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LOS ALAMOS SCIENTIFIC LABORATORY
LOS ALAMOS of the NEW MEXICO
University of California

**An Integrated Series of Crystallographic
Computer Programs
VIII. Thermal Ellipsoid Orientation**

APPROVED FOR PUBLIC RELEASE

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An Integrated Series of Crystallographic
Computer Programs
VIII. Thermal Ellipsoid Orientation

by

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Abstract

The procedures employed and the computer program used for determining the principal axes and the orientation of anisotropic thermal ellipsoids relative to crystallographic axes are described. This information is often useful in correlating the thermal vibrations of the atoms of a single crystal with its various other physical properties.

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Introduction to the Series of Reports

The program described in this report is one of an integrated series of crystallographic computer programs. This series encompasses the entire subject of single-crystal structure analysis and includes programs for such items as:

- (1) crystal orientation for the collection of intensity data
- (2) processing of collected data to allow correction for Lorentz-polarization, absorption, background, and crystal-shape effects
- (3) comparison of processed data over equivalent reflections to ascertain the general validity of the data and to obtain a set of relative F^2 (F has the conventional structure factor meaning)
- (4) a Fourier series analysis coupled with a plotting routine for obtaining Patterson vector maps and electron density maps of the Fourier and difference Fourier types
- (5) a least-squares procedure for determining the positions and thermal motions (isotropic and/or anisotropic) of the atoms in a single crystal
- (6) various subroutines (two per space group) for the least-squares procedure

(7) miscellaneous procedures employed during and after a structure analysis, e. g., calculation of interatomic distances and angles, of the orientation relationship of thermal ellipsoid axes to the crystallographic axes of the crystal, and of the polyhedral coordination of atoms; and the ordering of calculated and observed structure factors to prepare tables for publication.

Since each of the above items involves many repetitious procedures and calculations, it has been the authors' philosophy to employ computer techniques wherever possible and as early in the process of a structure determination as it is feasible to do so. Following this philosophy greatly reduces manual labor, minimizes clerical errors, and allows the maximum information to be obtained from the data.

Introduction to the Present Report

One of the products of a general least-squares determination of a crystal structure may be the description of the anisotropic thermal motion of an atom. This motion is characterized by six parameters B_{ij} ($i, j = 1$ to 3) of a vibration ellipsoid and is given by

$$T = \exp \left[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl) \right]$$

It is often useful in making a complete analysis of a crystal structure to determine from the B_{ij} parameters the principal axes of the thermal ellipsoid and the orientation of these axes relative to the crystallographic

axes. This report gives a listing of these quantities and describes the use of a FORTRAN II program for their calculations.

The operating deck consists of a general program, BIJ, and two subroutines, ASIN and UNLOAD. A listing of BIJ is given in a later section of this report. ASIN and UNLOAD are listed and described in the first report of this series (IA-2974).

Three modes of operation are available for BIJ. Our least-squares program GENLES (IA-3259) may have prepared an input magnetic tape, tape 3 (B3). If this is the case (and normally it is), then no data or control cards are necessary. BIJ and tape 3 (B3) are processed through the Monitor system with BIJ obtaining all needed information from tape 3 (B3).

The following is a description of the complete Monitor deck:

* I.D. (Monitor Identification Card)

* XEQ (Monitor Card)

Binary Cards for BIJ

Binary Cards for ASIN

Binary Cards for UNLOAD

} from a compilation
of
FORTRAN II
and FAP programs

END OF JOB (Monitor Card)

The second mode of operation is card input which requires a computer self-run on line. The following is a description of the complete self-run deck:

START Card (General Designation)

* I.D.

* XEQ

Binary Cards for BIJ	}	from
Binary Cards for ASIN		a compilation
Binary Cards for UNLOAD		of
		FORTRAN II
		and FAP programs
END OF JOB Card		
END TAPE Card		
END CARD READER Card (Contains 8,9 punch in column #1)		
Experimental Data Cards		
Two Blank Cards		

For the on-line self run, Sense Switch 1 must be ON. This also provides an on-line listing of the results of the BIJ calculations.

The third mode of operation is a mixture of tape and card input and again requires a computer self-run on line with Sense Switch 1 ON and use of tape 3 (B3). The operating deck is identical with the one for card input exclusively, and information from tape 3 (B3) is obtained through control characters on the data cards.

Mathematical Equations

The problem treated by the computer program described in this report is the calculation of the principal axes and the orientation of the thermal vibration ellipsoid relative to the axes of a unit cell.

We start the calculation by defining an orthonormal reference system, having axes X Y Z, as

$$X = x\underline{a} + y\underline{b} \cos \gamma + z\underline{c} \sin \beta \quad (1)$$

$$Y = 0 + y\underline{b} \sin \alpha^* \sin \gamma + 0 \quad (2)$$

$$Z = 0 - y\underline{b} \cos \alpha^* \sin \gamma + z\underline{c} \sin \beta \quad (3)$$

where x, y, z is an arbitrary point in space in a unit cell described by the usual crystallographic quantities $\underline{a}, \underline{b}, \underline{c}, \alpha, \beta$, and γ . The orthonormal system is related to a triclinic unit cell by having X coincident with $\underline{a}$, Y perpendicular to the plane formed by $\underline{a}$ and $\underline{c}$, and Z lying in the plane defined by $\underline{a}$ and $\underline{c}$. For a monoclinic unit cell, Y is coincident with $\underline{b}$ whereas in a hexagonal unit cell Y makes an angle of 30° with $\underline{b}$. For orthorhombic, tetragonal, and cubic-unit cells, the axes of the orthonormal system are coincident with the usual crystallographic axes.

