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THE CRYSTAL STRUCTURE DETERMINATIONS OF trans-DICYANO TRIEN COBALT(III) PERCHLORATE AND POTASSIUM ANTIMONY(III) PENTACHLORIDE AND TWO PHASE DETERMINATION TECHNIQUES BASED ON PATTERSON DECONVOLUTION

Ph.D. Thesis Submitted to Iowa State University,
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The crystal structure determinations of trans-dicyano trien cobalt(III) perchlorate and potassium antimony(III) pentachloride and two phase determination techniques based on Patterson deconvolution

by

Robert Kingsley Wismer

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

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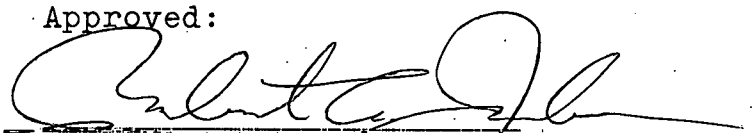

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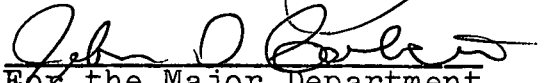

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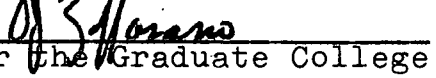

For the Graduate College

Iowa State University
Of Science and Technology
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The crystal structure determinations of trans-dicyano trien cobalt(III) perchlorate and potassium antimony(III) pentachloride and two phase determination techniques based on Patterson deconvolution*

Robert Kingsley Wismer

Under the supervision of R. A. Jacobson
From the Department of Chemistry
Iowa State University of Science and Technology

The crystal structure of trans-dicyano triethylene-tetramine cobalt(III) perchlorate (monoclinic, $P2_1/n$, a = 9.85, b = 22.35, c = 6.68 A, β = 100.9°, Z = 4, MoK_α radiation) has been determined by three-dimensional X-ray analysis. The structure was solved by conventional Patterson and Fourier techniques and refined by full matrix least squares to a final discrepancy factor of 0.123 for the 3314 observed reflections. The complex has a distorted octahedral configuration with the trien ligand equatorially coordinated. The bonding mode of the cyanide group is clearly through carbon.

The crystal structure of potassium antimony(III)

pentachloride (K_2SbCl_5, monoclinic, $P2_1/c$, $\underline{a}$ = 8.87, $\underline{b}$ = 12.46, $\underline{c}$ = 8.93 Å, β = 110.5°, Z = 4, MoKα radiation) has been determined by three-dimensional X-ray analysis. The structure was solved by conventional Patterson and Fourier techniques and refined by full matrix least squares to a final conventional discrepancy factor of 0.054 for the 1543 observed reflections. The $SbCl_5^=$ exhibits a distorted square pyramidal configuration in which the axial antimony - chloride bond (2.39 Å) is shorter than the mean basal antimony - chloride bond and two of the basal bonds are distorted by interionic and packing forces.

The superposition technique has been programmed for semi-automatic use in solving heavy atom and pseudo heavy atom problems. From a list of peaks, obtained by program analysis of a Patterson map, a heavy atom peak is chosen. This is then used as the origin for an in-core superposition. By utilizing the symmetry of the structure being solved, the program then determines the amount by which the origin of the resultant superposition map is shifted from the origin in electron density space, and computes the location of atoms in the unit cell. The program is written to handle inversion, mirror, glide, two-fold, and two-fold screw symmetry.

A method of phase determination which utilizes

both the Σ_2 relation and Patterson superposition techniques has been developed. Reflections input into the initial Σ_2 relation are used to compute a map upon which the Patterson is superimposed. The Fourier transform of the resultant map, with negative regions set equal to zero, yields reliable phases for the larger $|E|$ values. These are then extended and refined by usual direct method techniques. Application of this method to both a centric and an acentric structure is presented. Further refinements and extensions of the method are also discussed.

INTRODUCTION

This thesis describes the crystal structures of two compounds and details two methods for the determination of the phases of structure factors. The crystal structures were undertaken to extend the currently available knowledge of cobalt and antimony complexes.

The cobalt compound was believed by its discoverers to be cis-$\alpha(NC)_2$ trien cobalt(III) perchlorate. Thus, it would have been the sole known mononuclear cobalt complex in which the cyanide group was coordinated to cobalt through the nitrogen atom. The structure that was determined is actually trans-$(CN)_2$ trien cobalt(III) perchlorate and is one of the few examples in which a quadradentate ligand, not restricted by its own structure to be planar, is equatorially coordinated to cobalt.

The second structure described is that of K_2SbCl_5. The structure of the $SbCl_5^=$ anion has only been determined once previously, in the compound $(NH_4)_2SbCl_5$. In that instance, the disagreement between observed and calculated structure factors was such that the uncertainty in bond distances was 0.5 Å. Structures of antimony halides are known to be very sensitive to the cation present.

The first of the phase determining methods applies the techniques of pseudo heavy atom superposition and then uses space group symmetry to determine atomic

locations in electron density space. All of these operations are performed by a computer program with a minimum of human intervention.

The second phase determining method also uses superposition techniques, to enhance the phase determining properties of a pseudo electron density map which has been computed from origin-defining reflections. The coefficients of the Fourier transform of this modified map are then used to phase those reflections with the largest normalized unitary structure factors. This method greatly simplifies one of the major problems of direct methods, the expansion of the origin-defining set.

THE CRYSTAL AND MOLECULAR STRUCTURE OF TRANS-DICYANO TRIETHYLENETETRAMINE COBALT(III) PERCHLORATE

Introduction

The bonding mode of cyanide to cobalt has been the subject of considerable controversy in recent years. The energy difference between the cyano and isocyano coordinations is small enough to permit either to occur.[1] However, neutron diffraction studies of cyano-cobalt complexes[2,3,4] have regularly shown that the cyanide group bonds through carbon. Since it is ofttimes difficult to distinguish between atoms which differ by but one electron by X-ray diffraction, bonding via the carbon has sometimes been assumed.[5]

Kuroda and Gentile[6] recently have prepared what they characterize as an isocyano cobalt complex, cis-α-isocyano-triethylenetetramine cobalt(III) perchlorate. Their assignment of the isocyano coordination is based on visible and ultraviolet spectroscopy. Because there is some doubt as to the correctness of this assignment,[7] it was decided to carry out an X-ray structure determination of this compound.

Experimental

A sample of the compound, prepared by the method of Kuroda and Gentile,[6] was kindly supplied by Dr. James H.

Espenson. Amber-colored crystals were obtained by recrystallization from an aqueous solution. High resolution infrared spectra of the initial sample and of the recrystallized material, both in KBr pellets, were virtually identical, indicating that isomerization had not occurred during solution or recrystallization. Microscopic examination revealed that the crystals have sharply defined faces and are needle-like in appearance with a distorted hexagonal cross section in which alternate sides are of unequal lengths.

Crystals were selected and mounted on a glass fiber with Duco cement thinned with amyl acetate. Preliminary Weissenberg and precession photographs exhibited 2/m Laue symmetry, indicating a monoclinic space group. The following systematic absences were observed: $h0\ell$ when $h + \ell = 2n + 1$, and $0k0$ when $k = 2n + 1$. These absences are only consistent with the space group $P2_1/n$. The unit cell parameters at 25° C are $\underline{a} = 9.8544 \pm 0.0015$, $\underline{b} = 22.3529 \pm 0.0045$, $\underline{c} = 6.6766 \pm 0.0020$ Å, and $\beta = 100.85 \pm 0.03°$. These parameters and their standard deviations were obtained by a least squares fit[8] to the two-theta values of twelve independent reflections whose centers were determined by top-bottom, left-right beam splitting on a previously aligned Hilger-Watts four-circle diffractometer (MoKα radiation, $\lambda = 0.71069$ Å). Any

error in the instrumental zero was eliminated by centering the reflection at both plus two-theta and minus two-theta. A calculated density of 1.62 g/cc for four molecules per unit cell agrees quite well with an observed density of 1.65 $\pm$ 0.01 g/cc, which was determined by flotation techniques.

For data collection, a crystal was selected having approximate dimensions 0.1 x 0.1 x 0.9 mm along the a, b, and c crystal axes, respectively, and was mounted such that the c axis coincided with the ϕ axis of the diffractometer. Data were collected at room temperature using a Hilger-Watts four-circle diffractometer interfaced to an SDS 910 computer in a real time mode, equipped with a scintillation counter, and using Zr-filtered MoKα radiation. Within a two-theta sphere of 60° ($\sin\theta/\lambda$ = 0.704 Å^{-1}) all data in the $hk\ell$ and $\bar{h}k\ell$ octants were recorded using the θ-2θ scan technique with a take-off angle of 5.5°. Symmetric scan ranges of 1.2° in 2θ at low two-theta values to 2.0° at large two-theta values were used. Stationary-crystal, stationary-counter background counts of half the scan time were taken at the beginning and end of each scan. A counting rate of 0.4096 seconds per step of 0.01° in θ was employed. A total of 5081 reflections were measured in this way.

As a general check on electronic and crystal stability, the intensities of three standard reflections were remeasured periodically during the data collection period. These reflections did not vary to any significant degree during the entire period of data collection.

Based on a linear absorption coefficient of $\mu = 14.982\ cm^{-1}$, the maximum and minimum transmission factors[9] were 87.86% and 85.96% respectively, and no absorption correction was deemed necessary.

The intensity data were corrected for Lorentz-polarization effects. The estimated error in each intensity was calculated by

$$\sigma_I^2 = C_T + C_B + (0.03\ C_T)^2 + (0.03\ C_B)^2$$

where C_T and C_B are the total count and the background count, respectively. The factor 0.03 represents an estimate of non-statistical errors. The estimated deviations in the structure factors were calculated by the finite difference method.[10] Of the 4678 independent reflections, 3314 were considered observed ($> 3\sigma_F$).

Solution and Refinement

The positions of the cobalt and chlorine atoms were obtained from analysis of a sharpened Patterson function.[11] The remaining non-hydrogen atoms were found by successive structure factor[12] and electron density map calcula-

tions.[13,14] These atomic positions were then refined by a full matrix least squares procedure,[12] minimizing the function $\Sigma\omega(|F_o|-|F_c|)^2$, where $\omega = 1/\sigma_F^2$, to a conventional discrepancy factor of $R = \Sigma||F_o|-|F_c||/\Sigma|F_o| = 0.170$. The scattering factors used were those of Hanson et al.[15] with the cobalt and chlorine scattering factors modified for the real and imaginary parts of anomalous dispersion.[16]

An electron density difference map verified that all the non-hydrogen atoms had been accounted for, but indicated that some anisotropic motion, particularly of the cobalt and chlorine atoms, was present. Accordingly, anisotropic refinement was begun and after six cycles of refinement, values of R and $R\ (= \Sigma\omega(|F_o|-|F_c|)^2/\Sigma\omega|F_o|)^2)^{1/2})$ of 0.154 and 0.169, respectively, were obtained. The positions of the hydrogens bonded to carbons in the triethylenetetramine ligand were calculated with an H-C-C angle of 109.5° and a C-H distance of 1.07 Å. The hydrogen atoms were assigned isotropic thermal parameters of 3.0 $Å^2$. Two cycles of refinement with anisotropic thermal parameters for all non-hydrogen atoms, varying only the positional and thermal parameters of the non-hydrogen atoms and the overall scale factor, followed by a recalculation of the hydrogen atom positions and two further cycles of least squares refinement, yielded values for R and ωR of 0.123

and 0.156, respectively.

A final electron density difference map showed no peaks greater than 1.2 $e/\mathring{A}^3$. A final statistical analysis of the F_o and F_c values as a function of the scattering angle and magnitude of F_o revealed no unusual trends and suggests that the relative weighting scheme used is a reasonable one.

The bonding orientation of the two cyanide groups was determined after the final least squares refinement. The atom multipliers of the two cyanide group atoms were allowed to vary under two sets of conditions. In the first of these, carbon scattering factors were assigned to C(7) and C(8) and nitrogen scattering factors were assigned to N(5) and N(6). In the second instance, the scattering factor assignments were reversed. All four atom multipliers were initially set at a value of 1.00. The results of these refinements are shown in Table I and clearly indicate the correct assignments.

The final positional and thermal parameters for the non-hydrogen atoms are listed in Table II. The standard deviations were calculated from the inverse matrix of the final least squares refinement cycle. The calculated hydrogen atom positions are listed in Table III. Bond

Table I. Determination of the bonding mode of cyanide in trans-$(CN)_2$ trien $Co^{III}ClO_4$

Atom	Assigned Scattering Factor Table	Atom Multiplier Actual	Theoretical Co-C-N	Theoretical Co-N-C	R	ωR
C(7)	Carbon	1.033	1.0	1.17		
C(8)	Carbon	1.034	1.0	1.17		
N(5)	Nitrogen	1.026	1.0	0.86		
N(6)	Nitrogen	1.046	1.0	0.86	12.4	15.8
C(7)	Nitrogen	0.823	0.86	1.0		
C(8)	Nitrogen	0.825	0.86	1.0		
N(5)	Carbon	1.293	1.17	1.0		
N(6)	Carbon	1.314	1.17	1.0	12.4	15.8

Table II

Final positional and anisotropic thermal parameters of non-hydrogen atoms in trans-$(NC)_2$-trien $Co^{III}ClO_4$ [a,b]

Atom	x	y	z	$10^4\beta_{11}$	$10^4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$	$10^4\beta_{13}$	$10^4\beta_{23}$
Co	0.6629(1)	0.3488(1)	0.6552(2)	55.9(1.4)	9.2(0.2)	169.9(3.6)	1.1(0.5)	13.9(1.6)	0.7(0.9)
Cl	0.6616(3)	0.1285(1)	0.6466(6)	79.7(3.0)	15.6(0.6)	306.3(9.7)	3.6(1.1)	12.7(4.3)	6.1(2.2)
O(1)	0.6601(9)	0.0863(4)	0.4868(15)	139(12)	21(2)	360(32)	10(4)	-26(16)	11(7)
O(2)	0.5498(9)	0.1700(4)	0.5928(16)	121(12)	30(2)	486(39)	32(4)	-79(17)	43(8)
O(3)	0.7893(8)	0.1635(4)	0.6748(15)	92(10)	26(2)	386(32)	-5(4)	-7(14)	13(7)
O(4)	0.6586(11)	0.0988(5)	0.8283(16)	204(17)	34(3)	333(33)	-.2(5.6)	90(19)	-3(9)
N(1)	0.4727(8)	0.3159(4)	0.5898(14)	69(9)	14(2)	198(24)	-9(3)	2(12)	10(6)
N(2)	0.5927(8)	0.4122(3)	0.8075(12)	77(9)	11(2)	148(21)	3(3)	11(11)	4(5)
N(3)	0.8378(8)	0.3892(4)	0.7368(15)	66(9)	14(2)	224(26)	-4(3)	23(13)	-9(6)
N(4)	0.7579(9)	0.2898(4)	0.5051(13)	97(11)	14(2)	197(25)	8(4)	39(13)	7(6)
C(7)	0.6226(10)	0.3942(5)	0.4078(18)	68(11)	12(2)	205(30)	3(4)	17(15)	-.8(6.7)
C(8)	0.6997(10)	0.3013(4)	0.8952(18)	63(11)	9(2)	250(33)	-.7(3.5)	31(15)	-7(7)
C(1)	0.3914(11)	0.3494(6)	0.7122(20)	77(12)	22(3)	274(36)	-7(5)	15(17)	-.5(9)
C(2)	0.4392(11)	0.4144(5)	0.7393(20)	62(11)	20(3)	313(39)	10(4)	39(17)	15(9)
C(3)	0.6694(12)	0.4679(5)	0.7878(19)	93(13)	12(2)	280(37)	-4(4)	3(17)	-11(8)
C(4)	0.8173(13)	0.4545(5)	0.7531(24)	118(17)	16(3)	388(47)	-7(5)	11(22)	-19(9)
C(5)	0.9274(12)	0.3720(6)	0.6003(21)	81(13)	26(3)	289(40)	-5(5)	42(19)	-15(10)
C(6)	0.9102(13)	0.3046(5)	0.5589(23)	105(16)	26(3)	407(50)	18(6)	96(23)	14(11)
N(5)	0.6027(11)	0.4174(5)	0.2488(19)	116(13)	19(2)	349(38)	3(4)	27(18)	9(8)
N(6)	0.7204(10)	0.2762(4)	1.0540(15)	115(12)	16(2)	230(28)	3(4)	28(15)	5(7)

[a] In this and subsequent tables, numbers in parentheses represent standard deviations in the least significant digits.

