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Argonne National Laboratory

MODULATED RECIPROCAL CRYSTAL-LATTICE AND DIFFRACTOMETRIC COMPUTER PROGRAM

by

Masao Atoji and J. Gvildys

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IN NUCLEAR SCIENCE ABSTRACTS

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MODULATED RECIPROCAL CRYSTAL-LATTICE AND DIFFRACTOMETRIC COMPUTER PROGRAM

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Masao Atoji and J. Gvildys

ABSTRACT

The diffraction optics for all the conceivable modulations on the fundamental reciprocal-crystal lattice are interpreted in terms of a simple universal concept, the modulation reciprocal-lattice vector. The physical significance of this modulation vector is discussed in the following selected topics: the antiphase domain structure, the modulated magnetic-spin alignment, the structure imperfection, and the thermal diffuse scattering. Also presented is a computer program for calculating the basic diffractometry parameters for the modulated lattice and the crystal-detector setting angles in the four-circle, normal-beam, equatorial technique. The computer program, as well as our discussions on the modulation vector, are applicable to the X-ray, neutron, and electron-diffraction methods.

I. INTRODUCTION

The concept of the reciprocal system of vectors often provides a powerful tool in the interpretation of various physical properties. Our example here is the reciprocal space lattice whose primitive translation vectors are the reciprocals of those for the crystal lattice in real space. Many cases have been known in which the dynamical and kinematical properties of crystals and their intercorrelations with other physical systems are most elucidatively described in terms of the reciprocal lattice. In some instances, however, certain modulation of the reciprocal lattice is inevitable, and yet the resultant analysis provides itself the fruitfulness of the reciprocal-space description. In this report, the terminology "generalized reciprocal lattice" is also used to govern all possible modes of the modulated reciprocal lattice as well as the fundamental reciprocal lattice.

Perhaps the most pertinent topic on this subject is the reciprocal-lattice interpretation in the crystal-lattice diffraction optics of X-rays, neutrons, and electrons. We shall first discuss the role of the modulated

reciprocal lattice in these diffraction kinetics. The theoretical foundation on the diffraction process has been well established, and the mathematical derivation on the modulation case is frequently lengthy and intricate. Accordingly, they are described very concisely, leaning heavily on the cited references. Instead, the graphical illustrations are employed to emphasize the features of the modulations in the reciprocal lattices of the following representative cases: the antiphase domain structure, the sinusoidal magnetic-spin distribution, the thermal diffuse scattering, the order-disorder structure, and the related subjects.

When we confine ourselves to the geometry of the diffraction optics, practically all types of modulated reciprocal lattices can be represented by using the lattice vector that is a sum of the fundamental reciprocal-lattice vector and the modulation reciprocal-lattice vector. Based on this simple concept, a computer program for obtaining the basic diffractometric parameters for the generalized reciprocal lattice has been coded in the FORTRAN language. The program also calculated the single-crystal and detector-setting angles in the three-circle cone method with a normal-beam equatorial configuration. These geometrical-parameter computations are directly applicable to the X-ray and neutron diffractometries and with some limitations also to the electron-diffraction method.

It is now clear that our intention is not just to review the known phenomena, but also to seek the unified interpretation and formulae governing the characteristics of all conceivable modulations of the reciprocal lattice. Likewise, the computer program is also intended to be as universal as possible. The invariant and complete reciprocal representation of the diffraction optics of any crystal must be based on the generalized reciprocal lattice. For instance, even an ideally perfect and completely ordered crystal at 0°K gives rise to an off-site scattering effect due to the zero-point lattice vibrations which are by no means conformative to the fundamental reciprocal-lattice description.

II. FUNDAMENTAL AND MODULATED RECIPROCAL-LATTICE PARAMETERS

In the diffraction optics dealing with elastic scattering, the reciprocal-lattice vector, $\vec{H}$, is signified as a difference vector between the wave-propagation vector of the scattered radiation $\vec{k}$ and that for the incident radiation $\vec{k}_0$; that is, $\vec{H} = \vec{k} - \vec{k}_0$. Taking $|\vec{k}| = |\vec{k}_0| = 1/\lambda$, we have, $|\vec{H}| = (2 \sin \Theta)/\lambda = 1/D$, where Θ is a half of the scattering angle, λ is the radiation wavelength, D is the interplanar spacing, and $\vec{H}$ is expressed in terms of the primitive translation vectors of the reciprocal lattice, $\vec{a}^*$, $\vec{b}^*$, and $\vec{c}^*$, as follows:

$$\vec{H} = H\vec{a}^* + K\vec{b}^* + L\vec{c}^*. \quad (1)$$

Here, we must emphasize that H , K , and L are not necessarily integers. If they are integers, we may express Eq. (1) as

$$\vec{h} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^* \quad (2)$$

and $|\vec{h}| = (2 \sin \theta)/\lambda = 1/d$, in which θ is known as the Bragg angle. We have called the lattice expressed by Eq. (2) the fundamental reciprocal lattice, which may be regarded as a special case of Eq. (1) representing the generalized reciprocal lattice.

Certain integers can always be found for H , K , and L in Eq. (1) by adjusting the reciprocal-lattice unit-cell vectors, $\vec{a}^*$, $\vec{b}^*$, and $\vec{c}^*$. However, their reciprocal vectors, $\vec{a}$, $\vec{b}$, and $\vec{c}$ may have no physical significance at all. In other words, the lattice-vector assignment should not contradict the original definition that $\vec{a}$, $\vec{b}$, and $\vec{c}$ are the primitive translation vectors for the atomic repetition or those for the physical quantities assigned to the atoms in the crystal.

The modulation vector $\tau\vec{p}$ is now defined by

$$\vec{H} = \vec{h} + \tau\vec{p}, \quad (3)$$

where $|\vec{p}| = 1$, and hence τ is the modulus of the modulation vector. The modulation unit-vector $\vec{p}$, which specifies the direction of the shift from the fundamental lattice point, is expressed as

$$\vec{p} = u\frac{\vec{a}}{a} + v\frac{\vec{b}}{b} + w\frac{\vec{c}}{c}, \quad (4)$$

where u , v , and w are the direction parameters of $\vec{p}$ with respect to the unit-cell vectors, $\vec{a}$, $\vec{b}$, and $\vec{c}$, respectively. The physical significance of $\tau\vec{p}$ will be discussed in the following chapter. The magnitude of $\vec{H}$, $(2 \sin \theta)/\lambda$, is then obtainable from

$$\frac{4 \sin^2 \theta}{\lambda^2} = \frac{4 \sin^2 \theta}{\lambda^2} + \tau^2 + 2\tau\left(\frac{hu}{a} + \frac{kv}{b} + \frac{lw}{c}\right). \quad (5)$$

This relation is valid for any crystal system, since the orthogonality among $\vec{a}$, $\vec{b}$, and $\vec{c}$ is not assumed here. Equation (5) is convenient in computing the crystallographic parameters such as D , $(\sin \theta)/\lambda$, θ , etc. for a given set of u , v , w , and τ , as well as those for the $\tau = 0$ case.

When one is concerned with the vector components of $\tau\vec{p}$ with respect to the reciprocal-lattice coordinates, it is essential to use the formula,

$$\vec{p} = u^*\frac{\vec{a}^*}{a^*} + v^*\frac{\vec{b}^*}{b^*} + w^*\frac{\vec{c}^*}{c^*}, \quad (6)$$

where u^* , v^* , and w^* are the direction parameters of $\vec{p}$ with respect to $\vec{a}^*$, $\vec{b}^*$, and $\vec{c}^*$, respectively. From Eqs. (1), (3), and (6), we have

$$H = h + \frac{\tau u^*}{a^*}, \quad K = k + \frac{\tau v^*}{b^*}, \quad \text{and } L = \ell + \frac{\tau w^*}{c^*}. \quad (7)$$

Hence, the modulated reflection may be regarded as a satellite reflection associated with the fundamental reflection (hkl) .

The relationships among the direction parameters in the real space and those in the reciprocal space are as follows:

$$u^* = aa^*(u + v \cos \gamma + w \cos \beta),$$

$$v^* = bb^*(u \cos \gamma + v + w \cos \alpha),$$

and

$$w^* = cc^*(u \cos \beta + v \cos \alpha + w). \quad (8)$$

Likewise, we have

$$u = aa^*(u^* + v^* \cos \gamma^* + w^* \cos \beta^*),$$

$$v = bb^*(u^* \cos \gamma^* + v^* + w^* \cos \alpha^*),$$

and

$$w = cc^*(u^* \cos \beta^* + v^* \cos \alpha^* + w^*), \quad (9)$$

where $\alpha = \langle \vec{b}, \vec{c} \rangle$, $\beta = \langle \vec{c}, \vec{a} \rangle$, $\gamma = \langle \vec{a}, \vec{b} \rangle$, and α^* , β^* , and γ^* are the corresponding values for the reciprocal unit cell. Of course, we have

$$\vec{p} \cdot \vec{p} = \frac{uu^*}{aa^*} + \frac{vv^*}{bb^*} + \frac{ww^*}{cc^*} = 1. \quad (10)$$

Let M_a , M_b , and M_c denote the direction cosines of $\vec{p}$ relative to $\vec{a}$, $\vec{b}$, and $\vec{c}$, respectively. Then, the direction parameters in the reciprocal space are expressed as follows:

$$u^* = M_a aa^*, \quad v^* = M_b bb^*, \quad \text{and } w^* = M_c cc^*. \quad (11)$$

Similarly, we have

$$u = M_a^* aa^*, \quad v = M_b^* bb^*, \quad \text{and } w = M_c^* cc^*, \quad (12)$$

where M_a^* , M_b^* , and M_c^* are the direction cosines of $\vec{p}$ relative to $\vec{a}^*$, $\vec{b}^*$, and $\vec{c}^*$, respectively. In the orthogonal lattice, $\alpha = \beta = \gamma = \alpha^* = \beta^* = \gamma^* = 90^\circ$, $a^* = 1/a$, $b^* = 1/b$, $c^* = 1/c$, $u = u^* = M_a = M_a^*$, $v = v^* = M_b = M_b^*$, and $w = w^* = M_c = M_c^*$. Equations (3) to (12) are useful in computing the crystallographic parameters of the modulated lattice, and the setting angles for the single-crystal and the detector in the X-ray and neutron diffractometries.

III. EXAMPLES OF MODULATED RECIPROCAL LATTICE

A. Antiphase Domain Structure

Let us consider an antiphase domain structure having an antiphase boundary at the integral distances of Ma along $\vec{a}$ direction, where M is not always an integer.¹⁰ We then observe the reflections at $\vec{H} = \vec{h} \pm (2m+1)\vec{a}^*/(2M)$, where m is an integer and the intensity of the reflection is usually stronger for smaller m , that is, the strongest when $m = 0$. Here, the modulation vector $\tau\vec{p}$ is equal to $(2m+1)\vec{a}^*/(2M)$. The fundamental reflection takes place when M is very large or when Ma approximates a dimension of the coherent domain. Therefore, the antiphase-domain satellite reflections may be considered as a symmetrical splitting of the fundamental Bragg-Laue reflection for which $\vec{H} = \vec{h}$. In other words, the antiphase-domain reflections are also governed by the Laue function (Ref. 13, p. 4) and hence give rise to the sharp intensity distribution when the coherent domain is sufficiently large.