The anisotropic thermal motion of an atom is given by

$$T = \exp \left[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl) \right] \quad (4)$$

The terms B_{ij} represent the projection of the principal axes of the thermal vibration ellipsoid on (the axes and planes of) a reference system.

Let the three principal axes of the thermal vibration ellipsoid be given by q_i , ($i = 1, 2, 3$).

Let the direction cosines of these principal axes with respect to X, Y, Z of the orthonormal reference system be given by g_{ik} , ($i = 1, 2, 3$; $k = x, y, z$)

Then

$$B_{11} = \sum_i q_i^2 g_{ix}^2 x^2 \quad (5)$$

$$B_{22} = \sum_i q_i^2 g_{iy}^2 y^2 \quad (6)$$

$$B_{33} = \sum_i q_i^2 g_{iz}^2 z^2 \quad (7)$$

$$B_{12} = \sum_i 2q_i^2 g_{ix} g_{iy} x \cdot y \quad (8)$$

$$B_{13} = \sum_i 2q_i^2 g_{ix} g_{iz} x \cdot z \quad (9)$$

$$B_{23} = \sum_i 2q_i^2 g_{iy} g_{iz} y \cdot z \quad (10)$$

The principal axes q_i and the direction cosines g_{ik} are extracted from the parameters, B_{ij} , in the following manner.

A tensor of the second rank, $\underline{\underline{B}}$, is formed from the B_{ij} parameters

$$\underline{\underline{B}} = \begin{pmatrix} B_{11} & \frac{B_{12}}{2} & \frac{B_{13}}{2} \\ \frac{B_{12}}{2} & B_{22} & \frac{B_{23}}{2} \\ \frac{B_{13}}{2} & \frac{B_{23}}{2} & B_{33} \end{pmatrix} \quad (11)$$

This is operated on by the matrix $\underline{\underline{A}}$, (obtained from Eqs. (1), (2), and (3))

$$\underline{\underline{A}} = \begin{pmatrix} a & b \cos \gamma & c \sin \beta \\ 0 & b \sin \alpha^* \sin \gamma & 0 \\ 0 & -b \cos \alpha^* \sin \gamma & c \sin \beta \end{pmatrix} \quad (12)$$

and its transpose $\underline{\underline{A}}^T$, to yield another tensor, $\underline{\underline{U}}$,

$$\underline{\underline{U}} = \underline{\underline{A}}^T \underline{\underline{B}} \underline{\underline{A}} \quad (13)$$

$\underline{\underline{U}}$ is $\underline{\underline{B}}$ placed in the orthonormal reference system and is a 3 x 3 array.

$\underline{\underline{U}}$ is operated on by a rotation matrix, $\underline{\underline{C}}$, and its transpose, $\underline{\underline{C}}^T$, to yield a diagonal matrix, $\underline{\underline{D}}$

$$\underline{\underline{D}} = \underline{\underline{C}}^T \underline{\underline{U}} \underline{\underline{C}} \quad (14)$$

The diagonal elements of $\underline{\underline{D}}$, D_{ii} , are of the form

$$D_{ii} = 8 \pi^2 \bar{\mu}_i^2 \quad (15)$$

where $\bar{\mu}_i^2$ is the mean square amplitude of vibration along the i'th principal direction and $q_i = \sqrt{\bar{\mu}_i^2}$. All off-diagonal elements D_{ij} ($i \neq j$) are 0. The direction cosines g_{ik} are found in the i'th column and k'th row of the rotation matrix $\underline{\underline{C}}$.

The method used for the calculation of matrices $\underline{\underline{D}}$ and $\underline{\underline{C}}$ from $\underline{\underline{U}}$ is that given by Booth.* It consists (in n-dimensional space) of a series

* Numerical Methods, Booth, A. D., Academic Press Inc., New York, 1955.

of simple rotations about one axis (one dimension) at a time so as to eliminate the largest off-diagonal elements one at a time. This is an iterative procedure, but it does not take very many cycles to reduce all off-diagonal elements to below the level of significance. This method has a major advantage in that it gives both $\underline{\underline{C}}$ and $\underline{\underline{D}}$ at the same time and is quite well suited to automatic computer usage.

The matrix $\underline{\underline{C}}$ is equal to the continued product of matrices $\underline{\underline{R}}$ over m , the number of iterations performed, i.e.,

$$\underline{\underline{C}}_m = \prod_{i=1}^m \underline{\underline{R}}_i \quad (16)$$

The matrix $\underline{\underline{R}}_i$ has the general form

$$\underline{\underline{R}}_i = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & 0 & \\ 0 & 0 & + \cos \alpha & 0 & + \sin \alpha & 0 & \\ 0 & 0 & 0 & 1 & 0 & 0 & \\ 0 & 0 & - \sin \alpha & 0 & + \cos \alpha & 0 & \\ 0 & 0 & 0 & 0 & 0 & 1 & \\ \vdots & & & & & & \\ \vdots & & & & & & \\ \vdots & & & & & & \end{pmatrix} \quad (17)$$