[b] Anisotropic thermal parameters are defined by: $T = \exp[-(h^2\beta_{11} + k^2\beta_{22} + \ell^2\beta_{33} + 2hk\beta_{12} + 2k\ell\beta_{23} + 2h\ell\beta_{13})]$.

Table III. Calculated hydrogen atomic positions in trans-$(CN)_2$ trien $Co^{III}ClO_4$

Atom	x	y	z
H(AC1)	0.4041	0.3289	0.8624
H(BC1)	0.2834	0.3479	0.6404
H(AC2)	0.3934	0.4374	0.8519
H(BC2)	0.4113	0.4386	0.5960
H(AC3)	0.6762	0.4947	0.9921
H(BC3)	0.6135	0.4932	0.6569
H(AC4)	0.8303	0.4765	0.6143
H(BC4)	0.8906	0.4724	0.8798
H(AC5)	1.0339	0.3827	0.6673
H(BC5)	0.8990	0.3961	0.4566
H(AC6)	0.9606	0.2912	0.4366
H(BC6)	0.9593	0.2799	0.6960

lengths and bond angles, and significant non-bonded distances are listed in Tables IV and V, respectively, along with their standard deviations.[17] The final values of the observed and calculated structure factors are listed in Table VI.

Shortly after the data had been collected and the crystal removed from the diffractometer, the instrument was found to be slightly misaligned. Thus, the data are somewhat poorer than might be expected. However, since all the stereochemical features of interest were well determined and the electron density difference map was rather featureless, the data were not retaken.

Description of the Structure

The results clearly indicate that the bonding of cyanide to the cobalt is through the carbon and not the nitrogen, and that these groups are <u>trans</u> and not <u>cis</u> to one another, contrary to the predictions of Kuroda and Gentile.[6] Hence, the compound is <u>trans</u>-dicyanotriethylenetetramine cobalt(III) perchlorate, and is illustrated in Figure 1.[18] This configuration has been anticipated by Konya, Nishikawa, and Shibita[7] on the basis of spectroscopic examination of similar compounds. The <u>trans</u> configuration is also consistent with an exceedingly sharp band for the C-N stretching frequency at 2145 cm^{-1}, with no evidence of splitting.

Table IV. Selected bond distances and angles in angstroms and degrees for cis-$(CN)_2$ trien $Co^{III}ClO_4$

Cl-O(1)	1.427(9)	C(8)-N(6)	1.180(13)
Cl-O(2)	1.424(8)	N(1)-C(1)	1.462(15)
Cl-O(3)	1.456(9)	N(2)-C(2)	1.488(12)
Cl-O(4)	1.392(10)	N(2)-C(3)	1.476(13)
Co-N(1)	1.978(8)	N(3)-C(4)	1.484(14)
Co-N(2)	1.951(8)	N(3)-C(5)	1.444(15)
Co-N(3)	1.922(8)	N(4)-C(6)	1.506(15)
Co-N(4)	2.001(8)	C(1)-C(2)	1.527(16)
Co-C(7)	1.909(12)	C(3)-C(4)	1.551(17)
Co-C(8)	1.894(12)	C(5)-C(6)	1.536(18)
C(7)-N(5)	1.161(14)		

O(1)-Cl-O(2)	110.7(6)	N(4)-Co-C(8)	91.5(4)
O(1)-Cl-O(3)	109.1(6)	C(7)-Co-C(8)	177.9(4)
O(1)-Cl-O(4)	109.3(6)	Co-N(1)-C(1)	106.7(6)
O(2)-Cl-O(3)	107.1(6)	Co-N(2)-C(2)	108.1(7)
O(2)-Cl-O(4)	112.3(7)	Co-N(2)-C(3)	108.9(7)
O(3)-Cl-O(4)	108.4(6)	Co-N(3)-C(4)	110.8(7)
N(1)-Co-N(2)	88.0(4)	Co-N(3)-C(5)	109.0(7)
N(1)-Co-N(3)	172.5(4)	Co-N(4)-C(6)	106.3(7)
N(1)-Co-N(4)	99.4(4)	Co-C(7)-N(5)	173.7(10)
N(1)-Co-C(7)	89.2(4)	Co-C(8)-N(6)	174.1(9)

Table IV (Continued)

N(1)-Co-C(8)	89.2(4)	N(1)-C(1)-C(2)	111.3(9)
N(2)-Co-N(3)	84.5(4)	N(2)-C(2)-C(1)	105.9(8)
N(2)-Co-N(4)	172.6(4)	N(2)-C(3)-C(4)	111.4(8)
N(2)-Co-C(7)	91.8(4)	N(3)-C(4)-C(3)	110.2(9)
N(2)-Co-C(8)	89.6(4)	N(3)-C(5)-C(6)	108.3(10)
N(3)-Co-N(4)	88.1(4)	N(4)-C(6)-C(5)	109.1(9)
N(3)-Co-C(7)	90.7(4)	C(2)-N(2)-C(3)	116.8(8)
N(3)-Co-C(8)	91.0(4)	C(4)-N(3)-C(5)	114.5(10)
N(4)-Co-C(7)	87.3(4)		

Table V. Significant non-bonded distances in trans-$(CN)_2$ trien $Co^{III}ClO_4$[a]

C(7)-H(BC3)	2.870(10)
C(7)-H(AC4)	2.884(10)
C(8)-O(2)	2.694(13)
C(8)-O(3)	3.601(13)
N(4)-O(3)	3.034(12)
O(1)-H(AC5)'	2.34(1)
O(4)-H(BC1)'	2.49(1)

[a] Primed atoms indicate atoms in another molecule.

Table VI. Observed and calculated structure factors

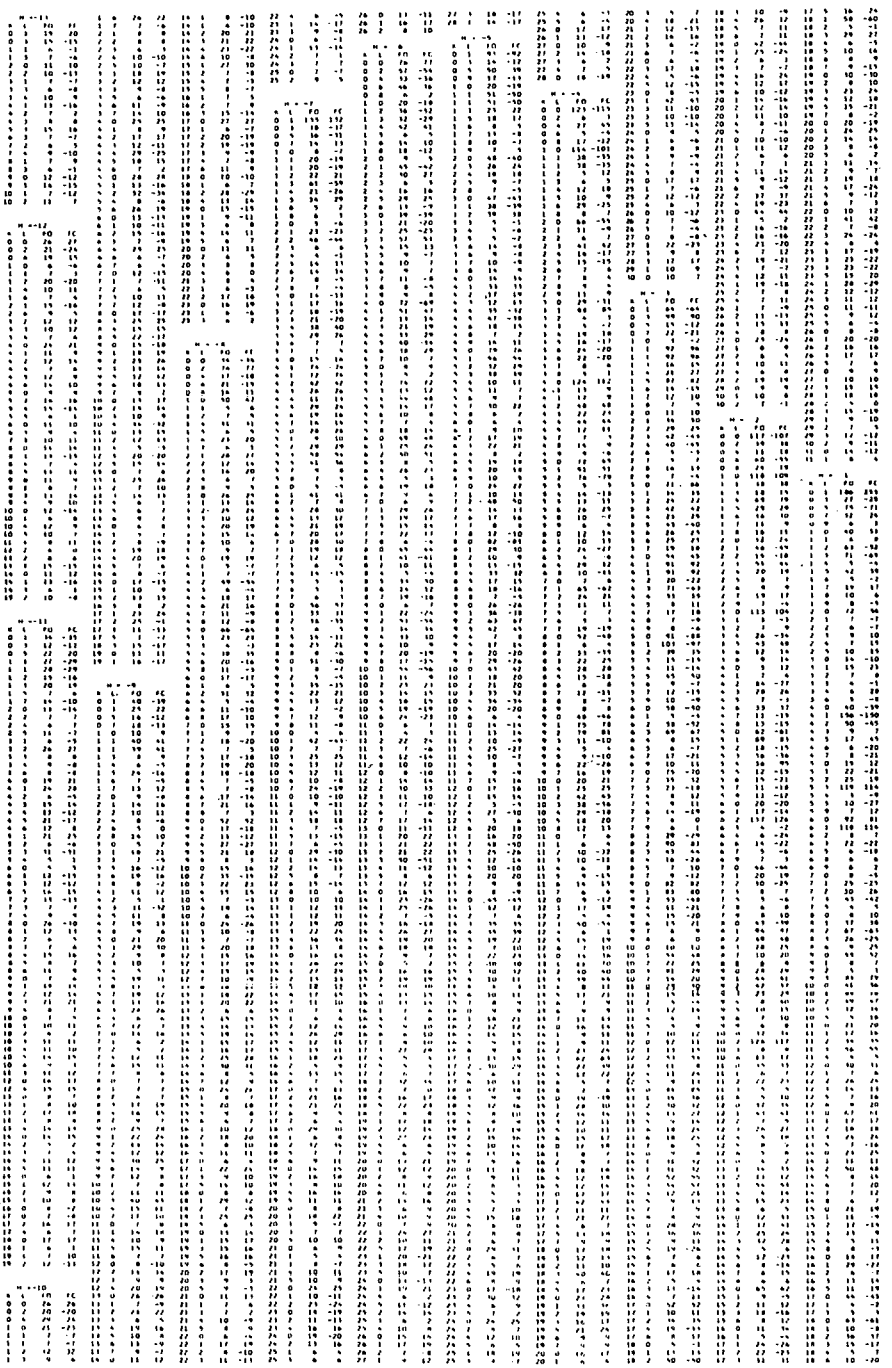
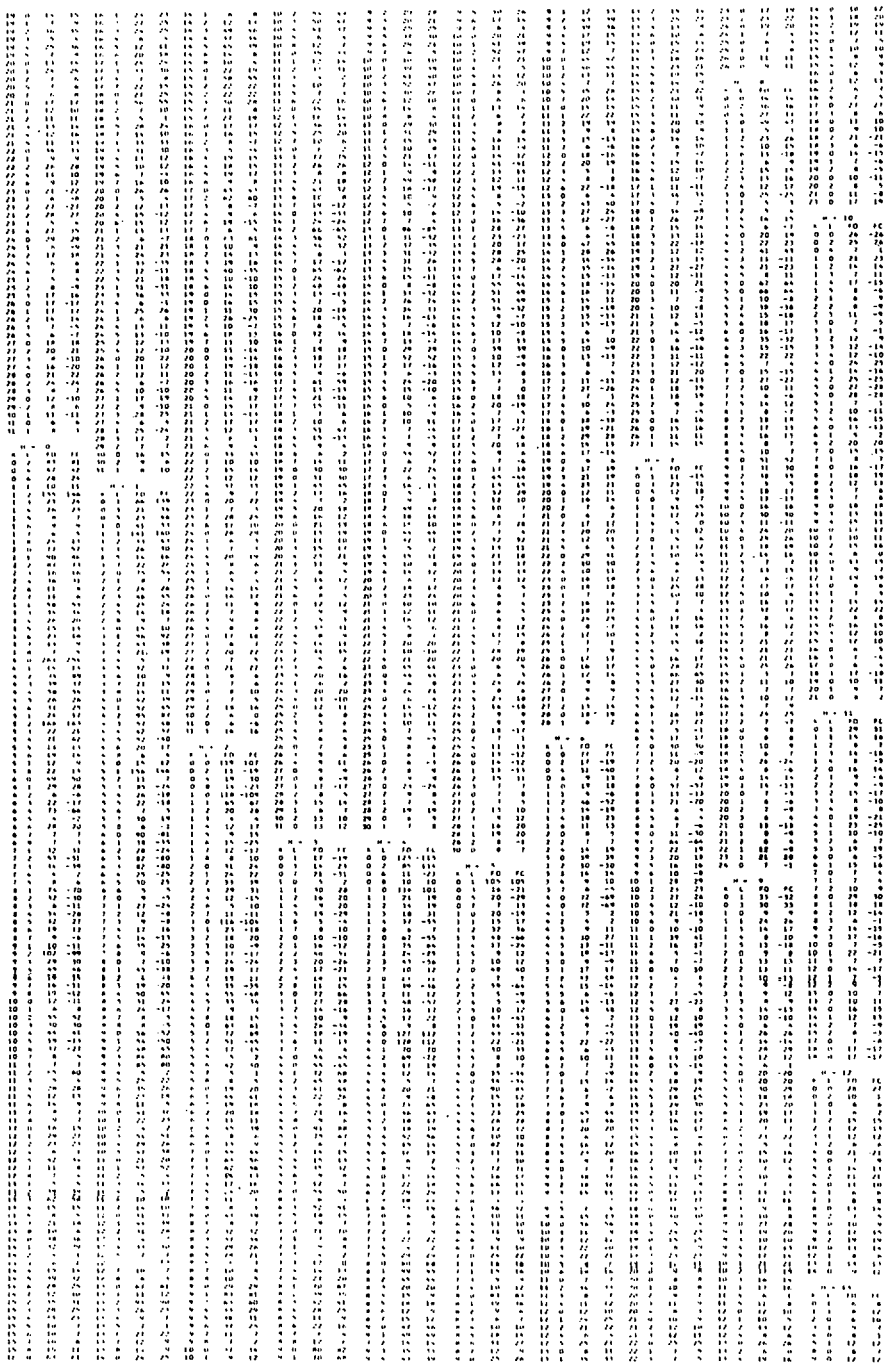


Table VI. (Continued)



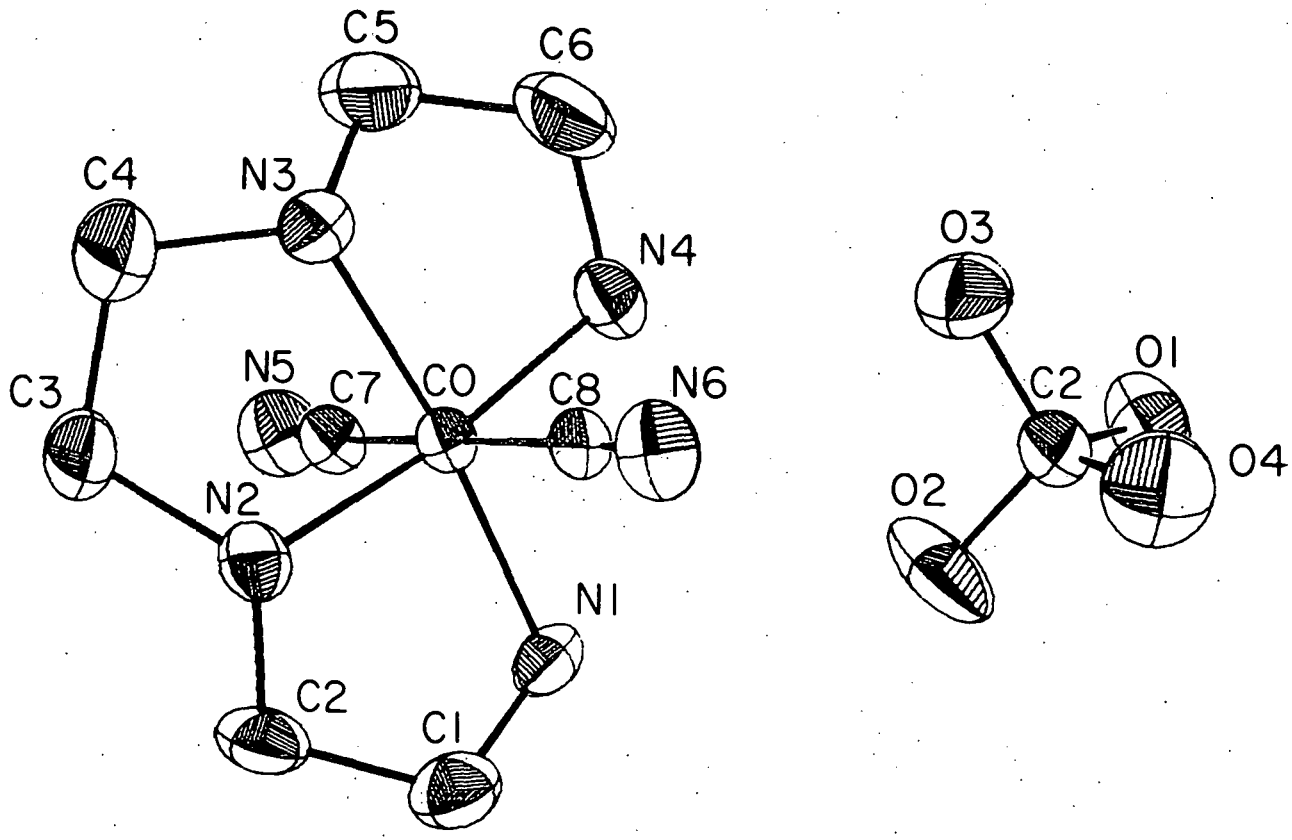


Figure 1. A formula unit of trans-cyano triethylenetetramine cobalt(III) perchlorate

The cyanide groups are within a degree of being perpendicular to the nitrogens of the trien ligand (Table IV), and the variations from an ideal octahedral configuration displayed by the N-Co-N angles appear to simply reflect the restrictions imposed by the quadradentate ligand (Figure 2). This trien ligand coordinated to cobalt in a cis configuration has been investigated by Freemen and Maxwell,[19] and Dwyler and Maxwell;[20] their results have been used as the basis of many of the comparisons which follow.