As an example, part of the modulated reciprocal lattice of Cu_3Pd is shown in Fig. 1. The two-dimensional satellites along the duplex reciprocal lines are due to the two-dimensional antiphase domains in the tetragonally-distorted cubic lattice.^{12,19,20} Numerous other examples of the reciprocal lattices modulated by the antiphase domain structure have been reported in Refs. 9, 18, and 23 and the references therein. A general theory on the subject has been given by Fujiwara.¹⁰

Fig. 1

The Reciprocal Lattice of Cu_3Pd as Revealed by the Electron and X-ray Diffraction Methods. The dashed duplex lines are due to the tetragonal distortion of the lattice, and the two-dimensional, antiphase domain structure generates the different pairs of satellites as indicated by the shaded and open small circles. (Redrawn from the figure given by Watanabe *et al.*²⁰.)

A new type of modulated reciprocal lattice found in Y_3C is schematically shown in Fig. 2 by selecting its $(h\bar{h}l)$ reciprocal plane. A set of shaded circles represents the intensity distribution due to the face-centered cubic lattice formed by the yttrium atoms. The fundamental lattice for the carbon atoms is a pseudocubic superstructure with $a' = 2a$, where a is the lattice constant of the yttrium matrix. The carbon-atom distribution follows a complex twin-domain modulation, which shifts each superstructure reciprocal-lattice point as shown in Fig. 2. In this schematic figure, the direction and magnitude of the modulation vector are represented by the arrow and the number of the arrowheads, respectively. Each arrowhead corresponds to a very small shift, $\tau = 0.015 (a')^*$, and only a very careful observation of the experimental data could have revealed this type of modulation. In the shifting modes, the following symmetry characteristics may be noted: The shifting direction is parallel or antiparallel to the reciprocal axis for $(h\bar{h}h)$ or the one for $(h\bar{h}0)$; the magnitude of the displacement is proportional to the distance from the $(h\bar{h}h)$, or equivalent reciprocal points, toward which the shifting takes place; the reciprocal axes for $(00l)$ and $(h\bar{h}0)$ possess two-fold symmetry. Further details will be published elsewhere.²

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Fig. 2. An Unusual Distribution of the Modulation Vectors Found in Y_3C

The antiphase or twin-domain modulation occurs not only in the atomic structure but has also been reported as regards the electronic spin alignment in the magnetic crystal and the electric-dipole configurations in the ferro-, ferri-, and antiferroelectric crystals.

B. Neutron Diffraction of Magnetic Crystal

The scattering process between the neutron magnetic moment and the atomic magnetic moment involves a spin vector-vector interaction. Moreover, the symmetry of the magnetic-moment distribution in crystal frequently differs from the symmetry of the atomic structure.³ Nevertheless, the neutron magnetic-diffraction optics are also best interpretable in terms of the reciprocal lattice derived from the magnetic unit cell.

In the magnetic-moment alignment, we set $\tau = \phi/(360^\circ d)$ in $\text{\AA}^{-1}$, where ϕ is the differential angle in degrees between the moment-vector phase angles assigned to the nearest neighboring magnetic atoms along $\vec{p}$, and d in $\text{\AA}$ is the distance between these two atoms. When $\phi = 360^\circ$, and hence $\tau = 1/d$, the magnetic alignment along $\vec{p}$ is ferromagnetic, and the magnetic lattice repetition in this direction is equivalent to the atomic lattice repetition. When $\phi = 180^\circ$, and therefore $\tau = 1/2d$, we have an antiferromagnetic array along $\vec{p}$, and subsequently the primitive translation along $\vec{p}$ has to be doubled. When ϕ takes other angles, the magnetic alignment may be said to be sinusoidally modulated. In other words, the moment components perpendicular to $\vec{p}$ are spiraling along $\vec{p}$ with the successive one-directional rotation angle of ϕ and without changing the magnitude. The magnitude of the moment component parallel to $\vec{p}$ is modulated sinusoidally, including the direction antiparallel to $\vec{p}$. Suppose $\phi = 20^\circ$, and hence $\tau = (18d)^{-1}$. The magnetic repetition along $\vec{p}$ has a large unit spacing, $18d$ $\text{\AA}$. The reciprocal-lattice representation of this seemingly complex structure is simply given by two satellites associated with each fundamental lattice point.

The magnetic-spin alignment may be considered as a classical equilibrium configuration of the spin-density wave. In this fashion, $\vec{p}$ may be called the spin-propagation unit-vector, and $2\pi\tau\vec{p}$ corresponds to the wave-number vector of the spin-density wave. As discussed above, the sinusoidal modulation generates a pair of satellite reflections at $\vec{h} \pm \tau\vec{p}$, and their intensity distribution is subjected to the Laue function. The weaker satellites at $\vec{h} \pm 2\tau\vec{p}$ and much weaker satellites corresponding to higher harmonics may also coexist. Hence, the similarity between the modulation due to the antiphase domain and that caused by the sinusoidal alignment is remarkable. In fact, the elucidation of these two types of spin structures requires an exceedingly careful examination of the intensity relation among the satellites.

The experimental results on the sinusoidal modulation in the rare-earth metals have been reviewed by Koehler,¹⁴ and other references have been briefly reviewed by Atoji.³ As regards the theoretical interpretation, one may refer to Koehler,¹⁵ Bacon,⁸ and Hastings and Corliss.¹¹

Our example is the tetragonal TbC_2 , which becomes antiferromagnetic below 64°K .⁴ The magnetic structure consists of three different configurations, one of which is shown in Fig. 3, where a dual sinusoidal modulation takes place as regards the y and z components of the magnetic moment. The modulation vector $\vec{p}$ is parallel to $\vec{a}$ and hence to $\vec{a}^*$, and τ is equal to $\vec{a}^*/4$. The y and z components of the Bohr magneton moment of Tb are, respectively, $(0; 7.1)$ at the atomic position (000) , $(1.6; 0)$ at $(\frac{1}{4}00)$, $(-1.6/\sqrt{2}; -7.1/\sqrt{2})$ at $(\frac{1}{8}\frac{1}{2}\frac{1}{2})$, etc. This moment correlation results in the extinction of the satellites associated with the reflection for which $h + k + l = 2n$. The magnetic reciprocal lattice of TbC_2 represents these configurations in a succinct manner (Fig. 4).

121-432 Rev. 1

Fig. 3. The Antiferromagnetic Structure of TbC_2 . The dumbbells represent the C_2 groups. The arrow indicating the relative magnitude of moment and its direction is placed at the Tb atom.

121-433

Fig. 4

The Reciprocal Lattice of the Antiferromagnetic TbC_2 . The magnetic reflections take place at the small circles.

C. Diffuse Reflections

The diffuse reflections have been discussed comprehensively by James,¹³ Wooster,²² and the references cited in these two books. A few comments are added here to stress our concept of the modulation vector.

In the thermal diffuse scattering due to the lattice vibrations, $2\pi\vec{p}$ is simply the wave number vector of the elastic wave propagating in the lattice.²² An outstanding example, the thermal diffuse scattering of ice, is shown in Fig. 5. When the rotation of the atomic groups takes place in the crystal, the modulation vector for the resultant diffuse scattering is a function of the geometrical parameters of the rotating atomic groups, and the modulation-vector distribution is strongly dependent on the symmetry of the potential around them.^{6,7} An idealized figure representing the modulation of the reciprocal lattice due to the order-disorder arrangement in AuCu_3 is shown in Fig. 6 (Ref. 22, p. 133). The inelastic scattering of the neutrons can also be described most efficiently by using a moment modulation vector in the reciprocal lattice.⁸ Countless other cases exist as regards the modulated reciprocal, and all their basic geometrical characteristics can be systematically described in terms of the modulation reciprocal-lattice vector. Accordingly, our computer program given in the following chapter should have a vast area of application.

121-407

Fig. 5. The Thermal-vibration Modulation-vector Distribution in the $(hk0)$ Reciprocal Plane of the Hexagonal Ice, as Revealed by the X-ray Method. The weak diffuse streaks bridging the fundamental lattice points are shown by the dotted lines, and the stronger diffuse spots are indicated by the short heavy lines; $\vec{a}_1^*$ and $\vec{a}_2^*$ correspond, respectively, to $\vec{a}^*$ and $\vec{b}^*$ in our notation (reproduced from the figure given by Owston¹⁷).

Fig. 6

A Part of the Reciprocal Lattice of AuCu_3 . The shaded circles represent the fundamental lattice points, and the isodiffuse contours indicate the disk-like distribution of the modulation vectors due to the imperfection in the atomic arrangement. (A modified drawing of the figure given by Wooster,²² through courtesy of the Clarendon Press.)

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IV. COMPUTER PROGRAM

Our computer program may be regarded as an extended form of the one developed by Mueller *et al.*¹⁶ for the fundamental reciprocal lattice, although the computer coding has been almost completely rewritten. The program computes D , $1/D^2$, $\sin^2 \theta$, $(\sin \theta)/\lambda$, $(\sin^2 \theta)/\lambda^2$, θ , and 2θ . The input data are the modulation parameter set, (u, v, w, τ) , or an alternate set, (u^*, v^*, w^*, τ) , as well as a , b , c , α , β , γ , and λ . Up to 40 different sets of modulation parameters could be accommodated in a single computing process. The program always generates the data for the set, $\vec{h}$, $\vec{h} + \tau\vec{p}$, and $\vec{h} - \tau\vec{p}$, which are denoted by (hkl) , $+(hkl)$, and $-(hkl)$, respectively. The calculations include various Lorenz or Lorenz-polarization factors directly applicable to the X-ray and neutron diffractometries, and the angles for the single-crystal and detector settings in the three-circle cone method. The extinction rules and the symmetry characteristics on (hkl) could also be applied to eliminate unnecessary output data. Optional input controls can be made on the sorting sequence, the termination of the calculation at the given angle or indices, and the experimental angular corrections to be applied to the crystal-detector settings. The outputs could be made on the printed form, the punched cards, or both. In the computer coding, τ has been denoted as t .