All diagonal elements are 1, and all off-diagonal elements are 0, except for those axes (dimensions) that are being rotated through angle α so as to eliminate an off-diagonal term in the $\underline{\underline{U}}$ tensor. Since in a 3×3 array there are three off-diagonal terms, we have three $\underline{\underline{R}}_i$ matrices which are for the elimination of:

the 13 element (rotation about the 22 dimension)

$$\begin{pmatrix} + \cos \alpha & 0 & + \sin \alpha \\ 0 & 1 & 0 \\ - \sin \alpha & 0 & + \cos \alpha \end{pmatrix} \quad (18)$$

the 12 element (rotation about the 33 dimension)

$$\begin{pmatrix} + \cos \alpha & + \sin \alpha & 0 \\ - \sin \alpha & + \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (19)$$

the 23 element (rotation about the 11 dimension)

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & + \cos \alpha & + \sin \alpha \\ 0 & - \sin \alpha & + \cos \alpha \end{pmatrix} \quad (20)$$

The matrix $\underline{\underline{D}}$ is the limit approached by the intermediate matrix $\underline{\underline{T}}_{\underline{\underline{i}}}$ in the series

$$\begin{aligned} \underline{\underline{T}}_1 &= \underline{\underline{R}}_1^{-1} \underline{\underline{U}} \underline{\underline{R}}_1 \\ \underline{\underline{T}}_2 &= \underline{\underline{C}}_2^{-1} \underline{\underline{U}} \underline{\underline{C}}_2 & (\underline{\underline{C}}_2 &= \underline{\underline{R}}_1 \underline{\underline{R}}_2) \\ \underline{\underline{T}}_3 &= \underline{\underline{C}}_3^{-1} \underline{\underline{U}} \underline{\underline{C}}_3 & (\underline{\underline{C}}_3 &= \underline{\underline{C}}_2 \underline{\underline{R}}_3) \\ &\vdots & \\ &\vdots & \\ \underline{\underline{D}} &= \underline{\underline{C}}_m^{-1} \underline{\underline{U}} \underline{\underline{C}}_m & (\underline{\underline{C}}_m &= \text{Eq. (16)}) \end{aligned} \quad (21)$$

The direction cosines relating the principal axes of the ellipsoid to the real lattice axes can be derived from the columns of $\underline{C}_m$ by the transformation

$$\underline{\epsilon}_i = \underline{E} \underline{C}_i \quad (22)$$

where $\underline{\epsilon}_i$ are the direction cosines of the i'th vector with respect to the real lattice vectors, $\underline{C}_i$ represents the i'th column of the matrix $\underline{C}_m$, and $\underline{E}$ represents the transformation matrix

$$\underline{E} = \begin{pmatrix} 1 & 0 & 0 \\ \cos \gamma & \sin \alpha^* \sin \gamma & -\cos \alpha^* \sin \gamma \\ \cos \beta & 0 & \sin \beta \end{pmatrix} \quad (23)$$

The evaluation of the derivatives used in this program is by numerical methods. That is

$$\frac{\partial F}{\partial \zeta_i} = \frac{F(\zeta_1, \dots, \zeta_n) - F(\zeta_1, \dots, \zeta_i + \Delta_i, \dots, \zeta_n)}{\Delta_i} \quad (24)$$

where F is the function, ζ_i is the i'th parameter, and $\Delta = B_{ij}/10000$ for our particular problem.

Glossary of Program Terms

CØR (2000) Correlation terms between all least-squares parameters read from GENLES output tape 3 (B3)

A (3,3)	Matrix used to determine the direction cosines of the principal axes of the thermal ellipsoid relative to the real lattice axes
AI (3,3)	Matrix used to convert the thermal tensor to an orthonormal system
AIT (3,3)	AI transpose
ATOM (12)	Identification of the various atoms
B (3,3)	B_{ij}
B1 (3,3)	Intermediate storage for $\underline{U} \underline{C}$
B4 (24)	Values of the various parameters to be printed
BK (1), B2 (3,3), BX (6)	Temporary storage for B_{ij}
C (3,3)	Rotation matrix
C1 (3,3), C2 (3,3)	Temporary storage for rotation matrix
D (6,6)	Correlation terms
D1 (6)	Standard deviations of B_{ij}
D3 (24,6)	Derivatives of each of the 24 output parameters with respect to each of the six B_{ij}
D4 (24)	Standard deviations of the B4 numbers
I11 (6)	Parameter number (see LA-3259) of the B_{ij}
IS (6)	Table used to keep track of symmetry-dependent B_{ij}
J2 (6)	Number of atoms of each kind
NA (12)	Problem identification from tape 3 (B3)
NAM (12)	Data set identification
NAME (12)	Problem identification
S (200)	Standard deviation read from tape 3 (B3)

X (3)	Temporary storage
AD	<u>a</u> axis
BD	<u>b</u> axis
CD	<u>c</u> axis
CA	Either α or $\cos \alpha$
CASTAR	$\cos \alpha^*$
CB	Either β or $\cos \beta$
CC	Either γ or $\cos \gamma$
CCSTAR	$\cos \gamma^*$
D36	The delta term used in the evaluation of the numerical derivatives
I1,J1	Indices of the currently largest off-diagonal element in the <u>U</u> matrix
I23	Index used to control the number of passes in the calculation of <u>D</u>
IA,IT	Bookkeeping variables used in the output
I,J,K,L	General indexing variables
MAXN	Number of parameters on tape 3 (B3)
N	Bookkeeping variable
N12	Identification of an atom as isotropic or anisotropic
N1	Number of data sets to be processed
N2	Control for input of standard deviations and correlation terms when data are read from cards
NJ	Number of types of atoms when data are read from tape 3 (B3)
SA	$\sin \alpha$