The N(1)-Co-N(2) and N(3)-Co-N(4) angles of 88.0 and 88.1° are reasonable and consistent with similar results obtained in other investigations of the trien ligand. A slight compression of the Co-N(2)-C(3)-C(4)-N(3) ring due to the equatorial coordination of the ligand adequately explains the somewhat small value of 84.5° for the N(2)-Co-N(3) angle. Hydrogen-hydrogen repulsions would be expected to produce an increase in the N(1)-Co-N(4) angle compared to the nominal 90°, and the 99° angle found is quite reasonable. A similar result was obtained during the investigation of a cobalt compound containing a homologous ligand.[21] The bond angles within the trien ligand, with the exception of the C-N-C angles, do not differ from the expected tetrahedral angles by more than three standard deviations. In addition, they fall within two standard deviations of the range of values of 108.4°

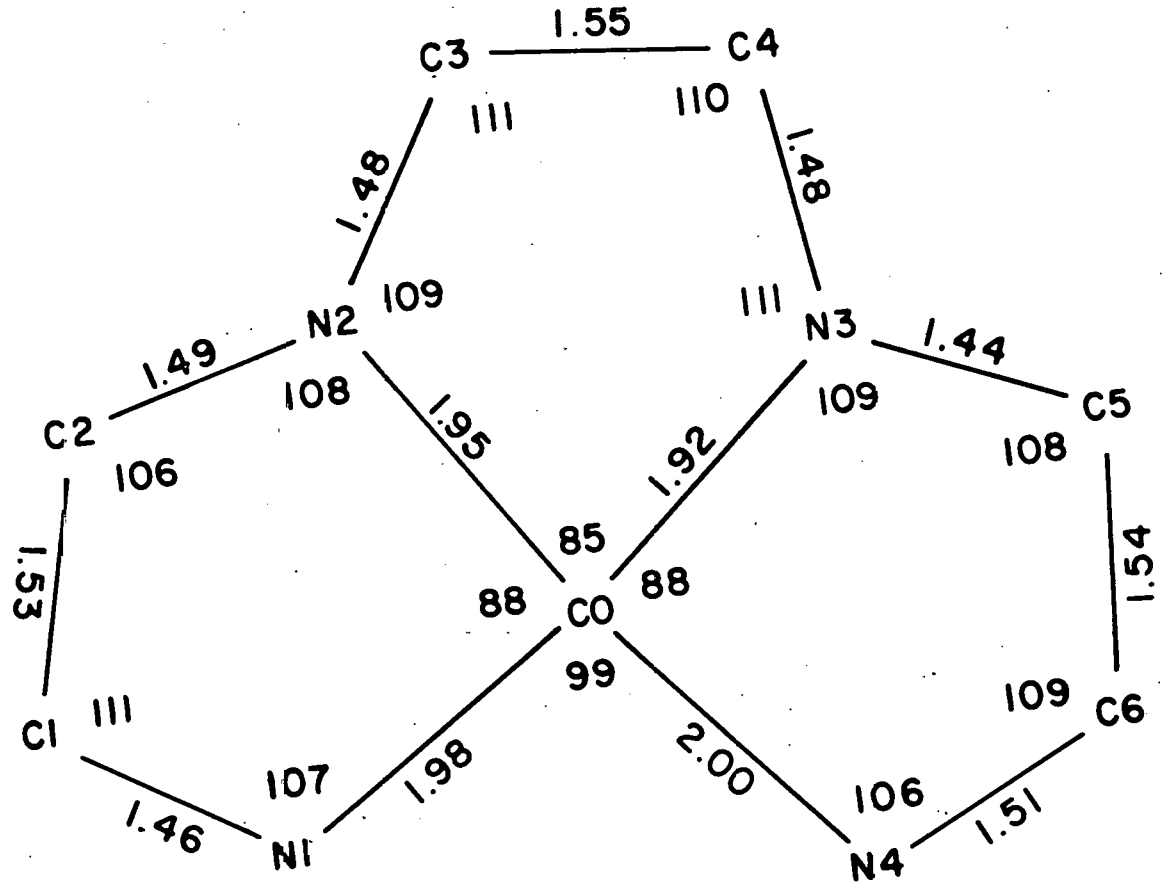


Figure 2. Bond distances and angles within the trien ligand

to 112.3° for Co-N-C bonds, and of 105.2° to 111.4° for N-C-C bonds reported by other investigators of this ligand. The C-N-C bond angles of 116.8° and 114.6° are also reasonable in view of the fact that the Co-N-C angles are, on the average, somewhat less than tetrahedral. These C-N-C angles also agree within three standard deviations with other results obtained in investigations of this ligand.

The bond distances within the trien ligand range from 1.92 to 2.00 Å for Co-N bonds, from 1.44 to 1.51 Å for N-C bonds, and from 1.53 to 1.55 Å for C-C bonds, with average values of 1.96, 1.48, and 1.54 Å, respectively. These distances in no instance differ significantly from previously reported values for other compounds involving the trien ligand coordinated to cobalt.

The four trien nitrogens and the cobalt atom all fall within 0.01 Å of the least squares plane. The three five-membered rings formed by the quadradentate ligand and the cobalt atom are not planar, however, as the carbon atoms are located above and below the N-Co-N planes. Nonetheless, all of the atoms in the trien ligand fall within 0.37 Å of a least squares plane.

As has been described above, the coordination of the cyanide groups to the cobalt is clearly through the carbon. The Co-C average bond distance of 1.90 Å is in good

agreement with previously published values. The average C-N distance of 1.17 Å also agrees quite well with the range of previously reported values, 1.15 to 1.18 Å.[2,22-24] The fact that no part of the chain N(6)-C(8)-Co-C(7)-N(5) is linear, with bond angles of N(6)-C(8)-Co, C(8)-Co-C(7), and Co-C(7)-N(5) of 174.1, 177.9, and 173.7°, respectively, is somewhat unusual but not surprising. Curry and Runciman[2] have already observed such a phenomenon. Much of this can be attributed to steric effects both inside the moiety and between moieties (Figure 3). Significant non-bonded distances are given in Table V.

The Cl-O bond distances in the perchlorate group average 1.42 Å and the angles average 109.5°. The relatively large thermal parameters, possibly due to spatial as well as temporal disorder probably account for the large individual deviations from the average values. However, these average values agree reasonably well with previously published values for this anion.[21] A weak hydrogen bond is possible between N(4) and O(3), which are 3.03 Å apart. Such a hydrogen bond would help stabilize the perchlorate group.

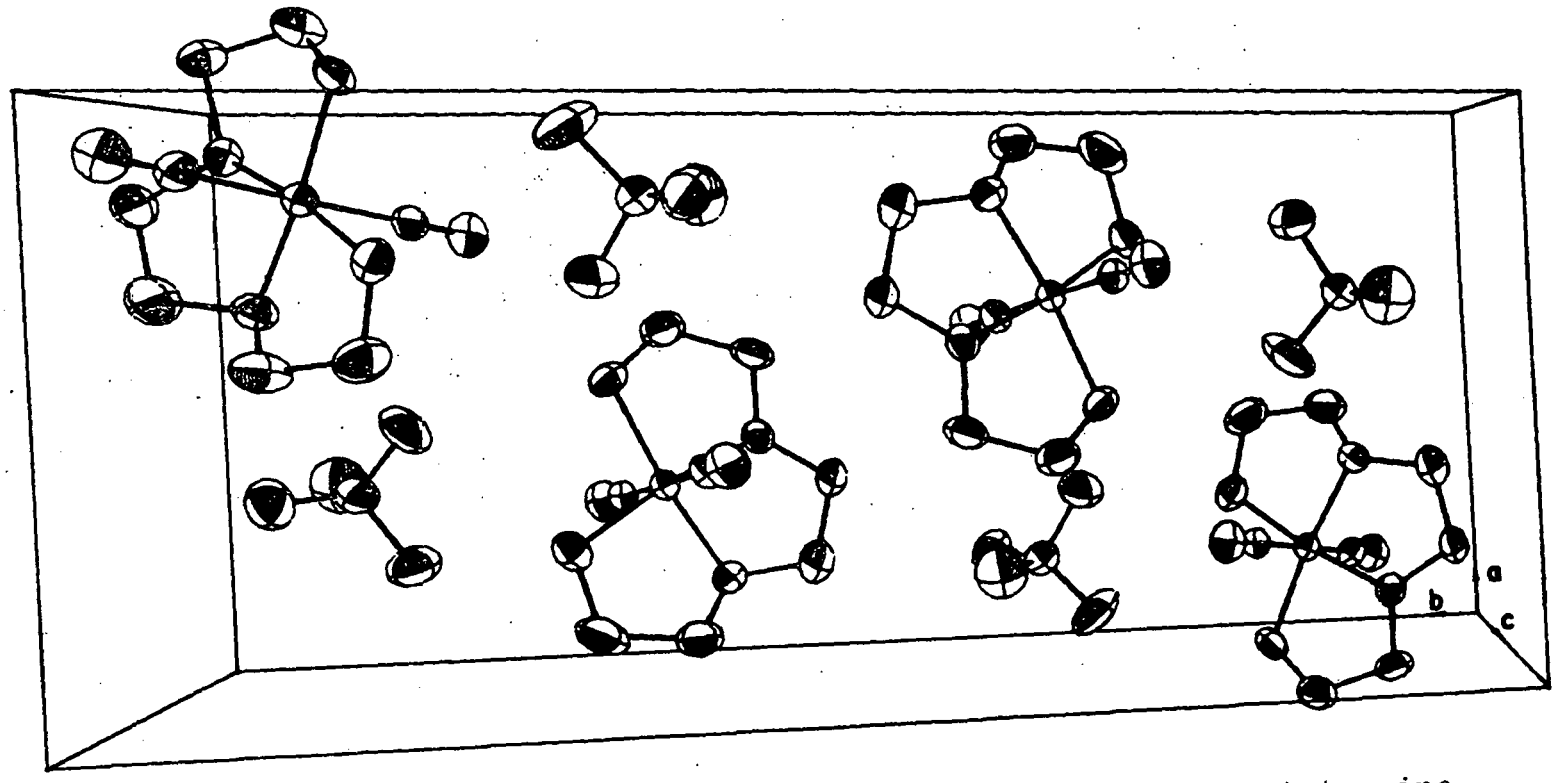


Figure 3. Unit cell showing packing of trans-cyano triethylenetetramine cobalt(III) perchlorate

THE STRUCTURE OF POTASSIUM ANTIMONY(III) PENTACHLORIDE

Introduction

Structural investigations of antimony halide complexes have been actively pursued in this laboratory during recent years, beginning with the work of Lawton and Jacobson.[25] The structures of species containing antimony-(III) are of particular interest because of questions concerning the stereochemical role of the lone pair of electrons.

Only a very few antimony(III) chloride structures have been reported in the literature. $SbCl_3$ exhibits a trigonal pyramid structure with antimony at the apex,[26] while in $(NH_4)_2SbCl_5$ the chlorine atoms are arranged in a square pyramidal coordination geometry around the antimony.[27] In $[C_5H_5NH][Sb^{III}Cl_4]$, the halogen configuration around the antimony can be described as tetragonally distorted octahedral with two of the equitorial atoms removed,[28] and $SbCl_6^{3-}$ forms perfect octahedra in $Co(NH_3)_6SbCl_6$.[29]

Because of the relatively poor determination (R = 0.24) of the structure of $(NH_4)_2SbCl_5$ and because of the seeming variety of structural geometries possible for antimony(III), it was decided to undertake a structure determination of K_2SbCl_5.

Experimental

A sample of K_2SbCl_5 was kindly supplied by Dr. Donald Macalady, who prepared the compound in the following manner: Two solutions, one of $SbCl_3$ in 3N HCl and one of KCl in 3N HCl, were combined so that the molar ratio of potassium to antimony in the resulting solution was 5:7. This solution was allowed to stand, and crystals formed by slow evaporation. Microscopic examination revealed many different crystal morphologies. Thin plates appeared to be the basic unit of all these morphologies, however.

A crystal was cut from one of these plates and mounted on the end of a glass fiber with Duco cement thinned with amyl acetate. Preliminary Weissenberg and precession photographs exhibited 2/m Laue symmetry, indicating a monoclinic space group. The following systematic absences were observed: $h0\ell$ when $\ell = 2n + 1$, and $0k0$ when $k = 2n + 1$. These absences are only consistent with the space group $P2_1/c$. The unit cell parameters at 25°C are $\underline{a} = 8.8686 \pm 0.0007$, $\underline{b} = 12.4577 \pm 0.0013$, $\underline{c} = 8.9280 \pm 0.0013$ Å and $\beta = 110.512 \pm 0.011°$. These parameters and their standard deviations were obtained by a least squares fit[8] to the 2θ values of sixteen independent reflections whose centers were determined by left-right, top-bottom beam splitting on a previously aligned four-circle diffractometer (MoKα radiation, $\lambda = 0.71069$ Å). A calculated

density of 2.711 g/cc for four molecules per unit cell agrees quite well with an observed density of 2.72 ± 0.01 g/cc, determined by flotation techniques.

For data collection the crystal described above, measuring approximately 0.2 mm along each of the crystal axes, was mounted so that the c axis coincided with the ø axis of the diffractometer. Data were collected at room temperature using an automated four-circle diffractometer designed and built in the Ames Laboratory. The upper full circle was purchased from STOE and is equipped with encoders (Baldwin Optical) and drive motors. The design of the base allows the encoders to be directly connected to the main θ and 2θ shafts, using solid and hollow shaft encoders, respectively. The diffractometer is interfaced to a PDP-15 computer in a real time mode and is equipped with a scintillation counter. Zirconium-filtered MoKα radiation was used for the data collection. A scan rate of 0.1 second per step of 0.01° in θ was employed with a variable scan range of 35 steps plus 1 step per degree theta. Stationary-crystal, stationary-counter background counts of a quarter of the scan time were taken at the beginning and end of each scan. Before the scan was made a peak height measurement was used to determine if the reflection was observed. To be scanned, the reflection had to exceed the background by

more than six counts. If the reflection met this criterion, the ω setting was then adjusted slightly, if necessary, to maximize the peak height. Within a two-theta sphere of 50° ($\sin\theta/\lambda$ = 0.595 Å^{-1}), all data in the $hk\ell$ and $\bar{h}k\ell$ octants were measured in this manner, using a take-off angle of 4.5°. Of the 1750 reflections examined, 1614 met the peak height criterion and were scanned.

As a general check on electronic and crystal stability, the intensities of three standard reflections were remeasured every twenty-five reflections. These reflections did not vary to any significant degree during the entire period of data collection.

The intensity data were corrected for Lorentz-polarization effects and for effects due to absorption. An absorption correction was made using the Tompa-Alcock absorption correction program[30,31] using a linear absorption coefficient of μ = 52.28 cm^{-1}. The maximum and minimum transmission factors were 43.95% and 55.98%, respectively. The estimated error in each intensity was calculated by

$$\sigma_I^2 = C_T + 2C_B + (0.03\ C_T)^2 + (0.03\ C_B)^2 + (0.03\ C_I)^2\ T_a^2,$$

where C_T, C_B, C_I, and T_a are the total count, the

background count, the net count, and the transmission factor, respectively, and the factor 0.03 represents an estimate of non-statistical errors. The estimated deviations in the structure factors were calculated by the finite difference method.[10] Of the 1614 independent reflections, 1543 were considered observed ($> 2.0\sigma_F$).