The formulas used in the programming have been given as Eqs. (3) to (9). The formulas for the crystal-setting angles, Φ and χ , in the fundamental lattice have been given by Willis,²¹ and those for the generalized lattice are summarized as follows:

$$(\tan \Phi)_{c-a} = \frac{(kb^* \pm \tau v^*) \sin \gamma^* - (lc^* \pm \tau w^*) \cos \alpha \sin \beta^*}{ha^* \pm \tau u^* + (kb^* \pm \tau v^*) \cos \gamma^* + (lc^* \pm \tau w^*) \cos \beta^*};$$

$$(\tan \Phi)_{c-b} = \frac{(ha^* \pm \tau u^*) \sin \gamma^* - (lc^* \pm \tau w^*) \cos \beta \sin \alpha^*}{kb^* \pm \tau v^* + (ha^* \pm \tau u^*) \cos \gamma^* + (lc^* \pm \tau w^*) \cos \alpha^*};$$

$$(\tan \Phi)_{b-c} = \frac{(ha^* \pm \tau u^*) \sin \beta^* - (kb^* \pm \tau v^*) \cos \gamma \sin \alpha^*}{lc^* \pm \tau w^* + (ha^* \pm \tau u^*) \cos \beta^* + (kb^* \pm \tau v^*) \cos \alpha^*};$$

$$(\tan \Phi)_{b-a} = \frac{(lc^* \pm 3w^*) \sin \beta^* - (kb^* \pm 3v^*) \cos \alpha \sin \gamma^*}{ha^* \pm 3u^* + (lc^* \pm 3w^*) \cos \beta^* + (kb^* \pm 3v^*) \cos \gamma^*};$$

$$(\tan \Phi)_{a-b} = \frac{(lc^* \pm \tau w^*) \sin \alpha^* - (ha^* \pm \tau u^*) \cos \beta \sin \gamma^*}{kb^* \pm \tau v^* + (lc^* \pm \tau w^*) \cos \alpha^* + (ha^* \pm \tau u^*) \cos \gamma^*};$$

$$(\tan \Phi)_{a-c} = \frac{(kb^* \pm \tau v^*) \sin \alpha^* - (ha^* \pm \tau u^*) \cos \gamma \sin \beta^*}{lc^* \pm \tau w^* + (kb^* \pm \tau v^*) \cos \alpha^* + (ha^* \pm \tau u^*) \cos \beta^*};$$

$$\sin \chi_a = (ha^* \pm \tau u^*) D \sin \beta \sin \gamma^*;$$

$$\sin \chi_b = (kb^* \pm \tau v^*) D \sin \gamma \sin \alpha^*;$$

$$\sin \chi_c = (lc^* \pm \tau w^*) D \sin \alpha \sin \beta^*.$$

In the above equations, $\pm$ corresponds to that in $\vec{h} \pm \tau \vec{p}$. The subscripts a, b, and c follow the definitions by Mueller *et al.*¹⁶: in Φ 's, the first subscript is the axis of the crystal along the Φ axis, and the second subscript represents the reciprocal axis of the crystal in the χ -circle plane; in χ 's, the subscript letter indicates the crystal axis parallel to the Φ axis. In the computation of the trigonometric functions regarding α^* , β^* , and γ^* , the following relations are utilized:

$$a^* \sin \gamma^* = (a \sin \beta)^{-1}, \quad a^* \sin \beta^* = (a \sin \gamma)^{-1};$$

$$b^* \sin \alpha^* = (b \sin \gamma)^{-1}, \quad b^* \sin \gamma^* = (b \sin \alpha)^{-1};$$

$$c^* \sin \alpha^* = (c \sin \beta)^{-1}, \quad c^* \sin \beta^* = (c \sin \alpha)^{-1}.$$

An obvious extension of the program is to implicate the arbitrary axial setting of the sample crystal. The formulas for this general case are excessively complex even in the $\tau = 0$ case. Accordingly, in the satellite-reflection study, the experimental procedures and the data interpretations could be made much simpler by prealigning the crystal along one of the principal axes.

The input-card format described in Table I is self-explanatory and gives the detailed scope of the program. An example of the input format is given in Fig. 7, and the output data are tabulated in Tables II and III. The sample case is the magnetic spin structure of TbC_2 . For searching u , v , w , and τ values in the neutron powder analysis, the monographs for $\sin \Theta$ vs. τ are computed for several appropriate sets of u , v , and w and are compared with the preliminary experimental $\sin \Theta$ values. The input and output

704 INPUT DATA

FORM I

COST CODE 52200-02-120-360

PROGRAM B187

PROBLEM TBC2

ORIGINATOR M. ATOJI

DATE 12/13/65

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[illegible]

Fig. 7. An Example of the Input Format with the Multiple Modulation Parameters

data used for preparing these monographs are given in Fig. 7 and Table II, respectively. For this type of calculation, the output may be arranged with respect to h , k , and l as executed in this sample case.

When u , v , w , and τ are determined accurately from the interpretation of the preliminary data, an entire set of data may be calculated with the output arranged in order of decreasing D value. Such output data are given in Table III. The symbolic program listing is given in Table IV. For the output-card format, see Refs. 1 and 5. The program is to be run on the CDC 3600 computer with SCOPE monitor system and a 65K core storage.

TABLE I. Input-card Format

The following card types are required as input information to this program and are listed in the order in which they must appear in the data deck.

Card Type	Columns	Format	Code Name	Description
1	1-72	72H		Title: Column 1 must be blank.
2	1-9	9F0.0	WAD	α in degrees.
	10-18		WBD	β in degrees.
	19-27		WCD	γ in degrees.
	28-36		A	a in Å.
	37-45		B	b in Å.
	46-54		C	c in Å.
	55-63		XL	λ in Å: The wavelength of the observation.
3	1-9	8F9.0	OUTPUT	Output control constant. 0. No optional output. 1. Optional output on punched cards.
	10-18		FINAL	Criteria for limit selection. 0. $1/D \leq 1/\lambda$. 1. $1/D \leq (2/\lambda) \sin \theta_{\max}$. 2. $ h \leq h_{\max}$, $ k \leq k_{\max}$, $ l \leq l_{\max}$. NOTE: In the last case, program limits are $1/D \leq 2/\lambda$.
	19-27		TMAX	$\theta_{\max}$ in degrees; used only if FINAL = 1.
	28-36		FINALH	$h_{\max}$.
	37-45		FINALK	$k_{\max}$.
	46-54		FINALL	$l_{\max}$.
	55-63		SORTK	Control parameter to determine the order of output. 0. Output in order of increasing $ l $, $ k $, $ h $; each octant separately. 1. Output for h , k , l 's associated with increasing values of θ ; all octants together. 2. Output for h , k , l 's associated with decreasing values of θ ; all octants together.

TABLE I (Contd.)

Card Type	Columns	Format	Code Name	Description
3	64-72		UVW	The number of different modulation vectors used in the program. The sign of UVW indicates what cards of Type 4 are to be read next: positive UVW, cards Type 4a; negative UVW, cards Type 4b. If UVW = 0, card of Type 4 is omitted.
4a	1-9 10-18 19-27 28-36	8F9.0	UX(1) VX(1) WX(1) TX(1)	u_1 v_1 w_1 } Direction parameters of the modulation vector. τ_1 The modulus of the modulation vector in $(\text{\AA})^{-1}$.
	37-45 46-54 55-63 64-72		UX(2) VX(2) WX(2) TX(2)	u_2 v_2 w_2 τ_2
4b	1-9 10-18 19-27 28-36 37-45 46-54 55-63 64-72	8F9.0	US(1) VS(1) WS(1) TX(1) US(2) VS(2) WS(2) TX(2)	u_1^* v_1^* w_1^* } Reciprocal direction parameters of the modulation vector. τ_1 The modulus of the modulation vector. u_2^* v_2^* w_2^* τ_2
5		2111, 2F9.0		NOTE: Use as many cards of Type 4 (4a or 4b) as required. Two sets of (u, v, w, τ) per card.
	1		LB	Columns 1-10 determine the extinction criteria; i.e., the calculations are only done for specified h, k, ℓ relationships. 0 No extinction criteria are used in the program. 1 The following nine tests LX(i), i = 1 to 9, are checked in the program.
	2		LX(1)	h k ℓ selection. 0 Omit this test. 1 $h + k + \ell = 2n$, condition for nonextinction. 2 $h + k = 2n$. 3 $h + \ell = 2n$. 4 $k + \ell = 2n$. 5 $h + k = 2n$, $h + \ell = 2n$, and $k + \ell = 2n$. 6 $-h + k + \ell = 3n$. 7 $h + k + \ell = 3n$.
	3		LX(2)	0 k ℓ selection. 0 Omit this test. 1 $k = 2n$. 2 $\ell = 2n$. 3 $k + \ell = 2n$. 4 $k + \ell = 4n$.

TABLE I (Contd.)

Card Type	Columns	Format	Code Name	Description
5	4		LX(3)	h 0 ℓ selection. 0 Omit this test. 1 $h = 2n$. 2 $\ell = 2n$. 3 $h + \ell = 2n$. 4 $h + \ell = 4n$.
	5		LX(4)	h k 0 selection. 0 Omit this test. 1 $h = 2n$. 2 $k = 2n$. 3 $h + k = 2n$. 4 $h + k = 4n$.
	6		LX(5)	h h ℓ selection. 0 Omit this test. 1 $\ell = 2n$. 2 $h = 2n$. 3 $h + \ell = 2n$. 4 $2h + \ell = 4n$.
	7		LX(6)	h 0 0 selection. 0 Omit this test. 1 $h = 2n$. 2 $h = 4n$.
	8		LX(7)	0 k 0 selection. 0 Omit this test. 1 $k = 2n$. 2 $k = 4n$.
	9		LX(8)	0 0 ℓ selection. 0 Omit this test. 1 $\ell = 2n$. 2 $\ell = 3n$. 3 $\ell = 4n$. 4 $\ell = 6n$.
	10		LX(9)	h h 0 selection. 0 Omit this test. 1 $h = 2n$.
	11		NP	ϕ Angle calculation. 0 Omit this calculation. 1 Calculate ϕ_{c-a} . 2 Calculate ϕ_{c-b} . 3 Calculate ϕ_{b-c} . 4 Calculate ϕ_{b-a} . 5 Calculate ϕ_{a-b} . 6 Calculate ϕ_{a-c} .
	12		NC	χ Angle calculation. 0 Omit this calculation. 1 Calculate χ_c . 2 Calculate χ_b . 3 Calculate χ_a .

TABLE I (Contd.)