SASTAR	$\sin \alpha^*$
SB	$\sin \beta$
SC	$\sin \gamma$
SCSTAR	$\sin \gamma^*$
SS1	Control for location of data
V	Value of the largest off-diagonal element in <u>D</u>
Y	The arctan of Y1
Y1	The tangent of the angle through which the matrix is rotated to eliminate the largest off-diagonal term
Y2	$\cos^2 Y$

Data Cards and/or Tape Description

As mentioned in the Introduction to the Present Report, normal input to BIJ consists of a magnetic tape, tape 3 (B3), that has been prepared as part of our least-squares program (IA-3259).

An alternative input consists exclusively of cards that are read on-line with Sense Switch 1 ON.

Card 1: Contains the control characters N1 and N2 in I5 fields.

N1 = number of anisotropic atoms to be processed for the unit cell described on Card 3

N2 = -1, sets all standard deviations equal to 0.0;

= 0, uses standard deviation and correlation terms that are located on tape 3 (B3);

= 1, uses standard deviations and correlation terms that are on cards.

- Card 2: 72 Hollerith characters for problem identification
- Card 3: Contains the unit cell constants $a, b, c, \alpha, \beta, \gamma$ in format 6F10.5.
(Angles may be replaced by cosines if desired.)
- Card 4: 72 Hollerith characters for identification of a particular anisotropic atom data set:
- Card 5: Contains B11, B22, B33, B12, B13, B23 in format 6F10,5. (Not read if N2 = 0.)
- Card 6: If N2 = -1, Card 6 is not needed.
N2 = 0, contains the parameter number (see LA-3259) associated with each B_{ij} in format 6I5;
N2 = 1, three cards of type 6 contain the six standard deviations of B_{ij} and the fifteen correlation terms of B_{ij} in format 7F10.5. (See the Illustrative Example for proper ordering of standard deviations and correlation terms for B_{ij} .)

It should be noted that there are N1 sets of Cards 4, 5, and 6 in the input deck. Also, as intimated by Cards 1 and 6, a mixed card-tape input is possible.

Output Description

The output from BLJ consists of an off-line printout containing the following information listed in the order of its occurrence.

1. Problem identification
2. Identification of the particular atomic data set being

processed

3. The matrix of the input B_{ij} parameters
4. Unit cell constants
5. The correlation terms of the B_{ij} parameters
6. The standard deviation of the B_{ij} parameters
7. The principal axes, q_i ($i = 1$ to 3) with their standard deviations
8. The quantities B_i ($i = 1$ to 3) with their standard deviations. B_i is equal to $8\pi^2 q_i^2$, and the average B_i , $(B_1 + B_2 + B_3)/3$, is equivalent to the usual isotropic thermal parameter B .
9. The angles and standard deviations that the thermal ellipsoid axes make with the real lattice axes
10. The direction cosines of the thermal ellipsoid axes relative to the orthogonal reference system

These ten items are then repeated for each set of thermal data being processed.

Illustrative Example: Input

As an illustrative example of the use of this program we will consider the determination of the orientation of the anisotropic thermal ellipsoid for the Cu atom and the NH_3 group in the structure of $\text{CuCN} \cdot \text{NH}_3$. This structure was refined as the Illustrative Example in LA-3259. We will assume that tape 3 (B3) is not available and that input data will

be read exclusively from cards. Copper cyanide ammonia is monoclinic with $a = 5.814$, $b = 7.977$, $c = 8.193 \text{ \AA}$, and $\beta = 125.8^\circ$. The B_{ij} terms for the copper atom and the ammonia group are taken from LA-3259 and listed as follows

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Copper	0.03486	0.00826	0.01481	-0.00161	0.02733	-0.00452
Ammonia	0.02675	0.01031	0.01976	0.00146	0.02252	0.00138

The standard deviations of the B_{ij} terms are taken from the same source and are

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Copper	0.00074	0.00023	0.00035	0.00071	0.00081	0.00051
Ammonia	0.00428	0.00174	0.00234	0.00388	0.00533	0.00297

The fifteen B_{ij} correlation terms for each atom are obtained from Figure 6 of LA-3259. The correlation terms are arranged on the cards in the sequence

$(i)(j),$

$(i)(j+1), (i+1)(j+1), (i+2)(j+1), \dots$

$(i)(j+2), (i+1)(j+2), (i+2)(j+2), (i+3)(j+2), \dots$

where j is initially equal to $i+1$.

For example, the B_{ij} terms for the copper atoms are indexed as parameters (4) through (9). We can then construct the following table

		B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
(4)	B_{11}	1.0	(4)(5)	(4)(6)	(4)(7)	(4)(8)	(4)(9)
(5)	B_{22}		1.0	(5)(6)	(5)(7)	(5)(8)	(5)(9)
(6)	B_{33}			1.0	(6)(7)	(6)(8)	(6)(9)
(7)	B_{12}				1.0	(7)(8)	(7)(9)
(8)	B_{13}					1.0	(8)(9)
(9)	B_{23}						1.0

where (4)(5) is the correlation term between B_{11} and B_{22} , and the other (X)(X) terms have similar meanings.