Solution and Refinement

The position of the antimony atom was obtained from analysis of a sharpened three-dimensional Patterson function.[11] The remaining atoms were found by successive structure factor[12] and electron density map calculations.[14] These atomic positions were refined by a full matrix least squares procedure,[12] minimizing the function $\Sigma\omega(|F_o|-|F_c|)^2$, where $\omega = 1/\sigma_F^2$, to a conventional discrepancy factor of $R = 0.169$. The scattering factors used were those of Hanson *et al.*,[15] modified for the real and imaginary parts of anomalous dispersion.[16]

An electron density difference map verified that all the atoms had been accounted for, but indicated that some anisotropic motion, particularly of the antimony, was present. Accordingly, anisotropic refinement was begun and after four cycles of refinement, values of R and ωR of 0.054 and 0.078, respectively, were obtained.

A final electron density difference map showed no peaks greater than 0.9 e/Å^3. A final statistical analysis of $\overline{w\Delta^2}$, where $\Delta = (|F_o| - |F_c|)$, as a function of the scattering angle and magnitude of F_o revealed no unusual trends and suggests that the relative weighting scheme used is a reasonable one.

The final positional and thermal parameters are listed in Table VII. The standard deviations were calculated from the inverse matrix of the final least squares cycle. Bond lengths, bond angles, and significant non-bonded distances[17] are listed in Table VIII. The final values of the observed and calculated structure factors are listed in Table IX.

Description and Discussion

The configuration of $SbCl_5^=$ in K_2SbCl_5 is essentially that of a square pyramid which has been distorted by interionic and packing forces. The inversion-related anions are packed approximately base to base, as depicted in Figure 4.[18] The axial antimony-chlorine bond length is 2.385 Å, in good agreement with the axial distance in $(NH_4)_2SbCl_5$ (2.36 Å),[27] the shorter distance (2.38 Å) in in$[C_5H_5NH][Sb^{III}Cl_4]$,[28] and only slightly longer than the distance (2.32 Å) in $SbCl_3$.[26]

Table VII. Final atomic coordinates and thermal parameters (x 10^4) for K_2SbCl_5 [a]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Sb	0.1836(1)	-0.0068(1)	0.2025(1)	75(1)	42(1)	80(1)	-2(.4)	20(.8)	-3(.4)
Cl(1)	0.2414(3)	0.0959(2)	0.0510(3)	141(4)	55(2)	98(3)	-3(2)	47(3)	3(2)
Cl(2)	-0.0097(3)	0.1519(2)	0.2070(3)	90(3)	51(2)	160(4)	6(2)	47(3)	2(2)
Cl(3)	0.4157(3)	-0.1400(2)	0.2121(3)	143(4)	68(2)	115(4)	35(2)	41(3)	.8(2)
Cl(4)	0.3885(3)	0.1137(2)	0.3563(3)	89(3)	61(2)	99(3)	-17(2)	26(3)	-9(2)
Cl(5)	0.1706(3)	-0.0770(2)	0.4611(3)	118(4)	67(2)	100(3)	-11(2)	40(3)	16(2)
K(1)	0.1853(3)	0.1746(2)	0.5939(3)	135(3)	56(1)	112(3)	2(2)	52(3)	-1(2)
K(2)	0.3742(3)	-0.1285(2)	0.8452(3)	106(3)	94(2)	129(4)	5(2)	43(3)	-24(2)

[a] Anisotropic thermal parameters are defined by:

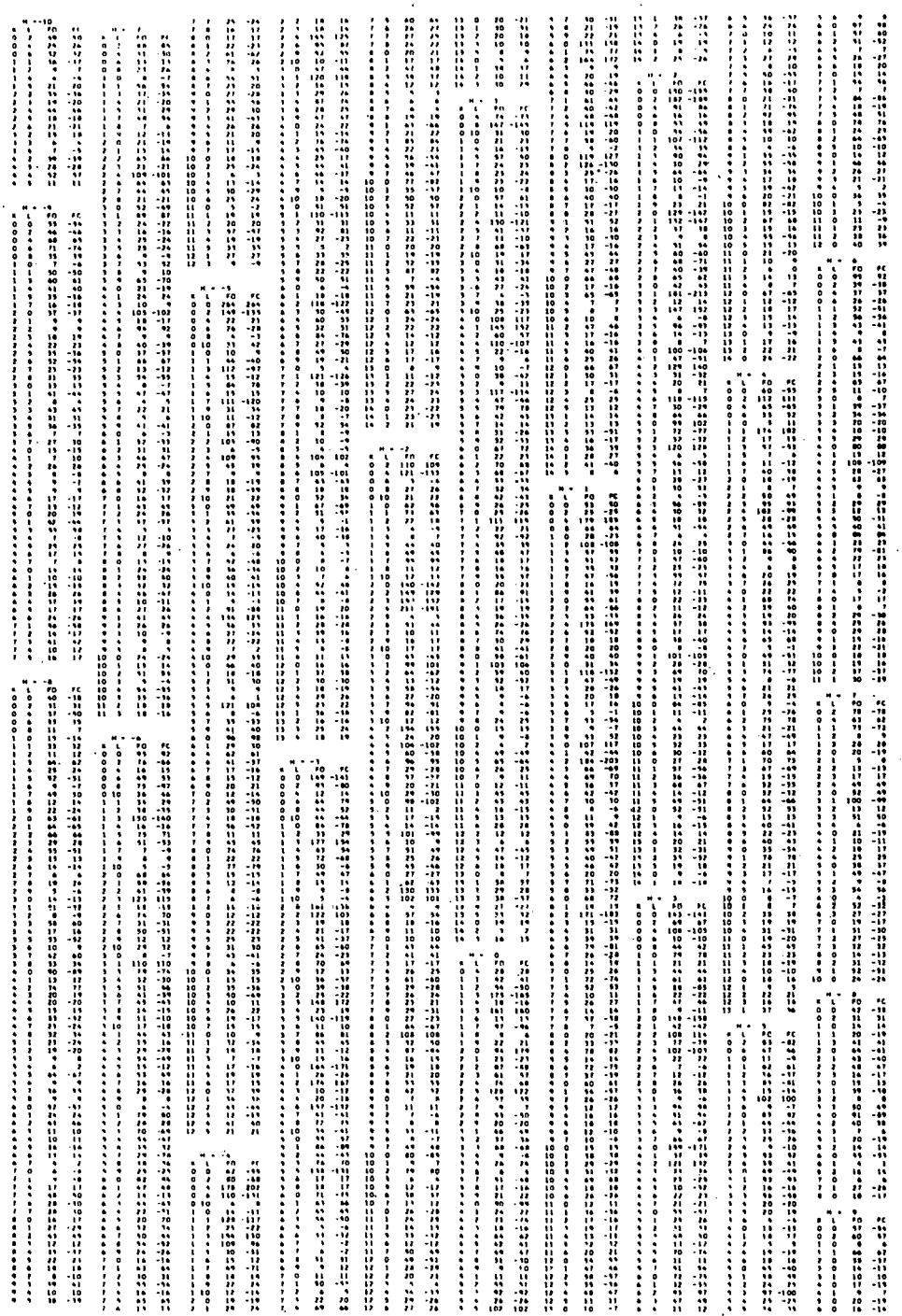
$$T = \exp -(h^2\beta_{11} + k^2\beta_{22} + \ell^2\beta_{33} + hk\beta_{12} + h\ell\beta_{13} + k\ell\beta_{23}) .$$

Table VIII. Bond lengths, bond angles, and significant non-bonded distances in K_2SbCl_5[a]

Sb-Cl(1)	2.799(2)	Sb-Cl(2)	2.625(2)
Sb-Cl(3)	2.622(2)	Sb-Cl(4)	2.385(2)
Sb-Cl(5)	2.509(2)		
Cl(4)-Sb-Cl(1)	81.92(7)	Cl(4)-Sb-Cl(2)	83.54(8)
Cl(4)-Sb-Cl(3)	87.06(8)	Cl(4)-Sb-Cl(5)	87.77(8)
Cl(1)-Sb-Cl(2)	88.50(7)	Cl(2)-Sb-Cl(5)	90.43(8)
Cl(5)-Sb-Cl(3)	92.19(3)	Cl(3)-Sb-Cl(1)	87.22(8)
Cl(1)-Sb-Cl(5)	169.69(8)	Cl(2)-Sb-Cl(3)	170.13(8)
Sb-Sb'	3.932(1)	Sb-Cl(2)'	3.881(3)
Cl(1)-Sb'	3.701(2)	Cl(1)-Cl(2)'	3.699(3)
$Cl(2)-Cl(5)_{i}$	3.768(3)	$Cl(1)-Cl(3)_{ii}$	3.832(4)
$Cl(1)-K(1)_{iii}$	3.187(3)	$Cl(1)-K(2)_{iii}$	3.290(3)
$Cl(2)-K(2)_{iii}$	3.168(3)	$Cl(1)-K(1)_{iv}$	3.247(3)
$Cl(2)-K(1)_{iv}$	3.147(3)	$Cl(3)-K(2)_{v}$	3.190(4)
Cl(2)-K(1)	3.289(3)	Cl(4)-K(1)	3.317(3)

[a] Primed atoms are those related by the center of inversion, as in Figure 4. Other symmetry operations referred to are: (i) -x, ½+y, -z; (ii) x, y, z-1; (iii) x, ½-y, z-1; (iv) x, -½-y, z-1; (v) 1-x, -y, -z.

Table IX. Observed and calculated structure factors



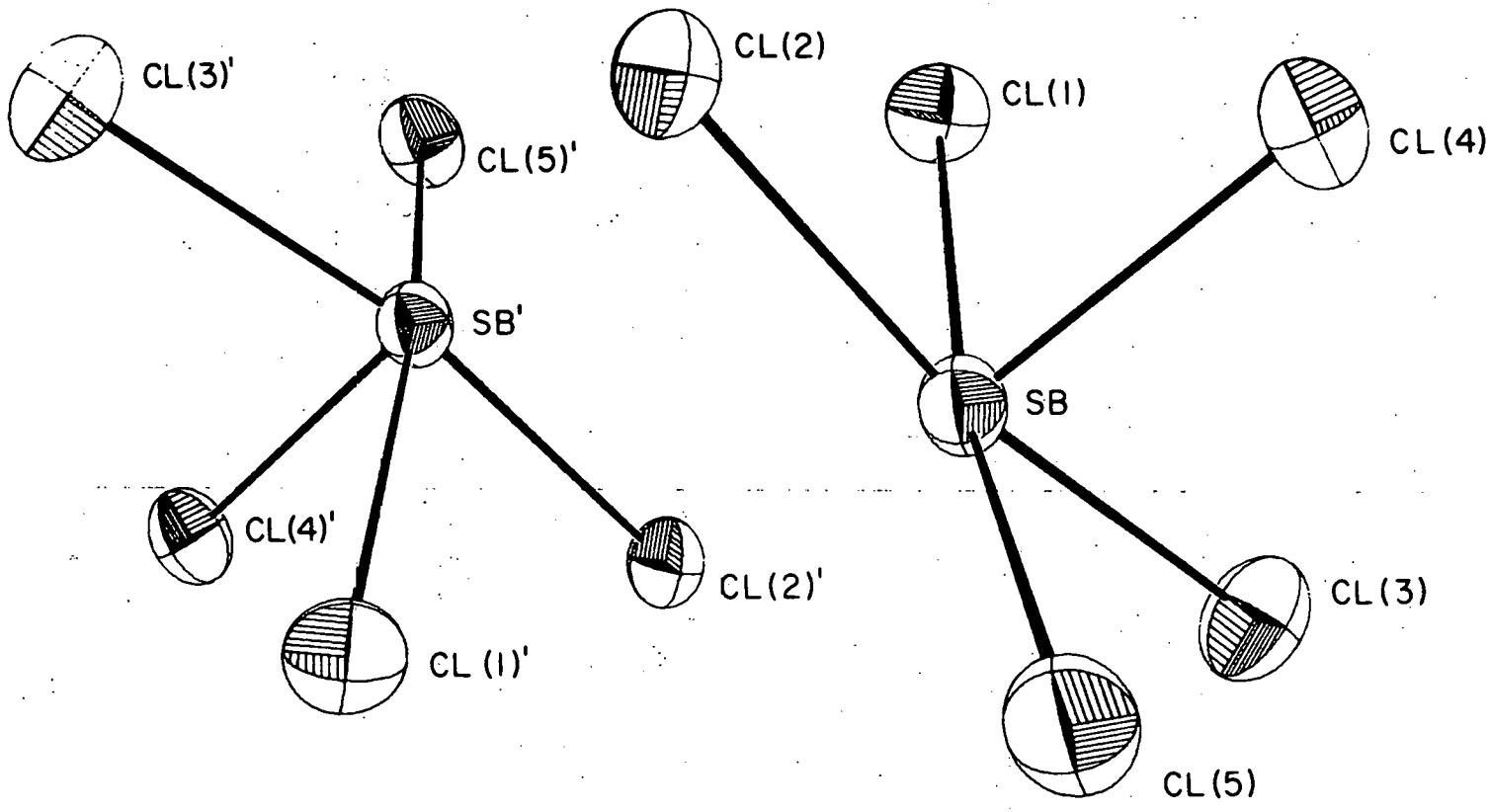


Figure 4. Two inversion-related $SbCl_5^=$ anions

The antimony-chlorine bond distances in the base are all considerably longer than the axial distance. Two of these distances are almost identical (2.622, 2.625 Å) and involve chlorines trans to each other. The other pair of chlorines form bonds of 2.799 and 2.509 Å length, with an average of 2.654 Å. In $(NH_4)_2SbCl_5$ all basal antimony-chlorine bonds were found to be essentially of equal length (2.62 Å average) while in $[C_5H_5NH][SbCl_4]$ the corresponding bond length for chlorines trans to one another is 2.63 Å.

In the present study, the lengthening of the Sb-Cl(1) distance to 2.799 Å appears to be due to electrostatic repulsions and packing effects, as it is this chlorine that is involved in the closest non-bonded contacts; significant non-bonded distances are given in Table VIII. An antimony atom is only 3.701 Å from Cl(1), whereas the sum of the van der Waal's radii is 4.0 Å. Also, the shortest chlorine-chlorine distance found, 3.699 Å, is between this chlorine and Cl(2)'. Both these distances would become significantly shorter if the Sb-Cl(1) bond were shortened. Thus, it can be inferred that this bond can be readily distorted if more efficient packing of the ions results. The shortening of the Sb-Cl(5) bond appears to be a trans effect in response to the lengthening of the Sb-Cl(1) bond.

The observed bond lengths of the basal antimony-chlorine bonds described above are consistent with characterizing the antimony bonding orbitals as being composed primarily of p-orbitals as in the three-center four-electron bonding scheme described by Porter and Jacobson.[32] The lone pair appears to have a comparatively small stereochemical effect. This is supported by the relatively short antimony-antimony distance of 3.932 Å, where localized lone pairs, if present, would have to be directed toward one another. Distortions of the Cl-Sb-Cl bond angles from the expected 90° (cf. Table VIII) can be explained by interionic repulsions between inversion-related complexes.

The arrangement of the $SbCl_5^=$ complexes in the unit cell is such that the chlorine atoms approximate a closest packed arrangement in the bc plane, as is evident in Figure 5, with the shortest chlorine-chlorine distances approximating the sum of the van der Waal's radii. None of the potassium ions lie between these planes, but rather are located among the $SbCl_5^=$ ions in the planes. The shortest potassium-chlorine distance is 3.147 Å.