Card Type	Columns	Format	Code Name	Description
5	13		LP	L or LP calculation. 0 Omit this calculation. 1 L for crystal face, symmetrical reflection. 2 L for Debye-Scherrer lines on cylindrical film. 3 LP for Debye-Scherrer lines on cylindrical film. 4 LP, equi-inclination, a-axis rotation. 5 LP, equi-inclination, b-axis rotation. 6 LP, equi-inclination, c-axis rotation.
				Multiplicity option. 0 No restriction. 1 Criteria $h \geq k \geq l \geq 0$ must be satisfied. 2 Criteria $h \geq k \geq 0$ must be satisfied.
				<u>Sign permutation control; octant selection.</u>
				0 Omit. 1 Calculate $\bar{h} k l$.
				0 Omit. 1 Calculate $h \bar{k} l$.
				0 Omit. 1 Calculate $\bar{h} \bar{k} l$.
				0 Omit. 1 Calculate $h k \bar{l}$.
				0 Omit. 1 Calculate $\bar{h} k \bar{l}$.
				0 Omit. 1 Calculate $h \bar{k} \bar{l}$.
				0 Omit. 1 Calculate $\bar{h} \bar{k} \bar{l}$.
	14		NCT	
6	1-9 10-18 19-27 28-36 37-45 46-54 55-63	8F9.0	INDEX(1)	0 Omit. 1 Calculate $\bar{h} k l$.
			INDEX(2)	0 Omit. 1 Calculate $h \bar{k} l$.
			INDEX(3)	0 Omit. 1 Calculate $\bar{h} \bar{k} l$.
			INDEX(4)	0 Omit. 1 Calculate $h k \bar{l}$.
			INDEX(5)	0 Omit. 1 Calculate $\bar{h} k \bar{l}$.
			INDEX(6)	0 Omit. 1 Calculate $h \bar{k} \bar{l}$.
			INDEX(7)	0 Omit. 1 Calculate $\bar{h} \bar{k} \bar{l}$.
			ADJP	$\Delta\phi$ Correction to be added to ϕ (in degrees).
			ADJC	$\Delta\chi$ Correction to be added to χ (in degrees).
				<u>Input required for punched-cards output.</u>
			ALPHA	α' For adjusting θ .
			TTPTAM	} $2\theta_{\max}$ Cards are punched only for $2\theta_{\min}$ $2\theta_{\max} \leq 2\theta \leq 2\theta_{\min}$
			TTMIN	
			BETA	β' Determines range of θ (output $2\theta - \beta'$ and $2\theta + \beta'$).
			GAMMA	γ' For adjusting ϕ .
			DELTA	Δ' For adjusting χ .
			STEP	Step angle in hundredths of a degree per unit.

NOTE: Card of Type 6 is omitted if OUTPUT = 0. (See card of Type 3.)

NOTE: Consecutive cases may be run.

TABLE II. An Example of the Printed Output Format for a
Single Modulation Parameter

B 187 ATOJI TBC2 TEMP 4K NEUTRON SINGLE MODULATION 12/23/65

ALPHA 90.00000 BETA 90.00000 GAMMA 90.00000 A 3.69000 B 3.69000 C 6.21700 LAMBDA 1.068700

C T U V W U* V* W*
1 0.04500 0.45460 0.45460 0.76590 0.45460 0.45460 0.76590

HKL OKL HCL HKO HFL HDO OKO OOL HHO PHI CHI COR NCT -KL H-L --L HK- -K- H-- --- ADJPHI ADJCHI T-MAX FINALH FINALK FINALL
0 0 0 0 0 0 0 0 0 1 1 1 2 1 1 0 1 0 0 0 -0.00 -0.00 15 -0 -0 -0

V CGSA* COSB* CCSG* A* B* C*
84.65129 0.000000 0.000000 0.000000 0.271003 0.271003 0.160849

C	H	K	L	O	1/CSO	SINTH	SINTHS	SINTL	SQTL5	THETA	2THETA	PHI	CHI	L-LP
0	0	0	0	0	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.0000	0.0000	0.0000	0.0000
-1	0	0	0	22.22222	0.02003	0.02405	0.00058	0.02250	0.00051	1.3719	2.7557	45.0000	310.0129	20.7997
1	0	0	0	22.22222	0.00203	0.02405	0.00058	0.02250	0.00051	1.3779	2.7557	45.0000	49.9871	20.7997
-1	0	0	1	7.71287	0.01681	0.06928	0.00480	0.06483	0.00420	3.9726	7.9453	45.0000	77.1054	7.2344
1	0	0	-1	7.71287	0.01681	0.06928	0.00480	0.06483	0.00420	3.9726	7.9453	45.0000	282.8946	7.2344
0	0	0	1	6.21700	0.02587	0.08595	0.00739	0.08042	0.00647	4.9306	9.8613	45.0000	90.0000	5.8390
0	0	0	-1	6.21700	0.02587	0.08595	0.00739	0.08042	0.00647	4.9306	9.8613	45.0000	270.0000	5.8390
1	0	0	1	5.06467	0.03898	0.10551	0.01113	0.09872	0.00975	6.0563	12.1126	45.0000	81.5737	4.7657
-1	0	0	-1	5.06467	0.03898	0.10551	0.01113	0.09872	0.00975	6.0563	12.1126	45.0000	278.4263	4.7657
-1	1	0	0	3.94117	0.06438	0.13558	0.01838	0.12687	0.01609	7.7922	15.5845	175.3322	352.1931	3.7222
1	-1	0	0	3.94117	0.06438	0.13558	0.01838	0.12687	0.01609	7.7922	15.5845	175.3322	7.8069	3.7222
0	1	0	0	3.69000	0.07344	0.14481	0.02097	0.13550	0.01836	8.3263	16.6526	0.0000	0.0000	3.4896
0	-1	0	0	3.69000	0.07344	0.14481	0.02097	0.13550	0.01836	8.3263	16.6526	0.0000	0.0000	3.4896
-1	1	0	1	3.55414	0.07916	0.15035	0.02260	0.14068	0.01979	8.6470	17.2939	175.3322	26.6914	3.3639
-1	0	0	2	3.46396	0.08334	0.15426	0.02380	0.14434	0.02083	8.8739	17.7477	45.0000	84.2480	3.2806
1	0	0	-2	3.46396	0.08334	0.15426	0.02380	0.14434	0.02083	8.8739	17.7477	45.0000	275.7520	3.2806
1	1	0	0	3.39902	0.08656	0.15721	0.02471	0.14710	0.02164	9.0448	18.0897	4.0149	6.7276	3.2206
-1	-1	0	0	3.39902	0.08656	0.15721	0.02471	0.14710	0.02164	9.0448	18.0897	4.0149	353.2724	3.2206
0	1	0	1	3.17317	0.09931	0.16840	0.02836	0.15757	0.02483	9.6946	19.3892	0.0000	30.6906	3.0122
0	-1	0	1	3.17317	0.09931	0.16840	0.02836	0.15757	0.02483	9.6946	19.3892	0.0000	30.6906	3.0122
0	1	0	-1	3.17317	0.09931	0.16840	0.02836	0.15757	0.02483	9.6946	19.3892	0.0000	329.3094	3.0122
1	-1	0	1	3.14131	0.10134	0.17010	0.02894	0.15917	0.02533	9.7939	19.5878	175.3322	37.8462	2.9828
-1	1	0	-1	3.14131	0.10134	0.17010	0.02894	0.15917	0.02533	9.7939	19.5878	175.3322	322.1538	2.9828
-1	-1	0	1	3.14130	0.10134	0.17010	0.02894	0.15917	0.02534	9.7939	19.5878	4.0149	23.3913	2.9828
1	1	0	-1	3.14130	0.10134	0.17010	0.02894	0.15917	0.02534	9.7939	19.5878	4.0149	336.6087	2.9828
0	0	0	2	3.10850	0.10349	0.17190	0.02555	0.16085	0.02587	9.8983	19.7966	45.0000	90.0000	2.9526
0	0	0	-2	3.10850	0.10349	0.17190	0.02555	0.16085	0.02587	9.8983	19.7966	45.0000	270.0000	2.9526
1	1	0	1	2.84538	0.12352	0.18780	0.03527	0.17572	0.03088	10.8242	21.6484	4.0149	33.7620	2.7107
-1	1	1	0	2.80901	0.12673	0.19023	0.03619	0.17800	0.03168	10.9661	21.9321	45.0000	354.4443	2.6773
1	0	0	2	2.79848	0.12769	0.19094	0.03646	0.17867	0.03192	11.0078	22.0157	45.0000	85.3557	2.6677
-1	0	0	-2	2.79848	0.12769	0.19094	0.03646	0.17867	0.03192	11.0078	22.0157	45.0000	274.6443	2.6677
-1	1	1	1	2.65823	0.14152	0.20102	0.04641	0.18810	0.03538	11.5965	23.1929	45.0000	19.6307	2.5392
-1	1	0	2	2.61986	0.14569	0.20396	0.04160	0.19085	0.03642	11.7687	23.5374	175.3322	48.8083	2.5041
0	1	1	0	2.60922	0.14688	0.20479	0.04194	0.19163	0.03672	11.8174	23.6347	45.0000	0.0000	2.4944
0	-1	1	0	2.60922	0.14688	0.20479	0.04194	0.19163	0.03672	11.8174	23.6347	125.0000	0.0000	2.4944
0	1	-1	0	2.60922	0.14688	0.20479	0.04194	0.19163	0.03672	11.8174	23.6347	135.0000	0.0000	2.4944
-1	-1	1	0	2.59142	0.14891	0.20620	0.04252	0.19294	0.03723	11.8997	23.7995	139.3169	354.8758	2.4781
1	-1	1	0	2.59142	0.14891	0.20620	0.04252	0.19294	0.03723	11.8997	23.7995	130.6831	5.1242	2.4781
-1	1	-1	0	2.59142	0.14891	0.20620	0.04252	0.19294	0.03723	11.8997	23.7995	139.3169	354.8758	2.4781
1	1	-1	0	2.59142	0.14891	0.20620	0.04252	0.19294	0.03723	11.8997	23.7995	139.3169	5.1242	2.4781
-1	-1	1	1	2.47162	0.16369	0.21619	0.04674	0.20230	0.04092	12.4856	24.9712	139.3169	18.2023	2.3688
-1	1	-1	1	2.47162	0.16369	0.21619	0.04674	0.20230	0.04092	12.4856	24.9712	130.6831	18.2023	2.3688
-1	1	1	-1	2.47163	0.16369	0.21619	0.04674	0.20230	0.04092	12.4856	24.9711	45.0000	331.1351	2.3688
-1	-1	0	2	2.44069	0.16787	0.21893	0.04793	0.20486	0.04197	12.6464	25.2928	4.0149	44.5111	2.3406
1	1	0	-2	2.44069	0.16787	0.21893	0.04793	0.20486	0.04197	12.6464	25.2928	4.0149	315.4889	2.3406
1	1	1	0	2.41765	0.17109	0.22102	0.04885	0.20681	0.04277	12.7690	25.5380	45.0000	4.7797	2.3196
0	1	1	1	2.40592	0.17276	0.22210	0.04933	0.20782	0.04319	12.8323	25.6645	45.0000	22.7674	2.3089
0	-1	1	1	2.40592	0.17276	0.22210	0.04933	0.20782	0.04319	12.8323	25.6645	135.0000	22.7674	2.3089
0	1	-1	1	2.40592	0.17276	0.22210	0.04933	0.20782	0.04319	12.8323	25.6645	135.0000	22.7674	2.3089
0	1	1	-1	2.40592	0.17276	0.22210	0.04933	0.20782	0.04319	12.8323	25.6645	45.0000	337.2326	2.3089
0	1	0	2	2.37737	0.17693	0.22477	0.05052	0.21032	0.04423	12.9891	25.9782	0.0000	49.8888	2.2830
0	-1	0	2	2.37737	0.17693	0.22477	0.05052	0.21032	0.04423	12.9891	25.9782	0.0000	49.8888	2.2830
0	1	0	-2	2.37737	0.17693	0.22477	0.05052	0.21032	0.04423	12.9891	25.9782	0.0000	310.1112	2.2830
1	-1	1	1	2.31951	0.18587	0.23037	0.05307	0.21556	0.04647	13.3190	26.6380	130.6931	26.9385	2.2304
1	1	-1	1	2.31951	0.18587	0.23037	0.05307	0.21556	0.04647	13.3190	26.6380	139.3169	26.9385	2.2304
1	1	1	-1	2.31950	0.18587	0.23037	0.05307	0.21556	0.04647	13.3190	26.6380	45.0000	342.9535	2.2304
1	-1	0	2	2.29389	0.19004	0.23295	0.05426	0.21797	0.04751	13.4705	26.9411	175.3322	54.7856	2.2071
-1	1	0	-2	2.29389	0.19004	0.23295	0.05426	0.21797	0.04751	13.4705	26.9411	175.3322	305.2144	2.2071
-1	0	0	3	2.22709	0.20161	0.23993	0.05757	0.22451	0.05040	13.8825	27.7650	45.0000	86.3055	2.1466
1	0	0	-3	2.22709	0.20161	0.23993	0.05757	0.22451	0.05040	13.8825	27.7650	45.0000	273.6945	2.1466
1	1	1	1	2.19241	0.20805	0.24373	0.05540	0.22806	0.05201	14.1067	28.2133	45.0000	25.3540	2.1153
-1	1	1	2	2.19239	0.20805	0.24373	0.05540	0.22806	0.05201	14.1068	28.2136	45.0000	39.0299	2.1152
1	1	0	2	2.17073	0.21222	0.24616	0.06060	0.23034	0.05306	14.2505	28.5009	4.0149	50.6365	2.0957
-1	-1	1	2	2.08413	0.23022	0.25639	0.06574	0.23991	0.05756	14.8560	29.7120	139.3169	36.7718	2.0176
-1	1	-1	2	2.08413	0.23022	0.25639	0.06574	0.23991	0.05756	14.8560	29.7120	130.6831	36.7718	2.0176
0	0	0	3	2.07233	0.23285	0.25785	0.06649	0.24127	0.05821	14.9425	29.8850	45.0000	90.0000	2.0070
0	0	0	-3	2.07233	0.23285	0.25785	0.06649	0.24127	0.05821	14.9425	29.8850	45.0000	270.0000	2.0070