From Figure 6 of LA-3259, the fifteen B_{ij} correlation terms for copper are

0.127	0.438	-0.014	0.736	0.019
	0.138	-0.000	0.078	-0.063
		-0.032	0.743	-0.049
			-0.040	0.532
				-0.021

and those for ammonia are

-0.215	0.091	-0.019	0.645	-0.023
	-0.227	0.008	-0.182	0.009
		-0.010	0.626	-0.002
			-0.021	0.507
				-0.023

The information given in the previous paragraphs is collected on punched cards as described in the data card section and is illustrated in Fig. 1.

[illegible]

Fig. 1. Input Data Cards for the Illustrative Example.

Illustrative Example: Output

Figure 2 is a reproduction of the output listing of the illustrative data processed by BIJ. The headings for the listed numbers are self-explanatory. It can be seen that the orientation of the anisotropic copper atom is fairly well described. However, the orientation of the ammonia group is not so well known. This is because the standard deviations associated with the B_{ij} 's of the ammonia group are much larger than those of the copper atom.

ANISOTROPIC ATOMS FROM REFINEMENT OF CU.CN.NH(3)
COPPER ATOM

THE INPUT B MATRIX

```
0.03485499 -3.0080500 0.01346500
-0.00080500 0.0026000 -0.0026000
0.01366500 -0.0026000 0.01461000
```

THE CELL CONSTANTS ARE

```
5.81400 7.97700 8.19300 0. -3.584570 0.
```

THE CORRELATION TERMS ARE

```
1.00E-00 1.27E-01 4.38E-01 -1.40E-02 7.36E-01 1.90E-02
1.27E-01 1.00E-00 1.38E-01 -9.0E-02 7.80E-02 -6.30E-02
4.38E-01 1.38E-01 1.00E-00 -3.20E-02 7.43E-01 -4.90E-02
-1.40E-02 -9.0E-02 -3.20E-02 1.00E-00 -4.00E-02 5.32E-01
7.36E-01 7.80E-02 7.43E-01 -4.00E-02 1.00E-00 -2.10E-02
1.90E-02 -6.30E-02 -4.90E-02 5.32E-01 -2.10E-02 1.00E-00
```

THE STANDARD DEVIATIONS ARE

```
7.400E-04 2.300E-04 3.500E-04 3.500E-04 4.050E-04 2.550E-04
```

I	ROOT MEAN SD		B.I.	SD	ANGLES THAT THE ELLIPSOID AXES MAKE WITH THE REAL LATTICE AXES				SD	DIRECTION COSINES OF ELLIPSOID AXES RELATIVE TO ORTHOGONAL LATTICE AXES						
	AMPLITUDE				A	SD	B	SD		C	SD	A	SD	B	SD	C
1	0.199	0.002	3.13	0.07	24.9	8.7	81.3	6.4	100.9	8.4	0.9069	0.0640	-0.0230	0.1125	0.4207	0.1322
2	0.149	0.003	1.75	0.07	102.6	2.1	54.1	2.2	56.9	2.2	-0.2184	0.0362	0.8281	0.0211	0.5163	0.0313
3	0.101	0.002	2.67	0.07	111.1	13.1	144.1	2.2	35.3	4.0	-0.3602	0.1650	-0.5601	0.0316	0.7460	0.0782

ANISOTROPIC ATOMS FROM REFINEMENT OF CU.CN.NH(3)
AMMONIA GROUP

THE INPUT B MATRIX

```
0.02676000 0.10672999 0.01126000
0.00072999 0.01030999 0.00069000
0.01126000 0.00069000 0.01996000
```

THE CELL CONSTANTS ARE

```
5.81400 7.97700 8.19300 0. -0.5849570 0.
```

THE CORRELATION TERMS ARE

```
1.00E-00 -2.15E-01 9.10E-02 -1.50E-02 6.45E-01 -2.30E-02
-2.15E-01 1.00E-00 -2.27E-01 8.00E-03 -1.52E-01 0.00E-03
9.10E-02 -2.27E-01 1.00E-00 -10.00E-03 6.26E-01 -2.00E-03
-1.50E-02 8.00E-03 -10.00E-03 1.00E-00 -2.10E-02 5.07E-01
6.45E-01 -1.52E-01 6.26E-01 -2.10E-02 1.00E-00 -2.30E-02
-2.30E-02 5.07E-03 -2.00E-03 5.07E-01 -2.30E-02 1.00E-00
```

THE STANDARD DEVIATIONS ARE

```
4.280E-03 1.740E-03 2.540E-03 1.940E-03 2.660E-03 1.485E-03
```

I	ROOT MEAN SD		B.I.	SD	ANGLES THAT THE ELLIPSOID AXES MAKE WITH THE REAL LATTICE AXES				SD	DIRECTION COSINES OF ELLIPSOID AXES RELATIVE TO ORTHOGONAL LATTICE AXES						
	AMPLITUDE				A	SD	B	SD		C	SD	A	SD	B	SD	C
1	0.172	0.014	2.34	0.08	41.3	28.5	111.1	53.9	89.5	11.4	0.7514	0.3333	-0.3608	0.8775	0.5525	0.2098
2	0.184	0.015	2.66	0.08	70.4	43.6	21.6	53.0	94.3	13.7	0.3359	0.7169	0.9298	0.3402	0.1304	0.5640
3	0.226	0.012	4.04	0.08	124.6	11.0	95.8	13.6	4.3	13.7	-0.5680	0.1576	0.0726	0.2355	0.6198	0.1073

Fig. 2. Illustrative Example of Output from BIJ.