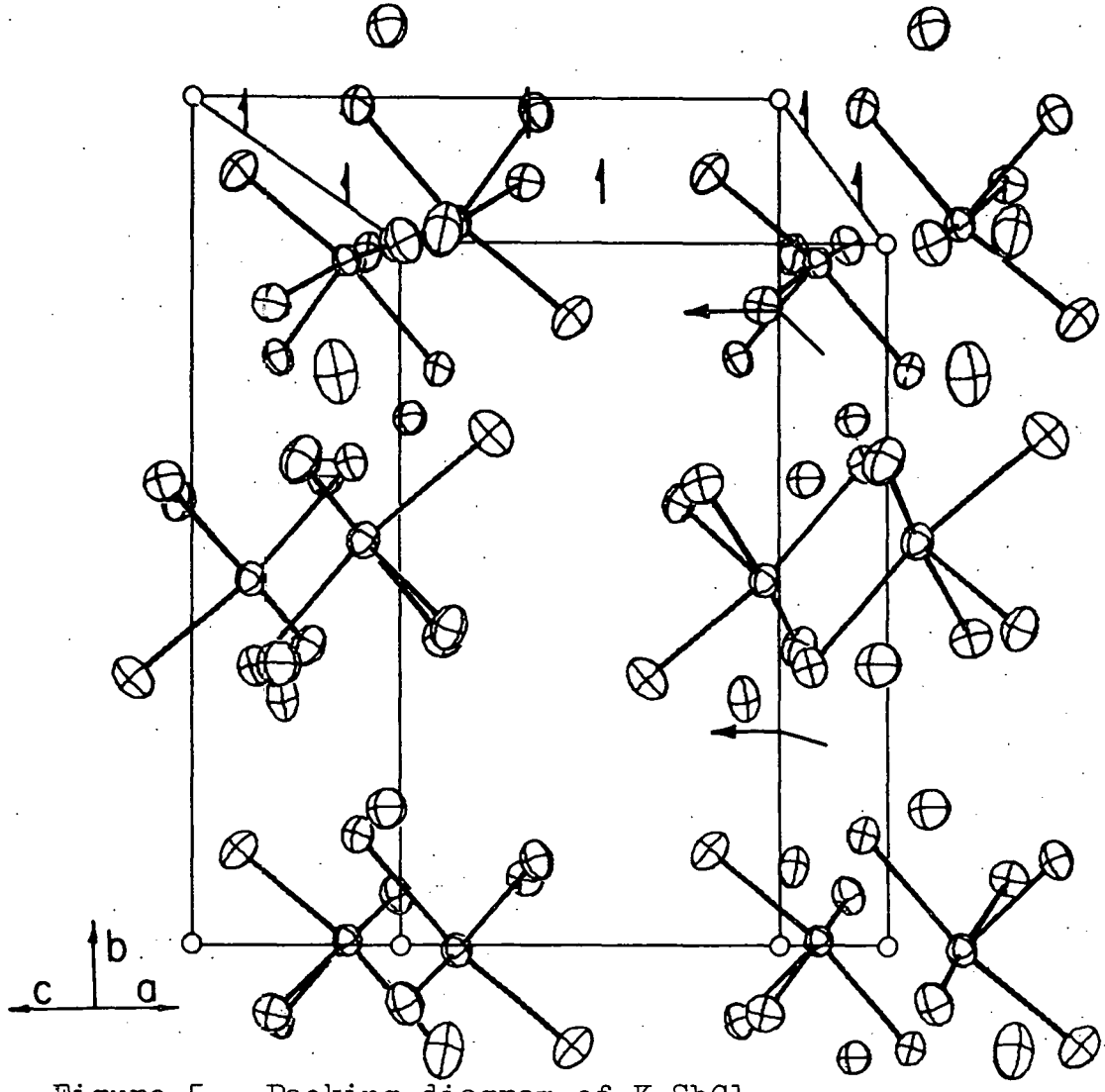


Figure 5. Packing diagram of K_2SbCl_5

ALOP: A PROGRAMMED, SEMI-AUTOMATIC VERSION OF THE PSEUDO HEAVY ATOM TECHNIQUE

Introduction

The increasing availability of high speed digital computers has enabled the crystallographer to make much more frequent use of mathematical techniques which previously were extremely time consuming. This fact has greatly enhanced the development and usage of direct methods, which recently have evolved to such an extent as to permit semi-automatic solution of crystal structures. In contrast, such indirect methods as Patterson superposition techniques have been employed more and more infrequently in recent times. Despite their great power, these latter methods require a great deal of human intervention and are somewhat tedious to perform. Clearly, what is required is a series of programs which would enable one to solve a structure using superposition techniques but requiring a minimum of human intervention.

This series of programs probably would have greatest applicability to, and thus should be specifically designed to solve, the pseudo heavy atom problem, in which the "heavy" atom does not contribute enough to the phasing to make heavy atom methods feasible. This problem occurs with compounds in which there are many light atoms and but

few heavy atoms, such as transition metal complexes or heavy atom derivatives of organic compounds.

In what follows, the essential features of this series of programs are detailed. The techniques employed naturally divide into two categories: (1) preparation of a Patterson map suitable for evaluation, and (2) utilization of this map to solve the structure.

Map Preparation

A sharpened Patterson map[11] is created on either tape or disk by the program ALFF[14] or any other similar Fourier series program. However, in this form the map is somewhat cumbersome to analyze. Hence, the program ALPP (Ames Laboratory Peak Picker) finds and outputs the heights and positions of all the peaks above a certain limit on the Patterson map. ALPP is divided into four subprocedures, the function of which is described below, and a main procedure, which controls the order of execution of the subprocedures. The program listing for ALPP is given in Appendix A.

Input to the first subprocedure, SETUP, consists of the size of the map and the minimum height of a peak which should be recognized. This subprocedure then reads and rewrites the map by layers, setting all points less than the minimum limit equal to zero.

The second subprocedure, LAYERS, reads these map layers and outputs layers with all non-peak grid points negated. The essence of this subprocedure is the subroutine PICKER, which is flowcharted in Figure 6. PICKER analyzes a line of the map point by point. The absolute value of each point is compared with that of the point before it. The lesser of the two is negated. LAYERS calls PICKER for each row and each column of the layer, and then compares points located diagonally to each point, negating those with smaller absolute values.

The next subprocedure, NTRLAY, compares the absolute value of a peak with those of the nine peaks adjacent to it in the next layer, again negating the smaller values. The only positive grid points which now remain are those of peaks. Next, these peak locations and heights are output and the modified map is printed, if desired for debugging purposes.

The final subprocedure, PKSORT, is a modified PL/I translation of QSTSRT. PKSORT sorts the peaks in order of decreasing height and outputs the ordered peaks.

The entire program runs in less core and requires somewhat less execution time than does ALFF. Thus, it is feasible to run the two programs back to back as one job.

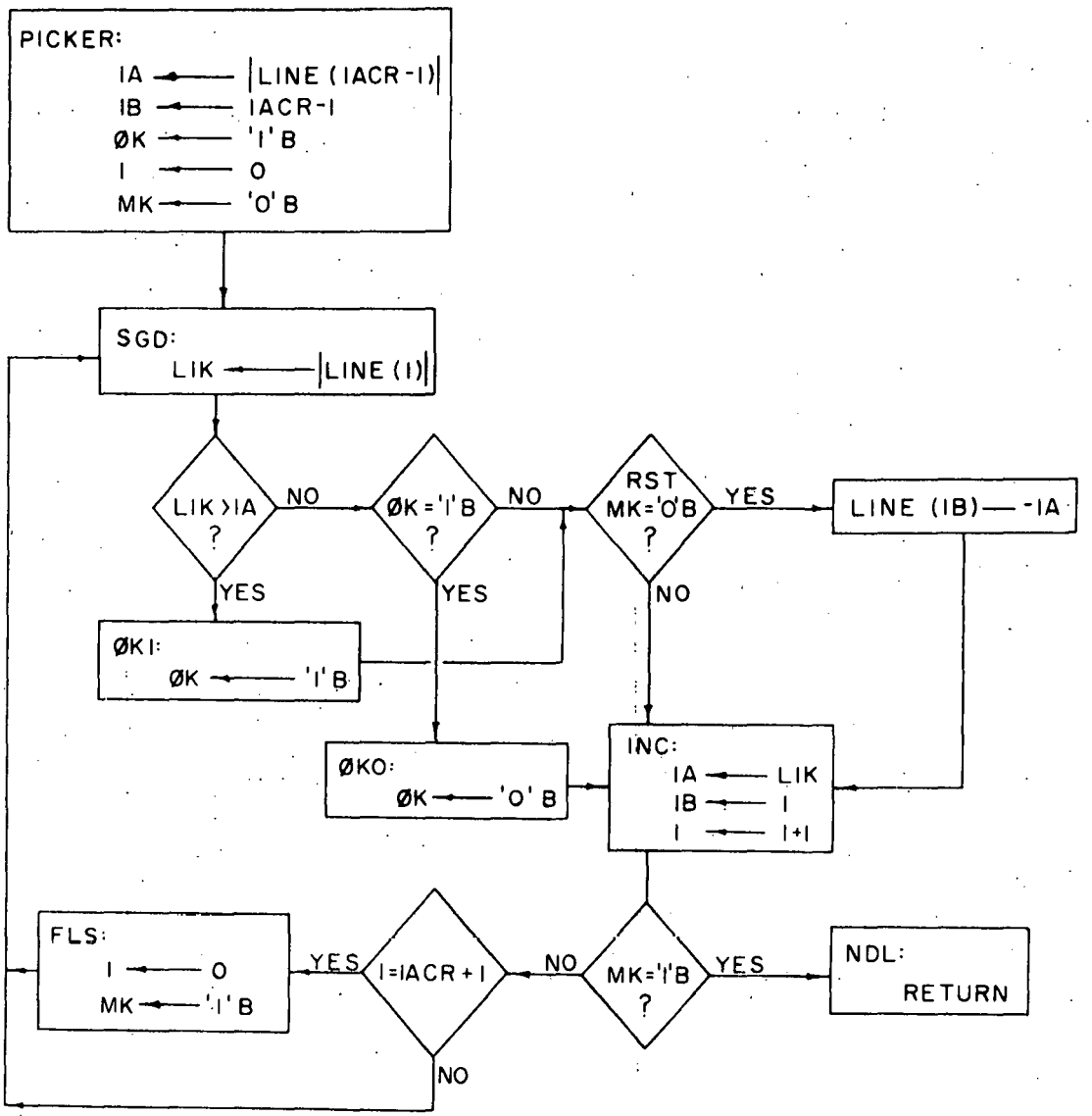


Figure 6. Flowchart of subroutine PICKER

Solution of the Structure

The main program of the series is ALOP (Ames Laboratory Origin Picker), and the program listing is given in Appendix B. ALOP is divided into a main procedure and seven subprocedures.

The main procedure reads in the size of the map, the number of peaks produced by ALPP, and the symmetry operations of the space group under consideration. These are in the form: $p_x x + q_x$, $p_y y + q_y$, $p_z z + q_z$, where p_x, p_y, p_z = 1 or -1 and q_x, q_y, q_z = 0 or ½. Thus one can represent an equivalent position produced by: an inversion, a two-fold axis, a two-fold screw axis, a mirror plane in one of the three crystal directions or an a-, b-, or c-glide plane. Any of the triclinic, monoclinic, or orthorhombic space groups can be represented by these five symmetry operations (except Fdd2 or Fddd). In addition, any of the other 230 crystallographic space groups can be converted into a space group which only uses these operations, although some loss of symmetry generally occurs.

The first subprocedure, PART1, searches the peaks produced by ALPP for a suitable heavy atom peak. This peak must be among the largest 20% of the peaks. In addition, if any of its coordinates, u, v, w, is equal to 0 or ½ of the unit cell, then it must be at least twice as large as the largest peak which has no one of u, v, w

equal to 0 or ½. These criteria assure that the heavy atom peak chosen is not solely a Harker vector, but allow the choice of a heavy atom which has 0 or ½ as one of its three coordinates, such as the antimony atom in K_2SbCl_5.

When PART1 finds a suitable heavy atom peak, it prints its coordinates, u_H, v_H, w_H, and uses it as the shift vector of an in-core algebraic superposition. For a peak u, v, w, to be retained, there must also be a peak at $u' = u + u_H$, $v' = v + v_H$, $w' = w + w_H$ in the list of peaks produced by ALPP. In practice, since ALPP only determines the maximum grid point, and not the center, of each peak, these requirements are somewhat too stringent and thus u', v', w' is permitted to be off by one grid point in each direction. The values of u', v', w' thus found are output for subsequent use.

PART2 assumes that the peaks produced by PART1 represent an electron density map of the compound, with its origin shifted to t_x, t_y, t_z, i.e., the following relations hold: $u_i = x_i + t_x$, $v_i = y_i + t_y$, $w_i = z_i + t_z$, where x_i, y_i, z_i are the coordinates of the peak in electron density space. When the symmetry operations defined above are applied to a peak at x, y, z they produce an equivalent peak at $p_x x + q_x$, $p_y y + q_y$, $p_z z + q_z$. Thus for every peak at $u = x + t_x$, $v = y + t_y$, $w = z + t_z$ there is an equivalent peak at $u' = p_x x + t_x + q_x$, $v' = p_y y + t_y$

$+ q_y$, $w' = p_z z + t_z + q_z$. In Table X the results of subtracting and adding u, v, w and u', v', w' are given for all permutations of p_x, p_y, p_z. The asterisked (*) sums determine values of t_x, t_y, and t_z. PART2 and PART3 accumulate all possible values of t_x, t_y, and t_z for the symmetry operations, as shown in Table XI. PART3 and PART4 write these values, along with the frequency of occurrence of each, on file SORTIN for future use. If any one of t_x, t_y, t_z is not determined, as is the case with all but inversion symmetry, it is set equal to -1. In addition to writing out the exact values of t_x, t_y, and t_z, those which are as much as one grid point off in each direction are also written out. Tables X and XI also demonstrate that values of t_x, t_y, t_z determined by two-folds, screws, mirrors, and glides have to meet criteria before they are acceptable, whereas inversions do not. Therefore, a greater weight is placed on these former values.

At this point, the following items may be present on file SORTIN: t_x, t_y, t_z triples; t_x, t_y; t_y, t_z; or t_x, t_z doubles; or t_x, t_y, or t_z singles. These are sorted by the IBM procedure IHESRTA within their different types in order of decreasing frequency of occurrence. PART5 reads and stores 1/64 of the triples, 1/16 of the doubles, and 1/4 of the singles, all of which have the largest frequencies. These singles, doubles, and triples

Table X. Relationships used in determining t_x, t_y, t_z

Quantity	u	v	w
U	$A = x + t_x$	$B = y + t_y$	$C = z + t_z$
U_0	$A + q_x$	$B + q_y$	$C + q_z$
$U_0 + U$	$2A + q_x$	$2B + q_y$	$2C + q_z$
$U_0 - U$	q_x	q_y	q_z
U_1	$-x + t_x + q_x$	$B + q_y$	$C + q_z$
$U_1 + U$	* $2t_x + q_x$	$2B + q_y$	$2C + q_z$
$U_1 - U$	$-2x + q_x$	q_y	q_z
U_2	$A + q_x$	$-y + t_y + q_y$	$C + q_z$
$U_2 + U$	$2A + q_x$	* $2t_y + q_y$	$2C + q_z$
$U_2 - U$	q_x	$-2y + q_y$	q_z
U_3	$-x + t_x + q_x$	$-y + t_y + q_y$	$C + q_z$
$U_3 + U$	* $2t_x + q_x$	* $2t_y + q_y$	$2C + q_z$
$U_3 - U$	$-2x + q_x$	$-2y + q_y$	q_z
U_4	$A + q_x$	$B + q_y$	$-z + t_z + q_z$
$U_4 + U$	$2A + q_x$	$2B + q_y$	* $2t_z + q_z$
$U_4 - U$	q_x	q_y	$-2z + q_z$
U_5	$-x + t_x + q_x$	$B + q_y$	$-z + t_z + q_z$
$U_5 + U$	* $2t_x + q_x$	$2B + q_y$	* $2t_z + q_z$
$U_5 - U$	$-2x + q_x$	q_y	$-2z + q_z$

Table X. (Continued)

Quantity	u	v	w
U_6	$A + q_x$	$-y + t_y + q_y$	$-z + t_z + q_z$
$U_6 + U$	$2A + q_x$	$* 2t_y + q_y$	$* 2t_z + q_z$
$U_6 - U$	q_x	$2y + q_y$	$2z + q_z$
U_7	$-x + t_x + q_x$	$-y + t_y + q_y$	$-z + t_z + q_z$
$U_7 + U$	$* 2t_x + q_x$	$* 2t_y + q_y$	$* 2t_z + q_z$
$U_7 - U$	$2x + q_x$	$2y + q_y$	$2z + t_z$

Table XI. Restrictions placed on the determination of t_x, t_y, t_z by the type of symmetry element

Type of symmetry element	Determines	Restrictions
Plane perpendicular to x	t_x	$v_1 - v = q_y$, $w_1 - w = q_z$
Plane perpendicular to y	t_y	$u_2 - u = q_x$, $w_2 - w = q_z$
Plane perpendicular to z	t_z	$u_4 - u = q_x$, $v_4 - v = q_y$
Axis in x	t_y, t_z	$u_6 - u = q_x$
Axis in y	t_x, t_z	$v_5 - v = q_y$
Axis in z	t_x, t_y	$w_3 - w = q_z$
Inversion	t_x, t_y, t_z	None

are then merged with each other as described in Table XII, with a latitude of one grid point allowed in each direction. Thus, if a single in t_x equals the t_x of a t_x, t_y double or is off by one grid point, then the frequency of the t_x, t_y double is increased by the frequency of the single. A record is kept of each such merge.