TABLE III. An Example of the Printed Output Format for the Multiple Modulation Parameters

B 187 ATCJ1 TBC2 TEMP 4K NEUTRON MULTIPLE MODULATION 12/23/65

ALPHA		BETA		GAMMA		A		B		C		LAMBDA													
90.00000		90.00000		90.00000		3.69000		3.69000		6.21700		1.068700													
C	T	U		V		W		U*		V*		W*													
1	0.02000	0.45460		0.45460		0.76590		0.45460		0.45460		0.76590													
2	0.04000	0.45460		0.45460		0.76590		0.45460		0.45460		0.76590													
3	0.06000	0.45460		0.45460		0.76590		0.45460		0.45460		0.76590													
4	0.08000	0.45460		0.45460		0.76590		0.45460		0.45460		0.76590													
5	0.10000	0.45460		0.45460		0.76590		0.45460		0.45460		0.76590													
HKL	OKL	HCL	HKO	HFL	HOO	OKO	OOL	HOO	PHI	CHI	COR	NCT	-KL	H-L	--L	HK-	-K-	H--	---	ADJPHI	ADJCHI	T-MAX	FINALH	FINALK	FINALL
0	0	0	0	0	0	0	0	0	1	1	1	2	1	1	0	1	0	0	0	-0.00	-0.00	15	-0	-0	-

V				CCSA*	COSB*	CCSG*	A*	B*	C*					
84.65129				0.000000	0.000000	0.000000	0.271003	0.271003	0.160849					
C	H	K	L	C	1/LSQ	SINTH	SINTHS	SINTL	SGTSL	THETA	2THETA	PHI	CHI	L-LP
0	0	0	0	0.000000	0.00000	0.00000	0.00000	0.00000	0.00000	0.0000	0.0000	0.0000	0.0000	0.0000
-1	0	0	0	50.00000	0.00040	0.01069	0.00011	0.01000	0.00010	0.6123	1.2247	45.0000	310.0129	46.7885
-2	0	0	0	25.00000	0.00160	0.02137	0.00046	0.02000	0.00040	1.2247	2.4495	45.0000	310.0129	23.4983
-3	0	0	0	16.66667	0.00360	0.03206	0.00103	0.03000	0.00090	1.8373	3.6745	45.0000	310.0129	15.6033
-4	0	0	0	12.50000	0.00640	0.04275	0.00183	0.04000	0.00160	2.4500	4.9001	45.0000	310.0129	11.7072
-5	0	0	0	10.00000	0.01000	0.05343	0.00286	0.05000	0.00250	3.0631	6.1261	45.0000	310.0129	9.3706
1	0	0	0	50.00000	0.00040	0.01069	0.00011	0.01000	0.00010	0.6123	1.2247	45.0000	49.9871	46.7885
2	0	0	0	25.00000	0.00160	0.02137	0.00046	0.02000	0.00040	1.2247	2.4495	45.0000	49.9871	23.3983
3	0	0	0	16.66667	0.00360	0.03206	0.00103	0.03000	0.00090	1.8373	3.6745	45.0000	49.9871	15.6033
4	0	0	0	12.50000	0.00640	0.04275	0.00183	0.04000	0.00160	2.4500	4.9001	45.0000	49.9871	11.7072
5	0	0	0	10.00000	0.01000	0.05343	0.00286	0.05000	0.00250	3.0631	6.1261	45.0000	49.9871	9.3706
0	1	0	0	3.69000	0.07344	0.14481	0.02097	0.13550	0.01836	8.3263	16.6526	0.0000	0.0000	3.4896
-1	1	0	0	3.80929	0.06891	0.14028	0.01668	0.13126	0.01723	8.0638	16.1276	178.0118	356.6548	3.6000
-2	1	0	0	3.91670	0.06519	0.13643	0.01661	0.12766	0.01630	7.8412	15.6825	175.8861	353.1084	3.6995
-3	1	0	0	4.00774	0.06226	0.13333	0.01778	0.12476	0.01556	7.6620	15.3241	173.6145	349.3871	3.7839
-4	1	0	0	4.07804	0.06013	0.13103	0.01717	0.12261	0.01503	7.5292	15.0584	171.1894	345.5302	3.8491
-5	1	0	0	4.12383	0.05880	0.12958	0.01679	0.12125	0.01470	7.4451	14.8902	168.6042	341.5882	3.8915
1	1	0	0	3.56302	0.07877	0.14997	0.02249	0.14033	0.01969	8.6252	17.2505	1.8592	3.1287	3.3721
2	1	0	0	3.43203	0.08490	0.15570	0.02424	0.14569	0.02122	8.9571	17.9142	3.5980	6.0354	3.2510
3	1	0	0	3.30002	0.09183	0.16192	0.02622	0.15151	0.02296	9.3185	18.6371	5.2249	8.7225	3.1292
4	1	0	0	3.16935	0.09955	0.16860	0.02843	0.15776	0.02489	9.7064	19.4128	6.7478	11.1976	3.0087
5	1	0	0	3.04175	0.10808	0.17567	0.03086	0.16438	0.02702	10.1178	20.2355	8.1746	13.4718	2.8912
0	1	1	0	2.60922	0.14688	0.20479	0.04194	0.19163	0.03672	11.8174	23.6347	45.0000	0.0000	2.4944
-1	1	1	0	2.69749	0.13743	0.19809	0.03524	0.18536	0.03436	11.4254	22.8507	45.0000	357.6319	2.5751
-2	1	1	0	2.78668	0.12877	0.19175	0.03677	0.17942	0.03219	11.0550	22.1100	45.0000	355.1025	2.6568
-3	1	1	0	2.87578	0.12092	0.18581	0.03453	0.17387	0.03023	10.7084	21.4168	45.0000	352.4059	2.7386
-4	1	1	0	2.96354	0.11386	0.18031	0.03251	0.16872	0.02847	10.3877	20.7754	45.0000	349.5381	2.8192
-5	1	1	0	3.04847	0.10761	0.17528	0.03072	0.16402	0.02690	10.0952	20.1904	45.0000	346.4978	2.8974
1	1	1	0	2.52264	0.15714	0.21182	0.04487	0.19820	0.03929	12.2291	24.4582	45.0000	2.2146	2.4153
2	1	1	0	2.43832	0.16820	0.21915	0.04803	0.20506	0.04205	12.6589	25.3178	45.0000	4.2840	2.3384
3	1	1	0	2.35668	0.18005	0.22674	0.05141	0.21216	0.04501	13.1051	26.2102	45.0000	6.2173	2.2642
4	1	1	0	2.27798	0.19271	0.23457	0.05502	0.21949	0.04816	13.5664	27.1328	45.0000	8.0233	2.1927
5	1	1	0	2.20239	0.20616	0.24262	0.05887	0.22703	0.05154	14.0414	28.0828	45.0000	9.7111	2.1243
0	0	0	1	6.21700	0.02587	0.08595	0.00739	0.08042	0.00647	4.9306	9.8612	45.0000	90.0000	5.0390
-1	0	0	1	6.84471	0.02134	0.07807	0.00609	0.07305	0.00534	4.4775	8.9550	45.0000	84.9504	6.4243
-2	0	0	1	7.53416	0.01762	0.07092	0.00503	0.06636	0.00440	4.0670	8.1341	45.0000	78.8273	7.0676
-3	0	0	1	8.25090	0.01469	0.06476	0.00419	0.06060	0.00367	3.7132	7.4264	45.0000	71.4399	7.7367
-4	0	0	1	8.92239	0.01256	0.05989	0.00359	0.05604	0.00314	3.4334	6.8668	45.0000	62.6813	8.3638
-5	0	0	1	9.43497	0.01123	0.05664	0.00321	0.05299	0.00281	3.2467	6.4934	45.0000	52.6537	8.8426
1	0	0	1	5.66136	0.03120	0.09439	0.00891	0.08832	0.00780	5.4159	10.8319	45.0000	85.8251	5.3212
2	0	0	1	5.17586	0.03733	0.10324	0.01066	0.09660	0.00933	5.9257	11.8514	45.0000	82.3504	4.8692
3	0	0	1	4.75351	0.04426	0.11241	0.01264	0.10519	0.01106	6.4544	12.9087	45.0000	79.4334	4.4763
4	0	0	1	4.38598	0.05198	0.12183	0.01484	0.11400	0.01300	6.9978	13.9956	45.0000	76.9618	4.1348
5	0	0	1	4.06520	0.06051	0.13145	0.01728	0.12300	0.01513	7.5531	15.1062	45.0000	74.8483	3.8372
0	1	0	1	3.17317	0.09931	0.16840	0.02836	0.15757	0.02483	9.6946	19.3892	0.0000	30.6906	3.0122
-1	1	0	1	3.35594	0.08986	0.16018	0.02566	0.14988	0.02246	9.2173	18.4346	178.0118	29.0442	3.1623
-2	1	0	1	3.50923	0.08120	0.15227	0.02219	0.14248	0.02030	8.7585	17.5170	175.8861	27.1904	3.3224
-3	1	0	1	3.69238	0.07335	0.14472	0.02094	0.13541	0.01834	8.3209	16.6418	173.6145	25.1024	3.4918
-4	1	0	1	3.88391	0.06629	0.13758	0.01893	0.12874	0.01657	7.9079	15.8157	171.1894	22.7524	3.6691
-5	1	0	1	4.08124	0.06004	0.13093	0.01714	0.12251	0.01501	7.5232	15.0465	168.6042	20.1136	3.8520
1	1	0	1	3.02101	0.10957	0.17688	0.03129	0.16551	0.02739	10.1879	20.3759	1.8592	32.1545	2.8721
2	1	0	1	2.87925	0.12063	0.18559	0.03444	0.17366	0.03016	10.6953	21.3907	3.5980	33.4585	2.7418
3	1	0	1	2.74740	0.13248	0.19449	0.03783	0.18199	0.03312	11.2151	22.4302	5.2249	34.6228	2.6208
4	1	0	1	2.62488	0.14514	0.20357	0.04144	0.19048	0.03628	11.7459	23.4917	6.7478	35.6668	2.5087
5	1	0	1	2.51106	0.15859	0.21280	0.04528	0.19912	0.03965	12.2864	24.5728	8.1746	36.6000	2.4047
0	1	1	1	2.40592	0.17276	0.22210	0.04933	0.20782	0.04319	12.8323	25.6645	45.0000	22.7674	2.3089
-1	1	1	1	2.51280	0.15837	0.21265	0.04522	0.19898	0.03959	12.2778	24.5555	45.0000	21.4501	2.4063
-2	1	1	1	2.62803	0.14479	0.20333	0.04134	0.19026	0.03620	11.7316	23.4632	45.0000	20.0112	2.5116
-3	1	1	1	2.75234	0.13201	0.19414	0.03769	0.18166	0.03300	11.1947	22.3894	45.0000	18.4351	2.6254
-4	1	1	1	2.88647	0.12002	0.18512	0.03427	0.17322	0.03001	10.6682	21.3365	45.0000	16.7040	2.7484
-5	1	1	1	3.03115	0.10884	0.17629	0.03108	0.16495	0.02721	10.1535	20.3071	45.0000	14.7974	2.8814
1	1	1	1	2.30669	0.18794	0.23165	0.05266	0.21676	0.04699	13.3944	26.7887	45.0000	23.9766	2.2188
2	1	1	1	2.21445	0.20392	0.24130	0.05823	0.22579	0.05098	13.9634	27.9268	45.0000	25.0895	2.1352
3	1	1	1	2.12858	0.22071	0.25104	0.06302	0.23490	0.05518	14.5388	29.0776	45.0000	26.1165	2.0576
0	0	0	2	3.10850	0.10349	0.17190	0.02555	0.16085	0.02587	9.8983	19.7966	45.0000	90.0000	2.9526
-1	0	0	2	3.26104	0.09403	0.16386	0.02685	0.15333	0.02351	9.4309	18.8619	45.0000	87.5966	3.0932
-2	0	0	2	3.42235	0.08538	0.15614	0.02438	0.14610	0.02134	8.9826	17.9653	45.0000	84.9504	3.2421
-3	0	0	2	3.59157	0.07752	0.14878	0.02214	0.13922	0.01938	8.5562	17.1124	45.0000	82.0358	3.3955
-4	0	0	2	3.76708	0.07047	0.14185	0.02012	0.13273	0.01762	8.1548	16.3095	45.0000	78.8273	3.5609
-5	0	0	2	3.94631	0.06421	0.13540	0.01833	0.12670	0.01605	7.7820	15.5641	45.0000	75.3015	3.7270
1	0	0	2	2.96506	0.11375	0.18022	0.03248	0.16863	0.02844	10.3823	20.7647	45.0000	87.8149	2.8205
2	0	0	2	2.83068	0.12480	0.18877	0.03563	0.17664	0.03120	10.8811	21.7621	45.0000	95.8251	2.6972