FØRTRAN II Listing of Program

On the following pages is the FØRTRAN II listing of the program described in this report. At statement 2001 +1 in the listing there is reference to FLUSH. FLUSH is a Los Alamos subroutine that empties the buffers of the packed output in our IØU system. Other installations using BIJ should remove this card before assembly.

CBIJ CALCULATION DECK

COMMENTS

C CARD 1 N1 AND N2 IN 15 FIELDS
 C N1 = NUMBER OF DATA SETS FOR THE CELL DESCRIBED ON CARD3
 C N2 = -1 TO SET ALL S.D. = 0.0
 C N2 = 0 FOR S.D. AND COR. ON TAPE 3(B3)
 C N2 = 1 FOR S.D. AND COR. ON CARDS
 C CARD 2 COMPOUND I. D. 12A6 FIELD
 C CARD 3 DESCRIPTION OF CELL. 6F10.5 FIELD
 C CELL CONSTANTS A, B, C, ALPHA, BETA, AND GAMMA OR THE
 C COSINES OF THESE ANGLES
 C CARD 4 DATA SET I. D. 12A6 FIELD
 C CARD 5 B11, B22, B33, B12, B13, B23 6F10.5 FIELD
 C CARD 6 N2 = -1 NO SUCH CARD
 C IF N2 = 0 LOCATION NUMBERS OF S. D.
 C IF N2 = 1 S.D. AND COR. TERMS ON 3 CARDS IN 7F10.5 FIELDS

1 FORMAT (7F10.5)
 2 FORMAT (8H0 ROOT22X30HANGLES THAT THE ELLIPSOID AXES7X47HDIRECTI
 1ON COSINES OF ELLIPSOID AXES RELATIVE TO/25H I MEAN SQ SD 8.1
 2 SD5X31HMAKE WITH THE REAL LATTICE AXES17X23HORTHOGONAL LATTICE AX
 3ES /11H AMPLITUDE19X1HA5X2HSD5X1HB5X2HSD5X1HC5X2HSD6X1HA5X2HSD7X1
 4HB5X2HSD7X1HC5X2HSD/3(/12,F7.3,F6.3,F6.2,F5.2,F7.1,F6.1,F7.1,F6.1,
 5F7.1,F6.1,F8.4,F7.4,F8.4,F7.4,F8.4,F7.4)
 3 FORMAT (12F8.3,6I2)
 4 FORMAT (25HOMATRIX FAILS TO CONVERGE/1H0)
 5 FORMAT (17HOPKRESENT B MATRIX/(1P3E20.8))
 6 FORMAT (12A6,6I2)
 7 FORMAT (1HG/(F10.3,14,F10.3,14))
 8 FORMAT (14I5)
 9 FORMAT (1H 12A6)
 10 FORMAT (26H0THE CORRELATION TERMS ARE/(1P6E10.2))
 11 FORMAT (28H0THE STANDARD DEVIATIONS ARE/1H 1P6E10.3)
 12 FORMAT (19H0THE INPUT B MATRIX/3(/3F14.8)/23H0THE CELL CONSTANTS A
 1RE//3F10.5,3F10.7)
 13 FORMAT(1H12A6)
 14 FORMAT (1H12A6,15,12X12A6)
 DIMENSION A(3,3),B(3,3),C(3,3),C1(3,3),C2(3,3),B1(3,3),
 1 AI(3,3),AIT(3,3), D(6,6),O1(6), B2(3,3),
 2 B4(24),D3(24,6),D4(24),NA(12),NAM(12),NAME(12),S(200),I11(6)
 3 ,COR(2000),BX(6),IS(6),BK(9)
 DIMENSION J2(6),ATOM(12),X(3)
 COMMON COR
 IF (SENSE SWITCH 1) 21,20
 20 SS1 = 0.0

```

      GO TO 30
21  SS1 = 1.0
50  READ 8,N1,N2
      READ 6,NAME
      READ 1,AD,BD,CD,CA,CB,CC
      IF ( N2 ) 33,30,33
30  REWIND 3
      READ TAPE 3,NA,N
      K=1
      DO 31 I=1,N
        L=K+I-1
        READ TAPE 3,(COR(J),J=K,L)
31  K=L+1
        READ TAPE 3,(S(J),J=1,N)
        MAXN=N
        IF ( SS1 ) 23,22,23
22  CONTINUE
        READ TAPE 3,AD,BD,CD,CA,CB,CC,NJ,(J2(I),I=1,NJ),ATOM,N1
        IT = 1
        IA = 0
        GO TO 33
23  CALL UNLOAD(3)
33  CONTINUE
        IF ( CA-1.0 ) 41,41,40
40  CA=COSF(CA/57.2958)
41  IF ( CB-1.0 ) 43,43,42
42  CB=COSF(CB/57.2958)
43  IF ( CC-1.0 ) 45,45,44
44  CC=COSF(CC/57.2958)
45  SA=SQRTF(1.0-CA**2)
        SB=SQRTF(1.0-CB**2)
        SC=SQRTF(1.0-CC**2)
        CASTAR=(CB*CC-CA)/(SB*SC)
        CCSTAR=(CA*CB-CC)/(SA*SB)
        SASTAR=SQRTF(1.0-CASTAR**2)
        SCSTAR=SQRTF(1.0-CCSTAR**2)
        AI(1)=AD*2.0
        AI(2)=0.0
        AI(3)=0.0
        AI(4)=BD*CC*2.0
        AI(5)=BD*SASTAR*SC*2.0
        AI(6)=-BD*CASTAR*SC*2.0
        AI(7)=CD*CB*2.0
        AI(8)=0.0
        AI(9)=CD*SB*2.0
        A(1)=1.0
        A(2)=CC
        A(3)=CB
        A(4)=0.0
        A(5)=SASTAR*SC
        A(6)=0.0
        A(7)=0.0
        A(8)=-CASTAR*SC
        A(9)=SB
57  IF ( SS1 ) 25,24,25
24  CONTINUE
        READ TAPE 3,X,B(1,1),B(2,2),B(3,3),B(1,2),B(1,3),B(2,3),N12,X,I11
        IA = IA+1
        IF ( IA-J2(1T) ) 29,29,28