This record is used in PART6, where all of the possible mergings for each symmetry element present are computed. Consider, as an example, the space group $P2_1/c$ which has an inversion producing a triple t_x, t_y, t_z, a two-fold screw axis producing a double in t_x, t_z and a c-glide producing a single in t_y. PART5 should have merged a single in t_y and a double in t_x, t_z with each triple and left a record of having done so. The values of the triples which were not suitably merged are eliminated, and the triple remaining with the highest frequency of occurrence is then output for use in PART7.

Sometimes, however, a space group may not have an inversion. If it has three two-fold or screw axes, these will produce three doubles: t_{x1} t_{y1}, t_{x2} t_{z2}, t_{y3} t_{z3}. In the cases where $t_{x1} = t_{x2}$, $t_{y1} = t_{y3}$, and $t_{z2} = t_{z3}$, a triple is created with a frequency equal to the sum of the frequencies of the three doubles. The highest such triple is then taken as the origin. If any one of t_x, t_y, or t_z is not determined by the above procedures, it

Table XII. Merging of singles and doubles into doubles and triples

Single or double	Double or triple merged into
t_x	$t_x\ t_y$, $t_x\ t_z$, $t_x\ t_y\ t_z$
t_y	$t_x\ t_y$, $t_y\ t_z$, $t_x\ t_y\ t_z$
t_z	$t_x\ t_z$, $t_y\ t_z$, $t_x\ t_y\ t_z$
$t_x\ t_y$	$t_x\ t_z$, $t_y\ t_z$, $t_x\ t_y\ t_z$
$t_x\ t_z$	$t_x\ t_y$, $t_y\ t_z$, $t_x\ t_y\ t_z$
$t_y\ t_z$	$t_x\ t_y$, $t_x\ t_z$, $t_x\ t_y\ t_z$

is set to zero, as the origin may have any value in that direction.

PART7 computes the electron density space coordinates of all the peaks found in PART1 by using the equations: $x_i = u_i - t_x$, $y_i = v_i - t_y$, $z_i = w_i - t_z$. For each peak, this procedure then attempts to find the symmetry equivalent peaks. If at least half of the equivalent peaks are present, a peak is output with the appropriate fractional coordinates.

ALOP uses less than 32K words of main core storage and runs in less than five minutes of CPU time for a 32 x 32 x 32 map with less than 500 peaks input from ALPP.

Results

The programs ALPP and ALOP were tried on two different problems and the technique was successful in both cases. In the first case, the structure of D-(1,5)-glucono lactone (space group $P2_12_12_1$)[33] was "chlorinated" by substituting chlorines for two of the hydrogens, yielding a molecule with two chlorines, six oxygens, and six carbons. The heavy atom ratio for this compound was $\Sigma Z^2_{heavy} / \Sigma (Z_{light})^2 = 0.963$. All of the non-hydrogen atoms were used in a structure factor calculation and a sharpened Patterson map was computed from these structure factors. ALPP found 502 off-origin peaks in this map with heights rang-

ing from 13 to 234. A heavy atom peak, which proved to be an oxygen-chlorine vector, was found at u = 30, v = 26, w = 3 with a height of 99 on the 32 x 32 x 32 map. In-core superposition retained 187 peaks with a minimum height of 23. This is a good demonstration of how the superposition process tends to eliminate spurious peaks. Multiple merging produced eleven possible origins, of which the one with the highest frequency of occurrence was $t_x = 14$, $t_y = 13$, $t_z = 12$. When this value was used as an origin, 33 symmetry independent peaks were retained. Subsequent least square refinement of the positional parameters and atom multipliers of these 33 positions through twelve least squares cycles resulted in a conventional discrepancy factor of R = 0.206. The scattering factor curve for this and the subsequent test case is defined by:

$$\hat{f}_i = \sum_{j=1}^{N} f_{ij} \Big/ \sum_{j=1}^{N} Z_j,$$

where f_{ij} is the normal scattering factor for the j^{th} atom over a range of $\sin\theta/\lambda$,[15] Z_j is the atomic number of the j^{th} atom, and the sum is over all the atoms in the unit cell.

The second test case was that of K_2SbCl_5 which crystallizes in space group $P2_1/c$ with four eight-atom moieties per unit cell. The heavy atom ratio for this compound is 1.200. ALPP found 258 off-origin peaks on the sharpened

Patterson map, ranging in height from 17 to 508. A heavy atom peak, which was produced by an antimony-antimony vector, was found at u = 20, v = 16, w = 3 with a height of 282 on the 32 x 32 x 32 map. In-core superposition retained 112 peaks. The origin with the highest frequency of occurrence was at t_x = 10, t_y = 0, t_z = 9, and its use yielded 20 symmetry independent peaks. Sixteen cycles of full matrix least squares refinement of the positional parameters and atom multipliers of these positions led to the removal of eleven of them as their atom multipliers dropped to less than 0.40. The remaining nine positions refined to yield a conventional discrepancy factor of R = 0.240.

PSST: A COMBINATION OF PATTERSON SUPERPOSITION AND SIGMA-2 TECHNIQUES FOR PHASE DETERMINATION

Introduction

At present there are two methods commonly used for solving structures of moderate complexity. Direct methods, such as those using the Σ_2 relation,[34] are primarily reciprocal space methods, while methods based on the deconvolution of the Patterson function (for a detailed bibliography see Buerger[35]) are primarily real space methods.

There is a certain parallelism between these two methods and both have their advantages and disadvantages. Both involve some initial choices which can greatly influence the success of the method. The Σ_2 relation can be readily programmed and many automatic or semi-automatic procedures have been developed based on this relation. However, it is usually difficult to make use of known structural information in this approach. Furthermore, if no reasonable structure is produced, the investigator has little recourse but to modify his choice of origin-determining reflections or to closely examine those phases selected at the early and most critial part of this phase determination procedure. With Patterson methods, on the other hand, there are usually a greater number of options initially available corresponding to differing modes of

selection of peaks for superposition. Also, known structural information can be more readily introduced, since a real space representation is being employed. For complex structures, however, large numbers of superpositions are generally required and severe degradation of the structural image can result due to the accumulation of errors in the atom position selections.

The advent of the fast Fourier transform technique and its application to crystallography[36] allows rapid real space - reciprocal space conversions. Thus, it is appropriate to consider whether a hybrid direct method - Patterson method approach having greater power than either method alone can be developed. It is just such a hybrid that is described here.

Theoretical Basis of the Method

In direct methods employing the Σ_2 relation, one starts with E's of large magnitude so that phases will be determined with reasonably high probabilities. Due to the fact that the initial contributors are few in number, erroneous phase indications may still result which then propagate in the phase determination procedure. Consider the map produced by a Fourier transform using as non-zero coefficients only those reflections input into the Σ_2 relation (henceforth this map will be referred to as the Σ_2 map). For the phase determination procedure to be successful, it

is necessary that the square of this Σ_2-map better resemble the true electron density function than does the Σ_2-map itself. If so, the phases of the transformed coefficients with larger magnitudes should be good approximations to the phases of the corresponding large $|E|$'s.

Since the initial set of E's is very small in number, possibly only the three origin-determining reflections, it is the characteristics of the Σ_2-map which should be closely examined. First, if large $|E|$'s are used, there is a high probability that atoms will lie on, or at least near, some of the maxima occurring on this map. Second, there will be a large number of extraneous maxima on the square of the Σ_2-map -- a number far exceeding the number of atoms in the cell. The first is an asset and the second a liability for successful phase determination. These extraneous peaks come from either maxima or minima on the Σ_2-map. It is the presence of these extra peaks that greatly inhibits the production of additional phase information.

One would like to modify the square of the Σ_2-map so that it better resembles the electron density function. An obvious such modification is to eliminate all negative regions (or possibly regions less than a certain lower bound) by setting these regions equal to zero before squaring. Indeed, this technique has been applied by Barrett

and Zwick[37] to some extent in the extension and refinement of crystallographic protein phases.

In the initial application of the Σ_2 relation, there are so few phased E's that even with the modification described above, there are large positive regions in many areas of the map which do not correspond to atomic locations. However, the Patterson function contains images of the structure with each atom in turn at the origin. Therefore, if an atomic position can be selected on the Σ_2-map, a superposition of the appropriately scaled Patterson map on this position should produce a map with considerably fewer extraneous peaks and with much better resemblance to the electron density function. If such a map is then squared to emphasize the higher peaks and transformed, better and more extensive phase information will result. Once a sufficiently large set of phased E's has been obtained, the remaining |E|'s can be efficiently phased by normal application of phase extension and refinement techniques of the Σ_2 type.

Application of the Method

Centric case

The compound β-picoline-N-oxide fumaric acid adduct[38] was chosen as a centrosymmetric test case. We felt this would be a good test case as the structure had previously been solved only with difficulty by use of a roving model --

vector verification technique after usual superposition and symbolic addition procedures had not proved successful.

This adduct crystallizes in the space group $P2_1/c$ with $\underline{a}$ = 3.888, $\underline{b}$ = 14.194, $\underline{c}$ = 14.666 Å and β = 98.85°. There are two adducts of formula $C_{16}H_{18}N_2O_{12}$ per unit cell, *i.e.*, the adduct has a center of symmetry. Values of $|E|$ were computed in the ordinary way and there were 270 $|E|$'s greater than 1.0. The three selected origin-determining reflections are given in Table XIII. These three, along with the symmetry-related reflections, were used in a Σ_2-map calculation (32 x 32 x 32 grid points). Some typical sections of this map are shown in Figure 7.

The positions of the five highest peaks on this map were noted and in each case checked by examining the Patterson for the presence of vectors between symmetry-related atoms. In each case, such vectors were found and indeed these peaks fell approximately (within 0.5 Å) at the positions of four carbons and a nitrogen in the structure.

All of the negative regions in the Σ_2-map were then set equal to zero and five independent superpositions were carried out by placing the origin of the Patterson at each of the five peak positions and the symmetry-related points. A sharpened Patterson function was used and the minimum procedure employed.[39] The scale of the Patterson was

Table XIII. Origin-determining reflections for the centric test case (β-picoline-N-oxide fumaric acid adduct)

h	k	l	|E|	Sign
1	0	2	4.17	+
3	1	3	2.53	-
1	14	-5	2.14	+

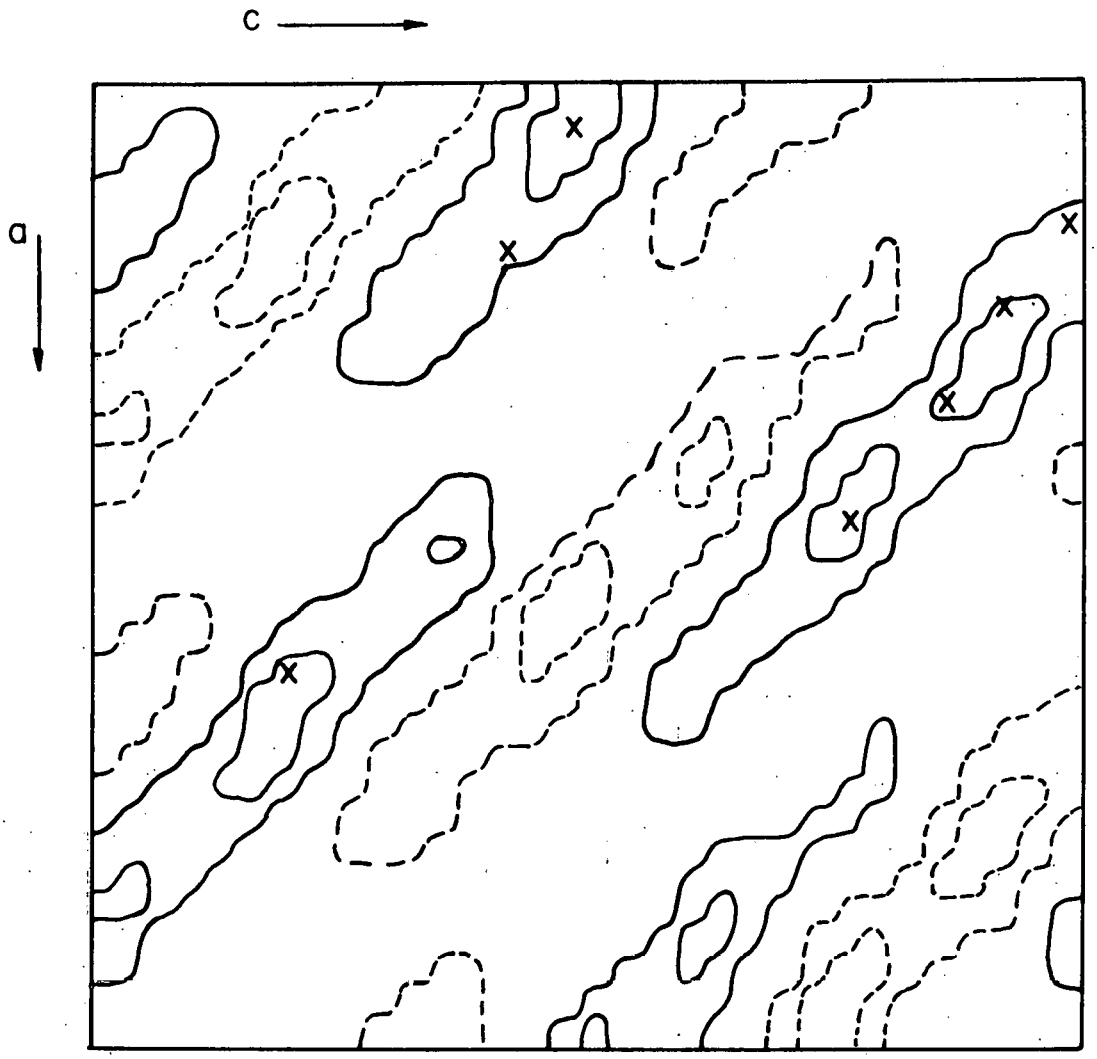


Figure 7a. Composite of layers 3,4,5 of a Σ_2-map for β-picoline-N-oxide fumaric acid adduct. —— contoured at 40 and 80. ---- contoured at -40 and -80. Atom positions indicated by X.