TABLE IV. Symbolic Program Listing

```

PROGRAM B1A7
DIMENSION FS(3),INDEX(7)
DIMENSION LX(9),LA(9)
DIMENSION TXP(81),KHT(81),TX(81),UX(81),VX(81),WX(81),
1UXA(81),VXB(81),WXC(81),US(81),VS(81),WS(81),SUM1(81),
2KFH(7500),ASORT(7500),FHKL(7500),TEMP(7500)
COMMON SINTH,XL,LX,LR,NP,LA,FA,FK,FL,AS,BS,CS,COSAS,COSBS,CGSCS,
1NC,V,A,R,C,BCMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP,
2ACJP,ADJC,KSORT,FHKL,TEMP,ISA,KSA,LSA,D,SUM,SINTHS,SINTL,SQTLS,
3THETA,TWOTH,PHI,CHI,SLP,TXP,KHT,SUM1,KFH,UXA,VXB,WXC,NB1,NE1,KXP,
4OUTPUT,US,VS,WS,SWAS,SWBS,SWCS,WON,NNN,ASORT,I,FS
501 FORMAT(72H
1
502 FORMAT(1H1)
503 FORMAT(8F9.0)
504 FORMAT(819)
505 FORMAT(21I1,2F9.0)
506 FORMAT(10A10 ALPHA BETA GAMMA A B
X C LAMBDA
507 FORMAT(6F10.5, F10.6 )
508 FORMAT(3H0 C,7X,1HT,11X,1HU,11X,1HV,11X,1HW,10X,2HU*,
110X,2HV*,10X,2HW*)
509 FORMAT(13,7F12.5)
510 FORMAT(*0 HKL OKL HOL HKO HHL HOC OKO OOL HHO PHI CHI COR NCT -
1KL H-L --L HK- -K- H-- --- ADJPHI ADJCHI T-MAX FINALH FINALK FI
2NALL*)
511 FORMAT(20(3X,1I1),1X,2F8.2,4F7.0)
512 FORMAT(94H0 V CCSA* COSB* CGSG*
X A* B* C*)
513 FORMAT(F16.5,6F13.6)
514 FORMAT(*0 C H K L D 1/DSQ SINTH SINTHS
1 SINTL SQTLS THETA D 2THETA PHI CHI L-LP*)
515 FORMAT(*0 C H K L D 1/CSQ SINTH SINTHS
1 SINTL SQTLS THETA D 2THETA *)
516 FORMAT(*0 C H K L D 1/CSQ SINTH SINTHS
1 SINTL SQTLS THETA D 2THETA L-LP *)
NNN=0
100 READ(60,501)
IF(EOF,60)400,102
102 CONTINUE
WRITE(61,502)
WRITE(61,501)
READ(60,503)WAD,WBD,WCD,A,B,C,XL
READ(60,503)OUTPUT,FINAL,TMAX,FINALH,FINALK,FINALL,SORTK,UVW
IF(FINAL-1.)104,106,104
104 TMAX=90.
106 WCN=TMAX/57.2957795
KSORT=SCRTK
TX(1)=0.
UX(1)=0.
VX(1)=0.
WX(1)=0.
US(1)=0.
VS(1)=0.
WS(1)=0.
IF(UVW)114,115,110
110 NUW=UVW
READ(60,503)(UX(I),VX(I),WX(I),TX(I),I=1,NUW)
GC TO 115
114 NUW=ABSF(UVW)
READ(60,503)(US(I),VS(I),WS(I),TX(I),I=1,NUW)
115 CONTINUE
READ(60,505)LR,(LX(I),I=1,9),NP,NC,LP,NCT,(INDEX(I),I=1,7),ADJP,
1ADJC
WRITE(61,506)
WRITE(61,507)WAD,WBD,WCD,A,B,C,XL
NUW1=NUW+1
NW1=NUW*2
NW=NW1+1
NE1=NW
NB1=1
NA=0
WA = WAD/57.2957795
WB = WBD/57.2957795
WC = WCD/57.2957795
CWA = COSF(WA)
CWB = COSF(WB)
CWC = COSF(WC)
SWA = SINF(WA)
SWB = SINF(WB)
SWC = SINF(WC)
BCMA=CWB*CWC-CWA
CAMB=CWC*CWA-CWB
ABMC=CWA*CWB-CWC
CGSAS=BCMA/(SWB*SWC)
COSBS=CAMB/(SWC*SWA)
CCSCS=ABMC/(SWA*SWB)
V = A*B*C*SQRTF(1.0+2.0*CWA*CWB*CWC-CWA*CWA-CWB*CWB-CWC*CWC)

```

TABLE IV (Contd.)

```

AS = B*C*SWA/V
BS = A*C*SWB/V
CS = A*B*SWC/V
SWAS=1./(B*BS*SWC)
SWBS=1./(A*AS*SWC)
SWCS=1./(A*AS*SWB)
TXP(1)=0.
KHT(1)=0.
UXA(1)=0.
VXB(1)=0.
WXC(1)=0.
IF(UVW)116,126,118
116 DO 117 I=1,NUVW
    UX(I)=A*AS*(US(I)+VS(I)*COSCS+WS(I)*COSBS)
    VX(I)=B*BS*(US(I)*COSCS+VS(I)+WS(I)*COSAS)
117 WX(I)=C*CS*(US(I)*COSBS+VS(I)*COSAS+WS(I))
    GO TO 120
118 DO 119 I=1,NUVW
    US(I)=AS*A*(UX(I)+VX(I)*CWC+WX(I)*CWB)
    VS(I)=BS*B*(UX(I)*CWC+VX(I)+WX(I)*CWA)
119 WS(I)=CS*C*(UX(I)*CWB+VX(I)*CWA+WX(I))
120 WRITE(61,508)
    WRITE(61,509)(I,TX(I),UX(I),VX(I),WX(I),US(I),VS(I),WS(I),
    I=1,NUVW)
    DO 124 I=2,NUVW1
        I1=I-1
        I2=I+NUVW
        TXP(I)=-TX(I1)
        TXP(I2)=TX(I1)
        KHT(I)=-I1
        KHT(I2)=I1
        UXA(I)=UX(I1)/A
        UXA(I2)=UXA(I)
        VXB(I)=VX(I1)/B
        VXB(I2)=VXB(I)
        WXC(I)=WX(I1)/C
        WXC(I2)=WXC(I)
        US(I)=US(I1)
        US(I2)=US(I)
        VS(I)=VS(I1)
        VS(I2)=VS(I)
        WS(I)=WS(I1)
        WS(I2)=WS(I)
124 CONTINUE
126 CONTINUE
    WRITE(61,510)
    WRITE(61,511)(LX(I),I=1,9),NP,NC,LP,NCT,(INDEX(I),I=1,7),ADJP,
    1ADJC,TMAX,FINALH,FINALK,FINALL
    CALL SUBRT
    WRITE(61,512)
    WRITE(61,513)V,COSAS,COSBS,COSCS,AS,BS,CS
132 IF(NP)400,132,134
134 IF(LP)400,136,138
    WRITE(61,514)
    GO TO 140
136 WRITE(61,515)
    GO TO 140
138 WRITE(61,516)
140 FS(1)=1.
    FS(2)=1.
    FS(3)=1.
    FS1=0.
    FS2=0.
    FS3=0.
    WON=SINF(WON)
    I=0
190 FH=FS1
    IF(FINAL-1.)220,220,200
200 FL=FS3
201 FK=FS2
203 CALL HKL
    FH=FH+1.0
    IF(FH-FINALH)203,203,204
204 FK=FK+1.0
202 FH=FS1
    IF(FK-FINALK)203,203,205
205 FL=FL+1.0
    IF(FL-FINALL)201,201,206
206 GO TO 234
220 FK=FS2
    FL=FS3
222 CALL HKL
    IF(NNN)226,224,226
224 FH=FH+1.0
    GO TO 222
226 FK=FK+1.0
    FH=FS1
    CALL HKL
    IF(NNN)228,224,228
228 FH=FS1
    FK=FS2
    FL = FL + 1.0