```

```

28 IT = IT+1
   IA = 1
29 CONTINUE
   IF ( N12 ) 1999,1999,51
25 CONTINUE
   REAC 6,NAM
60 READ 1,B(1,1),B(2,2),B(3,3),B(1,2),B(1,3),B(2,3)
51 DO 510 I=1,6
   IS(I) = 1
510 D1(I)=0.0
   DO 511 I=1,36
511 D(I) = 0.0
   IF ( SS1 ) 26,27,26
26 CONTINUE
   IF ( N2 ) 54,52,53
52 READ 8,I11
27 CONTINUE
   L=0
   DO 525 N=1,MAXN
   DO 524 J=1,6
   IF ( N-I11(J) ) 524,520,524
520 DO 523 I=1,6
   IF ( N-I11(I) ) 523,521,521
521 IF ( I11(I) ) 523,523,522
522 K = L+I11(I)
   D(J,I) = COR(K)
   D(I,J) = CCR(K)
523 CONTINUE
   K=I11(J)
   D1(J)=S(K)
524 CONTINUE
525 L = L+N
   DO 32 I=1,144
32 D3(I)=0.0
   GO TO 54
53 READ 1,(D1(I),I=1,6),((D(I+1,J),J=1,I),I=1,5)
   DO 530 I=1,6
   I11(I) = I
530 CONTINUE
54 DO 620 I=1,3
   DO 620 J=1,3
620 AIT(I,J)=AI(J,I)
   R(1,2)=B(1,2)/2.0
   B(1,3)=B(1,3)/2.0
   B(2,3)=B(2,3)/2.0
   B(2,1) = B(1,2)
   B(3,1) = B(1,3)
   B(3,2) = B(2,3)
   IF ( SS1 ) 202,201,202
201 CONTINUE
   WRITE OUTPUT TAPE 9,14,ATOM(2IT-1),ATOM(2IT),IA,NA
   GO TO 203
202 CONTINUE
   IF ( SENSE SWITCH 1 ) 58, 59
58 PRINT 9,NAME
   IF (N2) 159,158,159
158 PRINT 9,NA
159 PRINT 6,NAM
59 WRITE OUTPUT TAPE 9,13,NAME
   IF (N2) 161,160,161
160 WRITE OUTPUT TAPE 9,9,NA
161 WRITE OUTPUT TAPE 9,9,NAM

```



```

203 CONTINUE
  WRITE OUTPUT TAPE 9,12,B,AD,BD,CD,CA,CB,CC
  DO 63 I=4,6
63  D1(I)=D1(I)/2.0
    DO 62 I=1,6
      DO 61 J=1,I
61  D(J,I)=C(I,J)
62  D(I,I)=1.0
      BX(1)=B(1)
      BX(2)=B(5)
      BX(3)=B(9)
      BX(4)=B(4)
      BX(5) = B(7)
      BX(6) = B(8)
      DO 220 I=1,5
        K = I+1
        DO 220 J=K,6
          IF ( I11(I)-I11(J) ) 220,210,220
210  IS(J)=-I
220  CONTINUE
      55 WRITE OUTPUT TAPE 9,10,((D(I,J),I=1,6),J=1,6)
      WRITE OUTPUT TAPE 9,11,(D1(I),I=1,6)
      56 DO 64 I=1,6
64  B2(I) = BX(I)
      DO 600 I23=1,7
        IF ( I23-2 ) 73,71,70
      70 DO 700 I =1,6
700  BX(I) = B2(I)
      71 IF ( IS(I23-1) ) 600,72,72
      72 D36 = B2(I23-1)*0.0001
      DO 721 I=1,6
        IF ( I11(I23-1)-I11(I) ) 721,720,721
720  BX(I) = B2(I)*1.0001
721 CONTINUE
      73 B(1) = BX(1)
        B(2) = BX(4)
        B(3) = BX(5)
        B(4) = BX(4)
        B(5) = BX(2)
        B(6) = BX(6)
        B(7) = BX(5)
        B(8) = BX(6)
        B(9) = BX(3)
      DO 622 I=1,3
        DO 622 J=1,3
          B1(I,J)=0.0
          DO 622 K=1,3
622  B1(I,J)=B1(I,J)+B(K,J)*AI(I,K)
          DO 623 I=1,3
            DO 623 J=1,3
              B(I,J)=0.0
              DO 623 K=1,3
623  B(I,J)=B(I,J)+B1(I,K)*AIT(K,J)
            N=1
            DO 650 I=1,3
              DO 65 J=1,3
65  C1(I,J)=0.0
650  C1(I,I) = 1.0
            DO 624 I=1,4

