	1,208	1,719	470	4705	0,0913	0,3531	0,3130	0,0000
65	5	0	-1	2	0	-3	-7	-0	4	3,448	3,170	1,023	1,773	900	7571	0,0619	0,1484	0,2376	0,0000
79	2	0	-3	-13	-0	15	11	0	-12	3,170	2,068	1,644	1,709	407	5185	0,0436	0,0681	0,1778	0,0000
92	2	0	-7	9	0	-5	-11	-0	12	2,579	2,401	1,644	1,615	542	5590	0,0152	0,1944	0,0136	0,0000
73	4	0	-7	-27	-0	3	23	0	4	2,836	2,166	1,784	1,738	322	4331	-0,0017	0,1432	-0,0483	0,0000
67	9	0	-15	-18	-0	12	9	0	3	2,967	2,208	1,697	1,763	343	4478	-0,0348	0,0615	-0,1744	0,0000
61	3	0	2	-5	-0	-16	2	0	14	3,732	3,131	0,968	1,794	522	5158	-0,0341	0,4182	-0,2721	0,0000
80	3	0	2	-18	-0	12	15	0	-14	3,732	2,208	1,302	1,702	482	5013	-0,0630	0,3651	-0,3879	-1,0000
77	5	0	-1	-8	-0	-14	3	0	15	3,448	2,014	1,556	1,714	399	5140	-0,1782	0,1144	-0,8374	-1,0000
98	27	0	1	-23	-0	3	-4	0	-4	2,495	2,331	1,710	1,577	338	4721	-0,2433	0,0137	-1,1032	-1,0000

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13. ABSTRACT

Effective techniques leading from the values of the crystal structure invariants to the values of the individual phases have recently been obtained. In the present report a new formula expressing the structure invariants in terms of the observed crystal structure amplitudes is given, and a computer program is described which facilitates the computation of the invariants.

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