```

TABLE IV (Contd.)

```

CALL HKL
IF(NNN)230,224,230
230 FH=FH+1.
CALL HKL
IF(NNN)232,224,232
232 FH=FS1
FK.=FK + 1.0
CALL HKL
IF(NNN)234,224,234
234 NA=NA+1
FS1=0.
FS2=0.
FS3=0.
GO TO (241,243,245,247,249,251,253,260),NA
241 IF(INDEX(1))242,234,242
242 FS(1)=-1.
FS(2)=1.0
FS(3)=1.0
FS1=1.
GO TO 190
243 IF(INDEX(2))244,234,244
244 FS(1)= 1.
FS(2)=-1.0
FS(3)=1.0
FS2=1.
GO TO 190
245 IF(INDEX(3))246,234,246
246 FS(1)=-1.
FS(2)=-1.0
FS(3)=1.0
FS1=1.
FS2=1.
GO TO 190
247 IF(INDEX(4))248,234,248
248 FS(1)= 1.
FS(2)=1.0
FS(3)=-1.0
FS3=1.
GO TO 190
249 IF(INDEX(5))250,234,250
250 FS(1)=-1.
FS(2)=1.0
FS(3)=-1.0
FS1=1.
FS3=1.
GO TO 190
251 IF(INDEX(6))252,234,252
252 FS(1)= 1.
FS(2)=-1.0
FS(3)=-1.0
FS2=1.
FS3=1.
GO TO 190
253 IF(INDEX(7))254,234,254
254 FS(1)=-1.
FS(2)=-1.0
FS(3)=-1.0
FS1=1.
FS2=1.
FS3=1.
GO TO 190
260 IF(KSORT)100,100,300
300 N=1
CALLSORT (ASORT,TEMP,N,KSORT)
GO 320 I=1,N
FS(1)=1.0
FS(2)=1.0
FS(3)=1.0
I=I
IS=MOD F(ASORT(I),10000.0)
FH=MOD F(FHKL(IS), 512.0)
FHKL(IS)=(FHKL(IS)-FH)/ 512.0
FK=MOD F(FHKL(IS), 512.0)
FL=(FHKL(IS)-FK)/ 512.0-256.0
FK=FK-256.0
FH=FH-256.0
NB1=KFH(IS)
NE1=NB1
IF(FH)306,308,308
306 FS(1)=-1.
FH=-FH
308 IF(FK)310,312,312
310 FS(2)=-1.
FK=-FK
312 IF(FL)314,320,320
314 FS(3)=-1.
FL=-FL
320 CALL HKL1
GO TO 100
400 CALL EXIT
END

```

TABLE IV, (Contd.)

```

SUBROUTINE HKL
  DIMENSION FS(3)
  DIMENSION LX(9),LA(9)
  DIMENSION TXP(81),KHT(81),TX(81),UX(81),VX(81),WX(81),
1 UXA(81),VXB(81),WXC(81),US(81),VS(81),WS(81),SUM1(81),
2 KFH(7500),ASORT(7500),FHKL(7500),TEMP(7500)
  COMMON SINTH,XL,LX,LB,NP,LA,FH,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,
1 NC,V,A,B,C,BCMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP,
2 ADJP,ADJC,KSORT,FHKL,TEMP,ISA,KSA,LSA,D,SUM,SINTHS,SINTL,SOTLS,
3 THETA,TWOTH,PHI,CHI,SLP,TXP,KHT,SUM1,KFH,UXA,VXB,WXC,NB1,NE1,KXP,
4 OUTPUT,US,VS,WS,SWAS,SWBS,SWCS,WON,NNN,ASORT,I,FS
501 FORMAT(4I4,6F10.5,2F10.4)
502 FORMAT(4I4,6F10.5,3F10.4)
503 FORMAT(2I4,2I3,6F10.5,5F10.4)
  NNN=0
  FHS = FS(1)*FH
  FKS = FS(2)*FK
  FLS = FS(3)*FL
  SUM = (FHS*AS)**2 + (FKS*BS)**2 + (FLS*CS)**2 + 2.0*(FKS*FLS*BS*CS*
1 COSAS + FHS*FLS*CS*AS*COSBS + FHS*FKS*AS*BS*COSCS)
  NCN=0
  DO 190 J=NB1,NE1
    SUM1(J)=SUM+TXP(J)**2+2.0*(FHS*UXA(J)+FKS*VXB(J)+FLS*WXC(J))*TXP(J)
    SINTH=SQRT(SUM1(J)/4.)*XL
    IF(SINTH-WON)190,190,182
182 IF(NB1-NE1)186,184,184
184 NNN=1
    GO TO 600
186 NCN=NCN+1
    IF(NCN-NE1)190,184,184
190 CONTINUE
    IF(NCT-1)198,192,196
192 IF(FH-FK)600,194,194
194 IF(FK-FL)600,198,198
196 IF(FH-FK)600,198,198
198 CONTINUE
    DO 200 J=1,9
200 LA(J)=0
    IF(LB)420,420,301
301 LA(1)=1
    IF(FHS)303,302,303
302 LA(2)=1
303 IF(FKS)305,304,305
304 LA(3)=1
305 IF(FLS)307,306,307
306 LA(4)=1
307 IF(FHS-FKS)309,308,309
308 LA(5)=1
309 IF(FLS)312,310,312
310 IF(FKS)312,311,312
311 LA(6)=1
312 IF(FLS)315,313,315
313 IF(FHS)315,314,315
314 LA(7)=1
315 IF(FKS)318,316,318
316 IF(FHS)318,317,318
317 LA(8)=1
318 IF(FLS)321,319,321
319 IF(FHS-FKS)321,320,321
320 LA(9)=1
321 CONTINUE
    DO 400 J=1,9
    IF(LX(J))352,400,352
352 IF(LA(J))353,400,353
353 AH=FHS
    BH=FKS
    CH=FLS
    TH=2.
354 GO TO (361,362,363,364,365,366,367,368,369),J
361 GO TO (371,372,373,374,375,376,377),LX(J)
362 GO TO (372,373,371,378),LX(J)
363 GO TO (372,374,371,378),LX(J)
364 GO TO (373,374,371,378),LX(J)
365 GO TO (379,380,373,378),LX(J)
366 GO TO (371,378),LX(J)
367 GO TO (371,378),LX(J)
368 GO TO (371,377,378,381),LX(J)
369 GO TO 373
371 GO TO 390
372 CH=0.
    GO TO 390
373 BH=0.
    GO TO 390
374 AH=0.
    GO TO 390
375 AH=FHS+FKS
    BH=FHS+FLS
    CH=FKS+FLS

```

TABLE IV (Contd.)

```

GO TO 390
376 AH=-FHS
TH=3.
GO TO 390
377 TH=3.
GO TO 390
378 TH=4.
GO TO 390
379 AH=0.
BH=0.
GO TO 390
380 AH=0.
CH=0.
GO TO 390
381 TH=6.
GO TO 390
390 A7=ABSF(AH+BH+CH)
IF(A7)600,400,392
392 IF(A7-TH)600,400,394
394 A7=A7-TH
GO TO 392
400 CONTINUE
420 CONTINUE
IF(KSORT)450,450,423
423 CONTINUE
DO 440 J=NB1,NE1
SUM1(J)=SUM+TXP(J)**2+2.*(FHS*UXA(J)+FKS*VXB(J)+FLS*WXC(J))*TXP(J)
SQTLS=SUM1(J)/4.0
SINTL=SQRTF(SQTLS)
SINTH=SINTL*XL
IF(SINTH-WON)430,430,440
430 I=I+1
IF(I-7500)432,432,600
432 FHKL(I)=262144.*FLS+512.*FKS+FHS+67240192.
SOM=SUM1(J)
ASORT(I)=10000.0*INTF(50000.0*SOM)+FLOATF(I)
KFH(I)=J
440 CONTINUE
GO TO 600
ENTRY HKL1
FHS=FS(1)*FH
FKS=FS(2)*FK
FLS=FS(3)*FL
SUM = (FHS*AS)**2 + (FKS*BS)**2 + (FLS*CS)**2 +2.0*(FKS*FLS*BS*CS*
1COSAS +FHS*FLS*CS*AS*COSBS + FHS*FKS*AS*BS*COSCS)
450 CONTINUE
DO 498 J=NB1,NE1
SUM1(J)=SUM+TXP(J)**2+2.*(FHS*UXA(J)+FKS*VXB(J)+FLS*WXC(J))*TXP(J)
SQTLS=SUM1(J)/4.0
SINTL=SQRTF(SQTLS)
SINTH=SINTL*XL
IF(KSORT)452,452,459
452 IF(SINTH-WON)459,459,498
459 CONTINUE
ASH=AS*FHS+TXP(J)*US(J)
BSK=BS*FKS+TXP(J)*VS(J)
CSL=CS*FLS+TXP(J)*WS(J)
SINTHS=SINTH*SINTH
SLP=0.
CHI=0.
KXP=KHT(J)
D=1./SQRTF(SUM1(J))
THETA=ASINF(SINTH)
TWO TH=THETA*2.0
SN2TH = SIN(TWO TH)
IF(LP)468,468,460
460 GO TO(461,462,463,464,465,466),LP
461 SLP=1./SN2TH
GO TO 468
462 SLP=1./(SINTHS*2.*COSF(THETA))
GO TO 468
463 SLP=(1.0+COSF(TWO TH)**2)/(SINTHS*COSF(THETA))
GO TO 468
464 COSQMU=1.-((FH*XL)/(2.*A))**2
GO TO 467
465 COSQMU=1.-((FK*XL)/(2.*B))**2
GO TO 467
466 COSQMU=1.-((FL*XL)/(2.*C))**2
467 SLP = (2.0-SN2TH*SN2TH)*SINTH/(SN2TH*SQRTF(COSQMU+SINTHS-1.0))
468 CONTINUE
IF(NP)480,480,470
470 GO TO(471,472,473,474,475,476),NP
471 DNOM=(BSK*SWCS-CSL*CWA*SWBS)
DNOM= (ASH+BSK*COSCS+CSL*COSBS)
GO TO 477
472 DNOM=(ASH*SWCS-CSL*CWB*SWAS)
DNOM= (BSK+ASH*COSCS+CSL*COSAS)
GO TO 477
473 DNOM=(ASH*SWBS-BSK*CWC*SWAS)
DNOM= (CSL+ASH*COSBS+BSK*COSAS)
GO TO 477
474 DNOM=(CSL*SWCS-BSK*CWA*SWCS)