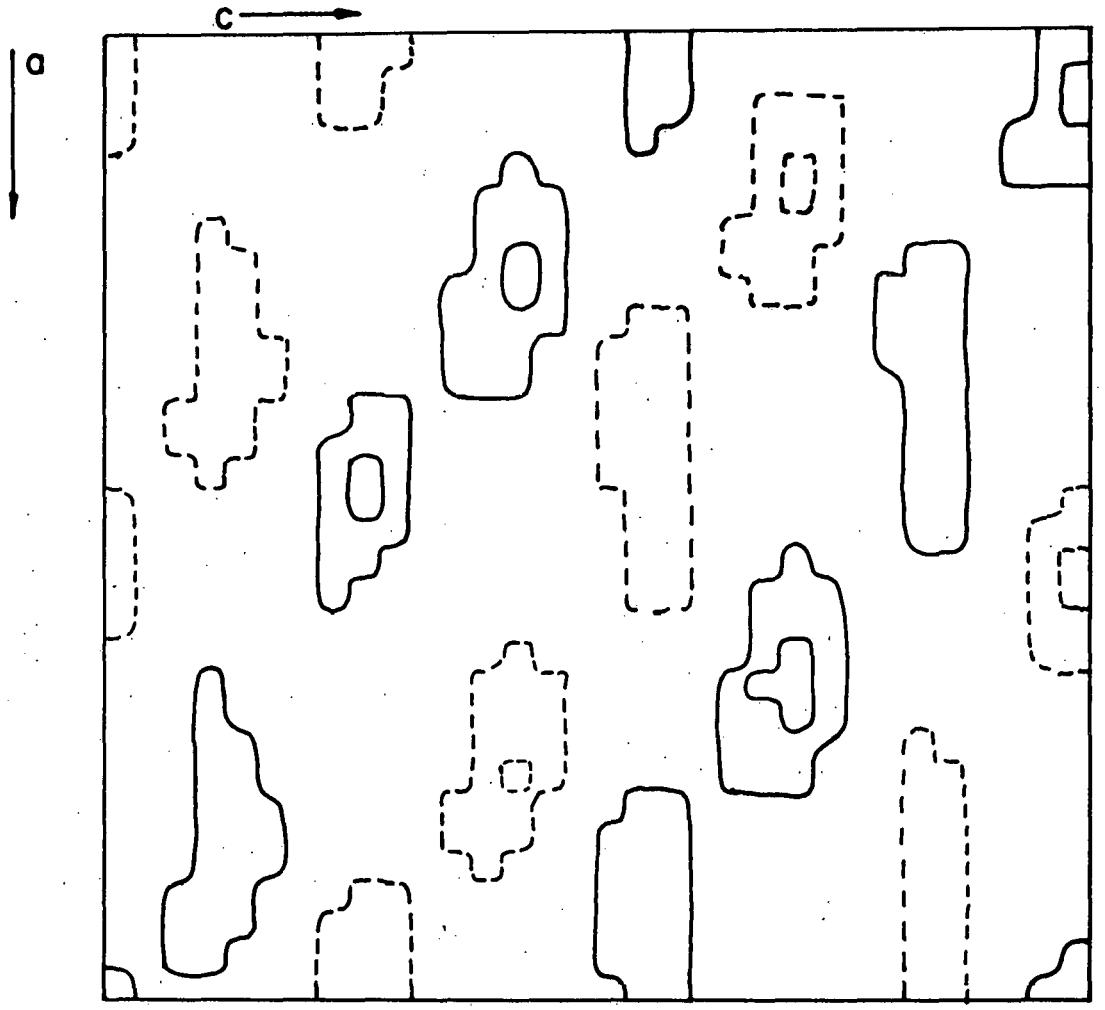


Figure 7b. Layer 9 of a Σ_2-map for β-picoline-N-oxide fumaric acid adduct. —— contoured at 15 and 25. ---- contoured at -15 and -25. No atoms in or near this section.

adjusted so that the value of the highest off-origin peak on the Patterson map was approximately equal to the value of the highest off-origin peak on the Σ_2-map. Figure 8 shows some typical results using the peak corresponding to the nitrogen atom position as the superposition point.

Each of the five maps was then squared and the resulting transform coefficients (G_{hkl}) calculated using a fast Fourier algorithm.[14] Only the 50 reflections with the largest values of the product $|E^*G|$ and with $|E| > 1.50$ were kept. Some typical results are shown in Table XIV. The signs determined for each hkl were then averaged. (In some cases more than 80% of the 50 largest $|E|$'s were signed correctly in the individual sets.) These signed reflections were then used to compute a new Σ_2-type map, and negative regions were set equal to zero. The transform of the square of this map was used to obtain signs (92% of which were correct) for input at the 90% confidence level into a phase extending program.[40] The resulting complete set of 270 phases was used to compute a map from which the positions of all the non-hydrogen atoms in the structure were readily determined. There were no significant spurious peaks on this map. This method has recently been used to solve the structure of diisopropyl-(2,3,4,5-tetraphenyl-cyclopenta-2,4-diene)-phosphate, which crystallizes in space group $P2_1/c$ with 160 non-

Table XIV. Representative results[a] obtained for a centric test case (β-picoline-N-oxide fumaric acid adduct)

h	k	l	|E|	Calculated signs 1	2	3	4	5	Known sign
-2	10	4	3.25	-	+	+	+	+	+
-1	11	7	3.13	-	+	+		+	+
0	11	9	3.00	-		+			+
0	12	4	2.94				+		-
-1	10	12	2.80	-	-	-	-	-	-
1	10	8	2.73	+	-	-		-	-
-2	4	12	2.63				+		+
1	11	7	2.55	+	-			-	-

[a] The absence of a calculated sign indicates that the value of | E*G | for that reflection was smaller than the limit used.

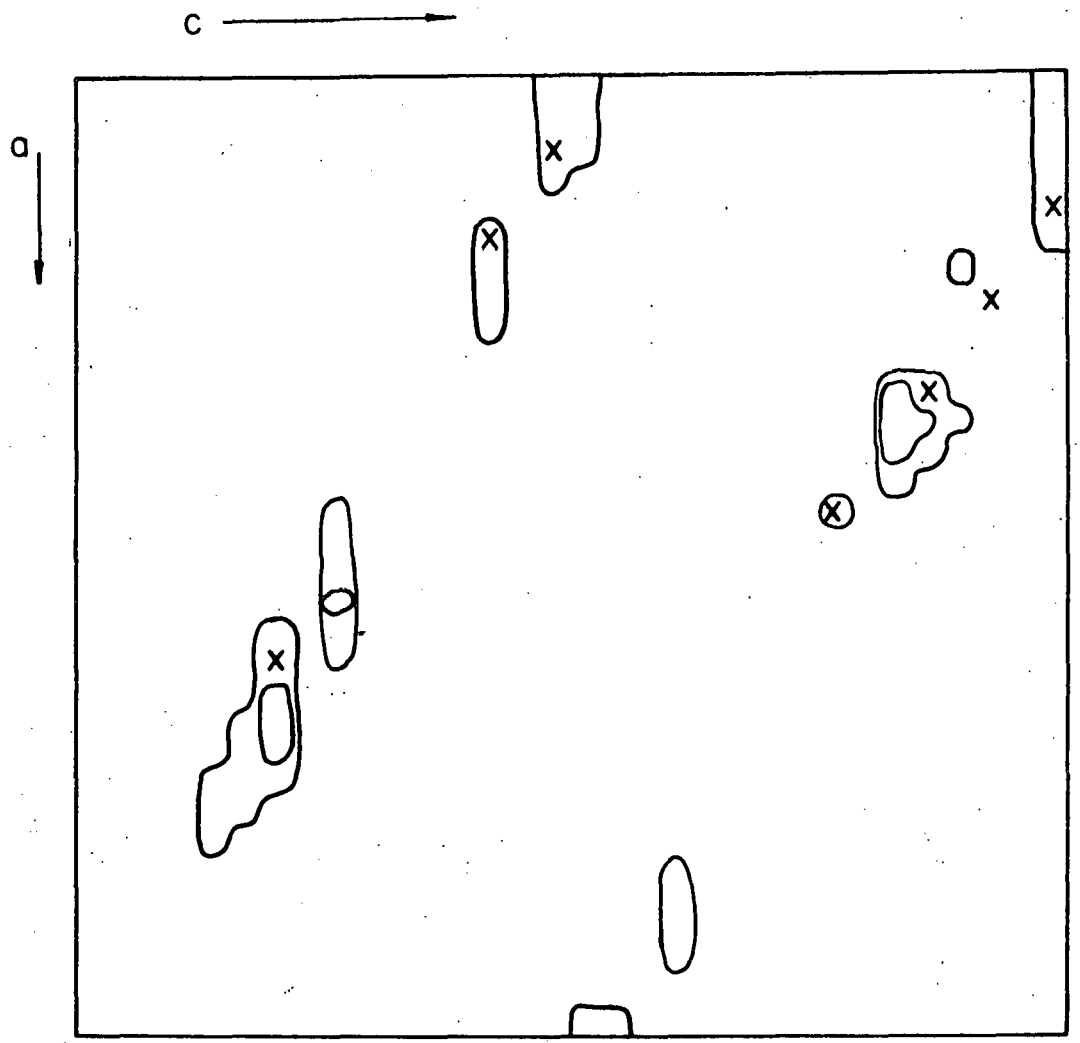


Figure 8a. Results of Patterson map superimposed on the Σ_2-map of Figure 7 at the four nitrogen equivalent positions. Composite of layers 3,4,5. —— contoured at 9 and 18. Atom positions indicated by X.

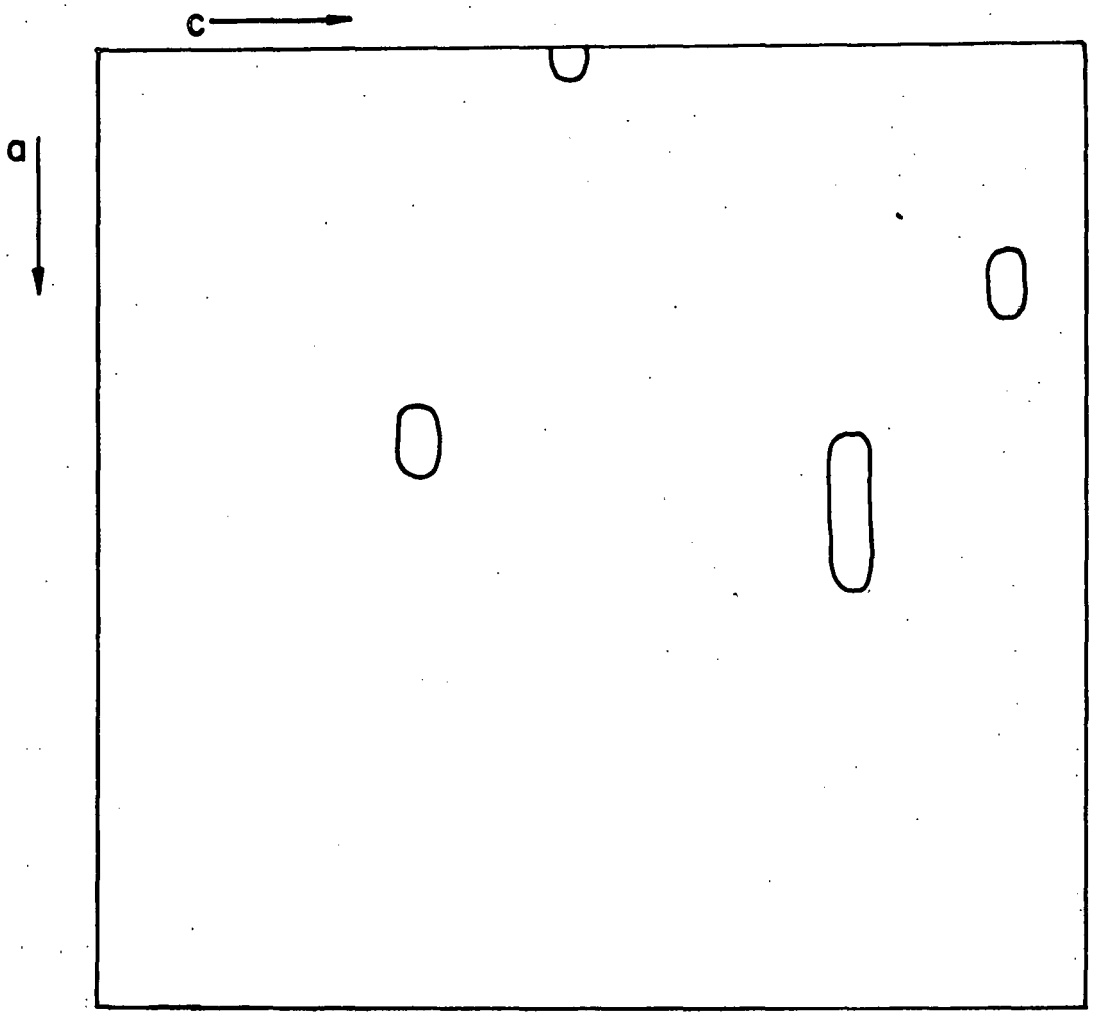


Figure 8b. Results of Patterson map superimposed on the Σ_2-map of Figure 7 at the four nitrogen equivalent positions. Layer 9. —— contoured at 5. No atoms in or near this section.

hydrogen atoms per cell.[41]

Acentric case

The compound chosen as a test for the acentric case was D-(1,5)-glucono lactone,[33] which crystallizes in the space group $P2_12_12_1$ with axial lengths $\underline{a}$ = 7.838, $\underline{b}$ = 12.322, $\underline{c}$ = 7.544 Å. Of the 1259 unique observed reflections, 435 have |E| greater than 1.0. Three origin-determining reflections were selected (|E| = 2.39, 2.51, 2.04), two of which were non-zonal reflections. To make the test a reasonably severe one, no enantiomorph-selecting reflection was included; the enantiomorph was chosen as part of the superposition procedure.

The Σ_2-map produced from these and their symmetry-related reflections showed more than 25 large peaks, all of which had relative heights between 120 and 185. The relative height of the other peaks on this map was less than 90. However, only eight of these 25 peaks generated appropriate Harker vectors on the Patterson. Of these eight, four were clearly in one enantiomorph, since they remained when the superposition point was a member of the set.

Using these four peaks and proceeding in a manner similar to the centric case above, the average phases of the 30 largest |E*G|'s with |E| > 1.40 were obtained. Some typical results for this acentric structure are given in

Table XV. The transform of the square of the expanded Σ_2-map yielded initial phases for the 50 largest $|E^*G|$'s with $|E| > 1.40$. These phased E's were then input into a phase-extending program at the 90% confidence level. In the resulting set of 410 phased E's, 390 were within 40° of the published phases and their transform readily revealed all the non-hydrogen atomic positions. As in the centric case, there were no significant spurious peaks on this final map.

Extensions of the Method

Since a reasonably severe test of the method was desired, only three origin-determining reflections were used for the initial Σ_2-map calculation in each case. Other reflections, phased by either Σ_2 or Σ_1 relations (and perhaps with appropriate weights), can also be included to produce peaks of greater reliability. In the centric case, those Σ_1 reflections which were determined with greater than 90% probability were included in the calculation of the Σ_2-map. Their addition improved the phase agreement to a small extent. The frequency check procedure[42] can also be applied to the Σ_2-map.

It is also possible to include an additional strong reflection in the origin-determining reflections, thus producing two Σ_2-maps in the centric case, for example. The resulting two sets of averaged phases could then be

Table XV. Representative results[a] obtained for an acentric test case (D-(1,5)-glucono lactone)

h	k	l	|E|	Calculated phases (°) 1	2	3	4	Known phase
0	3	6	3.48	270	270	270	270	270
0	4	3	2.67	0	180	180	180	180
0	7	9	2.58		90	90	90	90
0	11	2	2.36	89				90
2	2	6	2.22		277		256	296
1	7	5	2.19			276	284	293
4	-9	-1	2.04	230	243	220	256	252
0	4	0	1.95	179				0
3	-3	-7	1.77	179	171	182	177	197
3	4	2	1.64		261		278	316
1	-3	-2	1.59		83		90	81
0	2	3	1.58	179	0		0	180
2	4	6	1.56	84	88		91	114

[a] The absence of a calculated phase indicates that the value of $|E^*G|$ for that reflection was smaller than the limit used.

handled in a similar way as in those direct methods programs which produce multiple solutions.

Lower bounds different from zero can be used for modification of the resultant superposition map. Indeed, some calculations for the centric example have shown that use of a lower bound of 10% of the maximum peak height results in somewhat improved agreement.

From Tables XIV and XV, it is obvious that a straight average is a poor procedure compared to a more judicious method of averaging. Preliminary computations indicate that in the centric case a requirement of a net of two like signs produces a significant improvement in the percentage of correct signs selected.

The phases are also somewhat sensitive to grid point resolution of the maps. In the centric structure, calculations were run using a grid of 0.12 x 0.45 x 0.45 Å resolution. Results improve if a resolution of approximately 0.25 Å is used in all three directions.

Squaring the resultant superposition map appears to give the best phases compared with other powers which could be employed. All exponents from 0.2 to 6.6 in steps of 0.2 were examined for a typical run, with 2.0 appearing the most satisfactory.