```

```

624 BK(I) = B(I)
    SENSE LIGHT 0
80 U=0.
81 DO 100 I=1,2
    K = I+1
    DO 100 J=K,3
    IF ( ABSF(B(I,J)+B(J,I))-ABSF(U) ) 100,100,91
91 I1=I
    J1=J
    U = B(I,J)+B(J,I)
100 CONTINUE
    IF ( ABSF(U)-1.0E-6 ) 1000,1000,110
110 DO 120 I=1,3
    DO 111 J=1,3
111 C(I,J) = 0.0
120 C(I,I) = 1.0
    N=N+1
    IF (N-20) 121, 121, 3000
121 X=B(I1,I1)-B(J1,J1)
    IF ( X ) 123,122,123
122 Y=1.57079633
    GO TO 124
123 Y1 = U/X
    Y=ATANF(Y1)
124 C(I1,J1)=-SINF(Y/2.0)
    Y2=1.0-C(I1,J1)**2
    C(I1,I1)=SQRTF(Y2)
    C(J1,I1)=-C(I1,J1)
    C(J1,J1)=C(I1,I1)
3001 IF (SENSE LIGHT 1 ) 301,401
301 DO 400 I=1,3
    DO 400 J=1,3
    C1(I,J)=0.0
    DO 400 I2=1,3
400 C1(I,J)=C1(I,J)+C2(I,I2)*C(I2,J)
    DO 302 I=1,9
302 C(I) = C1(I)
    GO TO 403
401 DO 500 I=1,3
    DO 500 J=1,3
    C2(I,J)=0.0
    DO 500 I2=1,3
500 C2(I,J)=C2(I,J)+C1(I,I2)*C(I2,J)
    SENSE LIGHT 1
    DO 402 I=1,9
402 C(I) = C2(I)
403 DO 625 I=1,9
625 B(I) = BK(I)
    DO 200 I=1,3
    DO 200 J=1,3
    B1(I,J)=0.0
    DO 200 I2=1,3
200 B1(I,I)=B1(I,J)+B(I,I2)*C(I2,J)
    DO 300 I=1,3
    DO 300 J=1,3
    B(I,J)=0.0
    DO 300 I2=1,3
300 B(I,J)=B(I,J)+B1(I2,J)*C(I2,I)

```

```

      GO TO 80
1000 IF ( SENSE LIGHT 1 ) 1002,1004
1002 DO 1003 I=1,9
1003 C1(I)=C2(I)
1004 DO 1005 I=1,3
      DO 1005 J=1,3
      C(I,J)=0.0
      DO 1005 K=1,3
1005 C(I,J)=C(I,J)+A(I,K)*C1(K,J)
      GO TO (1010,1011,1011,1011,1011,1011,1011),I23
1010 DO 1006 I=1,3
      B4(I+3)=SQRTF(B(I,I)*0.01266515)
1006 B4(I)=B(I,I)
      DO 1007 I=7,15
      B4(I+9)=C1(I-6)
1007 B4(I)=90.0-ASINF(C(I-6))*57.29578
      IF ( N2 ) 601,600,600
1011 CONTINUE
      DO 1061 I=1,3
      D3(I+3,I23-1)=(SQRTF(B(I,I)*0.01266515)-B4(I+3))/D36
1061 D3(I,I23-1)=(B(I,I)-B4(I))/D36
      DO 1071 I=7,15
      D3(I+9,I23-1)=(C1(I-6)-B4(I+9))/D36
1071 D3(I,I23-1)=(90.0-ASINF(C(I-6))*57.29578-B4(I))/D36
      600 CONTINUE
      601 DO 1102 I=1,24
      D4(I)=0.0
      DO 1100 J=1,6
      DO 1100 K=1,6
1100 D4(I)=D4(I)+D3(I,J)*D3(I,K)*D1(J)*D1(K)*D(J,K)
1102 D4(I)=SQRTF(D4(I))
      IF ( SENSE SWITCH 1 ) 1101,1200
1101 PRINT 2,(I,B4(I+3),D4(I+3),B4(I),D4(I),
1 B4(3*I+4),D4(3*I+4),B4(3*I+5),D4(3*I+5),B4(3*I+6),D4(3*I+6),
2 B4(3*I+13),D4(3*I+13),B4(3*I+14),D4(3*I+14),B4(3*I+15),D4(3*I+15)
3 ,I=1,3)
1200 WRITE OUTPUT TAPE 9,2,(I,B4(I+3),D4(I+3),B4(I),D4(I),
1 B4(3*I+4),D4(3*I+4),B4(3*I+5),D4(3*I+5),B4(3*I+6),D4(3*I+6),
2 B4(3*I+13),D4(3*I+13),B4(3*I+14),D4(3*I+14),B4(3*I+15),D4(3*I+15)
3 ,I=1,3)
1999 N1=N1-1
      IF ( N1 ) 2000,2000,57
2000 IF ( SS1 ) 204,205,204
      204 CONTINUE
      IF ( SENSE SWITCH 6 ) 50,2001
      205 CONTINUE
      CALL EXIT
2001 CONTINUE
      CALL FLUSH
      PAUSE 77777
      GO TO 50
3000 PRINT 4
      WRITE OUTPUT TAPE 9,4
      WRITE OUTPUT TAPE 9,5,8
      GO TO 1999
      END

```