```


TABLE IV (Contd.)

```

      DNOM= (ASH+CSL*COSBS+BSK*COSCS)
      GO TO 477
475 DNUM=(CSL*SWAS-ASH*CWB*SWCS)
      DNOM= (BSK+CSL*COSAS+ASH*COSCS)
      GO TO 477
476 DNUM=(BSK*SWAS-ASH*CWC*SWBS)
      DNOM= (CSL+BSK*COSAS+ASH*COSBS)
477 DNM=DNUM/DNOM
      PHI=ATANF(DNM)*57.2957795
      PHI=PHI+ADJP
      IF(PHI)478,479,479
478 PHI=PHI+180.
      IF(PHI.GT.179.998) PHI=0.0
479 IF(NC)490,490,480
480 GO TO(481,482,483),NC
481 SNCC=CSL*D*SWA*SWBS
      GO TO 484
482 SNCC=BSK*D*SWC*SWAS
      GO TO 484
483 SNCC=ASH*D*SWB*SWLS
484 IF(ABSF(SNCC)-1.)486,486,485
485 SNCC=SIGNF(1.,SNCC)
486 CHI=ASINF(SNCC)*57.2957795
      IF(CHI)487,488,488
487 CHI=CHI+360.
488 CHI=CHI+ACJC
490 ISA=FHS
      KSA = FKS
      LSA = FLS
      THETA=THETA*57.2957795
      TWOTH = THETA*2.0
      IF(NP)491,491,494
491 IF(LP)492,492,493
492 WRITE(61,501)KXP,ISA,KSA,LSA,D,SUM1(J),SINTH,SINTHS,SINTL,
1SCTLS,THETA,TWOTH
      GO TO 495
493 WRITE(61,502)KXP,ISA,KSA,LSA,D,SUM1(J),SINTH,SINTHS,SINTL,
1SQTLS,THETA,TWOTH,SLP
      GO TO 495
494 WRITE(61,503)KXP,ISA,KSA,LSA,D,SUM1(J),SINTH,SINTHS,SINTL,
1SCTLS,THETA,TWOTH,PHI,CHI,SLP
495 CALL SUBRT
498 CONTINUE
600 RETURN
      END

```

```

C      SUBROUTINE SORT (A,TEMP,N,MODE)
      ALGEBRAIC SORT---SUBROUTINE SORT
      DIMENSION A(1), TEMP(1)
      N2HALF=1
10  N2=N2HALF+N2HALF
      IF (N2HALF-N) 20, 140, 140
20  NREM=XMODF(N,N2)
      N1=N-NREM
      IF (N1) 60, 60, 40
40  DO 50 I=1,N1,N2
      I1=I+N2HALF
50  CALL MERGE (A(I),N2HALF,A(I1),N2HALF,TEMP(I),MODE)
60  NREM1=NREM-N2HALF
      NLIMIT=N1
      IF (NREM1) 100, 100, 75
75  NLIMIT=N
      I1=N1+N2HALF
      CALL MERGE (A(N1+1),N2HALF,A(I1+1),NREM1,TEMP(N1+1),MODE)
100 DO 110 I=1,NLIMIT
110 A(I)=TEMP(I)
      N2HALF=N2HALF+N2HALF
      GO TO 10
140 RETURN
      END

```

TABLE IV (Contd.)

```

C      SUBROUTINE MERGE (JX,J,KX,K,LX,MODE)
      ALGEBRAIC SCRT---SUBROUTINE MERGE
      DIMENSION JX(1), KX(1), LX(1)
      L=J+K
      J1=1
      K1=1
      CO 130 L1=1,L
      IF (J1-J) 40, 40, 110
40    IF (K1-K) 50, 50, 80
50    GO TO (60,70), MODE
60    IF (KX(K1)-JX(J1)) 110, 110, 80
70    IF (KX(K1)-JX(J1)) 80, 80, 110
80    LX(L1)=JX(J1)
      J1=J1+1
      GO TO 130
110   LX(L1)=KX(K1)
      K1=K1+1
130   CONTINUE
      RETURN
      END

      SUBROUTINE SUBRT
      DIMENSION FS(3)
      DIMENSION LX(9),LA(9)
      DIMENSION TXP(81),KHT(81),TX(81),UX(81),VX(81),WX(81),
1    UXA(81),VXR(81),WXC(81),US(81),VS(81),WS(81),SUM1(81),
2    KFH(7500),ASORT(7500),FHKL(7500),TEMP(7500)
      COMMON SINTH,XL,LX,LB,NP,LA,FK,FL,AS,BS,CS,COSAS,COSBS,COSCS,
1    INC,V,A,B,C,ECMA,CAMB,ABMC,CWA,CWB,CWC,SWA,SWB,SWC,LP,NCT,ALPHAP,
2    ADJP,ADJC,KSORT,FHKL,TEMP,ISA,KSA,LSA,D,SUM,SINTHS,SINTL,SGTLS,
3    THETA,TWOTH,PHI,CHI,SLP,TXP,KHT,SUM1,KFH,UXA,VXB,WXC,NB1,NE1,KXP,
4    OUTPUT,US,VS,WS,SWAS,SWBS,SWCS,WON,NNN,ASORT,I,FS
501  FORMAT(8F9.0)
502  FORMAT(*0 PALPHA 2THETA-MAX 2THETA-MIN PBETA PGAM
1    MA PCDELTA STEP*)
503  FORMAT(6F12.2,I8)
504  FORMAT(1HE,I3,3I3,1HE,4(I5,1HE),2H11,I2,1HE,I5,1HE)
      IF(OUTPUT-1.120,2,3)
2    READ(60,501)ALPHA,TTPTAM,TTMIN,BETA,GAMMA,DELTA,STEP
      NSTEP=STEP
      OUTPUT=OUTPUT+1.
      WRITE(61,502)
      WRITE(61,503)ALPHA,TTPTAM,TTMIN,BETA,GAMMA,DELTA,NSTEP
      NSTEP=NSTEP+100
      PHI=0.
      CHI=0.
      GO TO 20
3    IF(TWOTH-TTPTAM)4,4,20
4    IF(TWOTH-TTMIN)20,5,5
5    TTPB=TWOTH+BETA
      IH=ISA+1000
      IK=KSA+1000
      IL=LSA+1000
      PHI=PHI+GAMMA
      CHI=CHI+DELTA
      TPA=THETA+ALPHA
      TTMB=TWOTH-BETA
      IF(PHI)6,7,7
6    PHI=PHI+360.0
7    IF(CHI)8,9,9
8    CHI=CHI+360.
9    IF(TPA)10,11,11
10   TPA=TPA+360.0
11   IF(TTMB)12,13,13
12   TTMB=TTMB+360.0
13   IF(TTPB)14,15,15
14   TTPB=TTPB+360.0
15   CONTINUE
      KPHI=100000.+100.*PHI+.5
      KCHI=100000.+100.*CHI+.5
      KTPA=100000.+100.*TPA+.5
      KTMB=100000.+100.*TTMB+.5
      KTPB=100000.+100.*TTPB+.5
      WRITE(62,504)KXP,IH,IK,IL,KCHI,KPHI,KTPA,KTMB,NSTEP,KTPB
20   RETURN
      END

```

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REFERENCES

1. Atoji, M., A Multipurpose Neutron Diffractometer, ANL-6920 (1964).
2. Atoji, M., Crystal Structure of Y_3C (to be published).
3. Atoji, M., Graphical Representation of Magnetic Space Groups, Am. J. Phys. 33, 212 (1965).
4. Atoji, M., Magnetic Structure of TbC_2 (to be published).
5. Atoji, M., Multipurpose Neutron-diffraction Instrumentations, Nucl. Instr. Methods 35, 13 (1965).
6. Atoji, M., and Lipscomb, W. N., The X-ray Scattering from a Hindered Rotator III, Acta Cryst. 7, 726 (1954).
7. Atoji, M., Watanabe, T., and Lipscomb, W. N., The X-ray Scattering from a Hindered Rotator II, Acta Cryst. 6, 62 (1953).
8. Bacon, G. E., Neutron Diffraction, 2nd. ed., Clarendon Press, Oxford (1962).
9. Fujime, S., Watanabe, D., and Ogawa, S., The Intensity of Satellite Reflections in Electron Diffraction Patterns from Evaporated Alloy Films with CuAu II Type Superstructure, J. Phys. Soc. Japan 19, 1881 (1964).
10. Fujiwara, K., On the Period of Out-of-Step of Ordered Alloys with Anti-phase Domain Structure, J. Phys. Soc. Japan 12, 7 (1957).
11. Hastings, J. M., and Corliss, L. M., Magnetic Structure of Manganese Chromite, Phys. Rev. 126, 556 (1962).
12. Hirabayashi, M., and Ogawa, S., On the Superstructure of the Ordered Alloy Cu_3Pd II. X-ray Diffraction Study, J. Phys. Soc. Japan 12, 259 (1957).
13. James, R. W., The Optical Principles of the Diffraction of X-rays, G. Bell and Sons, London (1950).
14. Koehler, W. C., Magnetic Properties of Rare-Earth Metals and Alloys, J. Appl. Phys. 36, 1078 (1965).
15. Koehler, W. C., Neutron Diffraction by Helical Spin Structures, Acta Cryst. 14, 535 (1961).
16. Mueller, M. H., Meyer, E. F. H., and Simonsen, S. H., Crystallographic D-space Computer Program, ANL-6519 (1962).
17. Owston, P. G., Diffuse Scattering of X-rays by Ice, Acta Cryst. 2, 222 (1949).
18. Sato, H., and Toth, R. S., Long-period Superlattices in Alloys. II, Phys. Rev. 127, 469 (1962).

19. Watanabe, D., Hirabayashi, M., and Ogawa, S., On the Superstructure of the Alloy Cu_3Pd , Acta Cryst. 8, 510 (1955).
20. Watanabe, D., and Ogawa, S., On the Superstructure of the Ordered Alloy Cu_3Pd , I. Electron Diffraction Study, J. Phys. Soc. Japan 11, 226 (1956).
21. Willis, B. T. M., Use of a Two-circle Device to Obtain Three-dimensional Neutron Diffraction Data, AERE-R-3308 (1960).
22. Wooster, W. A., Diffuse X-ray Reflections from Crystals, Clarendon Press, Oxford (1962).
23. Yamaguchi, S., Watanabe, D., and Ogawa, S., Study on Anti-phase Domains in Cu_3Au by Means of Electron Diffraction and Electron Microscopy, J. Phys. Soc. Japan 17, 1030 (1961).