RESEARCH PROPOSALS

The proposals for research given below suggested themselves during the course of the research described in this thesis. No claim of an exhaustive literature search for these ideas is implied, although it is the author's belief that they are not presently under investigation.

Due to the fact that more investigators without formal training are employing crystallography as a research tool, there is a desperate need for the development of computer programs which can make many of the routine decisions now requiring human intervention. ALPP eliminates, or at least makes much less tedious, the contouring of a map, and is an example of this type of program. Such a program should be developed to implement the PSST method. One could write a program to implement the heavy atom technique, which would work in conjunction with ALOP, by cycling structure factor and Fourier series calculations, at the same time deciding whether or not possible atomic positions should be retained. As well as being easy for the initiate to use, the above programs should also permit enough intervention so that the course of their execution can be altered by the more experienced user.

The prime difficulties in implementing direct methods are in choosing between various sets of phases

produced and in discriminating spurious from real atomic peaks. The first problem is being extensively researched and such methods as the comparison of absolute figures of merit and the psi zero test of MULTAN,[40] the absolute value of rho test reported by W. Ozbirn,[43] and a plot of psi zero *vs.* the absolute figure of merit as described by Cochran and Douglas[44] are all examples of possible solutions. A promising approach to the problem of peak discrimination should be the superposition of the Patterson on a likely atomic position, similar to the technique used in the PSST method. Another approach would be the development of a program which makes use of known interatomic vectors, such as those within a benzene ring, to choose peaks of chemical sense. A third would be the development of a more exact and easily used technique for producing three-dimensional models. A model constructed of wooden spheres suspended by fine lines from a perforated plate would satisfy these requirements.

The relative ease in determining the bonding mode of cyanide in *trans*-$(CN)_2$ trien cobalt (III) perchlorate indicates that X-ray diffraction data may be sensitive enough to distinguish between carbon and nitrogen. A more intensive effort on the part of investigators on this problem and perhaps even a reexamination of published data could be initiated.

The number of antimony (III) structures which have been determined is exceedingly small. The investigation of a number of different compounds of formula $M_2Sb^{III}X_5$ (M = Na, K, Rb, Cs; X = Cl, Br, I) would be of interest in determining the influence of the M^+ and the X^- on the configuration of the $SbX_5^=$ complex.

The Σ_2-map has a much wider applicability than is described in the PSST method. In combination with the discriminator function[45] to test possible atomic positions, it should have great power. In addition, using the expanded starting set of phased E's to produce a map which then would be used in place of the Σ_2-map, is an extension which has promise.

APPENDIX A

PROGRAM LISTING OF ALPP

```
//A375ALPP  JOB  A0310,WISMER,MSGLEVEL=(1,1)                              JCL-0010
//PICKPEAK  EXEC  PL1LFCL,PARM.PL1L='ATR,XREF,NOSTMT,OPT=02',             JCL-0020
//     TIME.PL1L=(0,45),REGION.PL1L=128K,                                 JCL-0030
//     TIME.LKED=(0,10),PARM.LKED='LIST,LET,OVLY'                         JCL-0040
//PL1L.SYSIN  DD  *                                                       JCL-0050
 /*  PICK PEAKS FROM AN ELECTRON DENSITY OR PATTERSON MAP              */ ALPP0010
 CONTOUR: PROCEDURE OPTIONS (MAIN);                                       ALPP0020
 /* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * ALPP0030
          THE PURPOSE OF THIS PROGRAM IS TO PICK PEAKS FROM EITHER AN     ALPP0040
     ELECTRON-DENSITY MAP OR A PATTERSON MAP.  THE MAP MAY BE PRODUCED    ALPP0050
     BY THE PROGRAM "FOUR" (ROGERS & JACOBSON, IS-2155), BY THE           ALPP0060
     PROGRAM "ALFF" (HUBBARD, QUICKSALL & JACOBSON, IS-2625), OR BY ANY   ALPP0070
     OTHER SUITABLE MAP-GENERATING PROGRAM.  THE MAP IS INPUT LINE BY     ALPP0080
     LINE FROM THE FILE "MAPIN".  FILE "MPOUT" IS A DIRECT-ACCESS        ALPP0090
     VERSION OF THE MAP, USED FOR INTERMEDIATE STORAGE.  FILE "PEAKS"    ALPP0100
     CONTAINS ALL OF THE PEAKS PICKED FROM THE MAP, IN ORDER OF          ALPP0110
     DESCENDING PEAK HEIGHT, IN THE FORM: IU, IV, IW, IHEIGHT, WHERE     ALPP0120
     ALL VARIABLES ARE FULL-WORD INTEGERS.                               ALPP0130
          THIS PROGRAM WAS WRITTEN IN FEBRUARY, 1972 BY R.K.WISMER.      ALPP0140
                                                                         ALPP0150
  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * ALPP0160
 CARD  COLUMN  VARIABLE  FORMAT  EXPLANATION                            ALPP0170
   1    1-80    TITLE     A(80)  ANY ALPHANUMERIC TITLE                  ALPP0180
   2    1- 4    PGM       A(4)   PROGRAM PRODUCING MAP, "ALFF" OR "FOUR" ALPP0190
        5- 8    IACR      F(4)   NUMBER OF GRIDS ACROSS FULL LINE.       ALPP0200
        9-12    IDWN      F(4)   NUMBER OF LINES DOWN FULL LAYER.        ALPP0210
       13-16    ILAY      F(4)   NUMBER OF LAYERS IN FULL MAP.           ALPP0220
       17-20    IPRT      F(4)   =1 PRINT THE MAP; =0 DO NOT PRINT THE MAP.ALPP0230
       21-24    LMT       F(4)   LOWER LIMIT, BELOW WHICH PEAK NOT ACCEPTEDALPP0240
       25-28    FW        F(4)   FIELD WIDTH FOR PRINTED MAP.           ALPP0250
       29-32    SP        F(4)   NUMBER OF SPACES BETWEEN LINES.        ALPP0260
 ***    NO PEAK ON THE MAP MAY EXCEED THE VALUE 2**14.                   ALPP0270
 ***    THE FULL CELL MAP IN ALL THREE DIRECTIONS MUST BE INPUT.         ALPP0280
 ***    THE INPUT MAP MAY HAVE ANY ORIENTATION.                          ALPP0290
  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */ALPP0300
          DECLARE  (IACR, IDWN, ILAY, IPRT, LMT, FW, SP, IACS, PMIN,     ALPP0310
                    PMAX, #PEAK)        FIXED BINARY (15);               ALPP0320
 /*                                                                      ALPP0330
          READ IN THE CONTROL CARDS AND INITIALIZE THE MAP               ALPP0340
                                                                       */ ALPP0350
          CALL SETUP (IACR,IDWN,ILAY,IPRT,LMT,FW,SP,IACS,PMIN,PMAX);     ALPP0360
 /*                                                                      ALPP0370
          PICK PEAKS FROM EACH LAYER                                     ALPP0380
                                                                       */ ALPP0390
          CALL LAYERS (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX);             ALPP0400
 /*                                                                      ALPP0410
          PICK PEAKS BETWEEN LAYERS AND OUTPUT PEAKS                     ALPP0420
                                                                       */ ALPP0430
          CALL NTRLAY (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX,#PEAK,IPRT); ALPP0440
 /*                                                                      ALPP0450
```

```
        SORT PEAKS INTO DESCENDING ORDER BY HEIGHT AND OUTPUT          ALPP0460
                                                                    */ ALPP0470
        CALL PKSORT(#PEAK);                                            ALPP0480
        PUT EDIT ('NORMAL PROGRAM TERMINATION')(PAGE,A);               ALPP0490
        END CONTOUR;                                                   ALPP0500



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                   STUP0010
 /*   READ IN THE CONTROL CARDS AND INITIALIZE THE MAP                */ STUP0020
 SETUP:   PROCEDURE (IACR,IDWN,ILAY,IPRT,LMT,FW,SP,IACS,PMIN,PMAX);    STUP0030
          DECLARE  (IACR, IDWN, ILAY, IPRT, LMT, FW, SP, IACS, PMIN,   STUP0040
                    PMAX, ISTP)          FIXED BINARY (15);          STUP0050
          DECLARE   LNALFF (0:IACR-1)   CONTROLLED FLOAT BINARY,       STUP0060
                   (LNFOUR(0:IACR), LAYER (0:IACR,0:IDWN))             STUP0070
                                        CONTROLLED FIXED BINARY (15);  STUP0080
          DECLARE   PGM                 CHARACTER (4);                 STUP0090
          DECLARE   XLM                 FLOAT BINARY;                  STUP0100
          DECLARE   TITLE               CHARACTER (80);                STUP0110
          DECLARE   MPOUT          FILE ENVIRONMENT (REGIONAL(1)) KEYED;STUP0120
          DECLARE   STAMP               CHARACTER (54) EXTERNAL;       STUP0130
          CALL TM_DT;                                                  STUP0140
 /*                                                                    STUP0150
          READ AND INTERPRET THE CONTROL CARDS                         STUP0160
                                                                    */ STUP0170
          GET EDIT (TITLE,PGM,IACR,IDWN,ILAY,IPRT,LMT,FW,SP,IMUD)      STUP0180
                   (A(80),A(4),7 F(4),X(44),F(4));                     STUP0190
          CLOSE FILE (SYSIN);                                          STUP0200
          PUT EDIT (TITLE, STAMP,                                      STUP0210
                    'NUMBER OF GRIDS ACROSS A FULL LINE =',IACR,       STUP0220
                    'NUMBER OF LINES DOWN A FULL LAYER = ',IDWN,       STUP0230
                    'NUMBER OF LAYERS IN A FULL MAP =',ILAY,           STUP0240
                    'LOWER LIMIT OF A RECOGNIZABLE PEAK = ',LMT)       STUP0250
                   (A(80),SKIP(2),X(20),A(54),4 (SKIP(2),X(25),A,      STUP0260
                    COL(65),F(4)));                                    STUP0270
          PUT EDIT ('THE GENERATING PROGRAM WAS "',PGM,'".')           STUP0280
                   (SKIP(2),X(20),A,A(4),A);                           STUP0290
          IACS = 0;                                                    STUP0300
          IF (IPRT=1)  THEN PRTR: DO;                                  STUP0310
               PUT EDIT ('THE MAP WILL BE PRINTED')(SKIP(2),X(25),A);  STUP0320
          PUT EDIT ('FIELD WIDTH =',FW,'SPACES BETWEEN LINES =',SP)    STUP0330
                   (2 (SKIP(2),X(25),A,F(4)));                         STUP0340
          CALL PRSETUP (IACS,IACR,FW,SP,PMIN,PMAX,ISTP);               STUP0350
          IF (ISTP=1)  THEN GO TO ABND;                    ELSE;       STUP0360
               END PRTR;  ELSE  PUT EDIT ('THE MAP WILL NOT BE PRINTED')STUP0370
                                (SKIP(2),X(25),A);                     STUP0380
          IF (PGM='ALFF')  THEN ALLOCATE LNALFF;                ELSE;  STUP0390
          ALLOCATE  LNFOUR, LAYER;                                     STUP0400
          PUT PAGE;                                                    STUP0410
```

```
          OPEN FILE (MAPIN) INPUT RECORD SEQUENTIAL,                          STUP0420
               FILE (MPOUT) OUTPUT RECORD SEQUENTIAL;                         STUP0430
/*                                                                            STUP0440
          READ MAP LINES, ZERO POINTS LESS THAN LMT, & WRITE MAP LAYERS       STUP0450
                                                                        */    STUP0460
          IF (PGM='ALFF')  THEN DO;      XLM = LMT;                           STUP0470
               NLAY = ILAY-1;       NDWN = IDWN-1;       END;                STUP0480
                          ELSE DO;                                          STUP0490
               NLAY = ILAY - 1;     NDWN = IDWN;         END;                STUP0500
LYLUP:    DO L = 0 TO NLAY BY 1;                                            STUP0510
LNLUP:    DO K = 0 TO NDWN BY 1;                                            STUP0520
          IF (PGM='ALFF')  THEN AL: DO;                                     STUP0530
               READ FILE (MAPIN) INTO (LNALFF);                             STUP0540
GDLUP:         DO J = 0 TO IACR-1 BY 1;                                     STUP0550
               IF (LNALFF(J)<=XLM)  THEN LAYER (J,K) = 0;                   STUP0560
                                    ELSE LAYER (J,K) = LNALFF(J);           STUP0570
               END GDLUP;                                                   STUP0580
               LAYER(IACR,K) = LAYER(0,K);                                  STUP0590
               END AL;                                                      STUP0600
                          ELSE FR: DO;                                      STUP0610
               READ FILE (MAPIN) INTO (LNFOUR);                             STUP0620
PTLUP:         DO J = 0 TO IACR BY 1;                                       STUP0630
               IF (LNFOUR(J)<=LMT)  THEN LAYER (J,K) = 0;                   STUP0640
                                    ELSE LAYER (J,K) = LNFOUR (J);          STUP0650
               END PTLUP;                                                   STUP0660
               END FR;                                                      STUP0670
          END LNLUP;                                                        STUP0680
          LAYER(*,IACR) = LAYER(*,0);                                       STUP0690
          WRITE FILE (MPOUT) FROM (LAYER) KEYFROM(L);                       STUP0700
          PUT EDIT ('LAYER NUMBER ',L,' WRITTEN OUT.')                      STUP0710
                   (SKIP,A,F(3),A);                                         STUP0720
          END LYLUP;                                                        STUP0730
          FREE LNALFF, LNFOUR, LAYER;                                       STUP0740
          CLOSE FILE (MAPIN),  FILE (MPOUT);                                STUP0750
          RETURN;                                                           STUP0760
ABND:     END SETUP;                                                        STUP0770


* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                         TMDT0010
 /* CREATES A TIME - DATE STAMP FOR FUTURE USE                        */     TMDT0020
 (SUBRG,STRG):  TM_DT:  PROCEDURE;                                          TMDT0030
 DECLARE STAMP CHARACTER(54) EXTERNAL,  AMPM CHARACTER(4);                  TMDT0040
 DECLARE MOS(12) CHARACTER(9) VARYING INITIAL ('JANUARY','FEBRUARY',        TMDT0050
         'MARCH','APRIL','MAY','JUNE','JULY','AUGUST','SEPTEMBER',         TMDT0060
         'OCTOBER','NOVEMBER','DECEMBER');                                  TMDT0070
 DECLARE TM CHARACTER(9), TMS(2) CHARACTER(2) DEFINED TM;  TM = TIME;       TMDT0080
 DECLARE DT CHARACTER(6), DS (3) CHARACTER(2) DEFINED DT;  DT = DATE;       TMDT0090
 IF (TMS(1) > 11)  THEN AMPM = 'P.M.';   ELSE AMPM = 'A.M.';                TMDT0100
```

```
STAMP = 'RUN ON ' || MOS(DS(2)) || ' ' || DS(3) || ', 19' || DS(1) ||   TMDT0110
    ', AT ' || TMS(1) || ' HOURS ' || TMS(2) || ' MINUTES ' || AMPM;   TMDT0120
END TM_DT;                                                             TMDT0130



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                    PRSU0010
 /*   A PROCEDURE TO CHECK THE PRINT PARAMETERS AND SET UP PRINTING  */ PRSU0020
 PRSETUP: PROCEDURE (ACRS,ACRE,FW,SP,PMIN,PMAX,ISTP);                  PRSU0030
          DECLARE  (ACRS, ACRE,     /* INITIAL & FINAL ACROSS GRIDS   */ PRSU0040
                    FW, SP,         /* FIELD WIDTH, SPACES BTWN LINES */ PRSU0050
                    PMIN, PMAX,     /* MINIMUM AND MAXIMUM PEAK HEIGHT*/ PRSU0060
                    ISTP, PMN, PMX)     FIXED BINARY (15);            PRSU0070
          DECLARE   XXX             CHARACTER (9);                     PRSU0080
          DECLARE   MN(2)           FIXED BIN INIT (-9,-99),           PRSU0090
                    MX(2)           FIXED BIN INIT (99,999);           PRSU0100
          DECLARE   NUMS(*)         CHAR(*) EXTERNAL CONTROLLED,       PRSU0110
                    HEAD            CHAR (132) STATIC EXTERNAL;        PRSU0120
          IF (FW*(ACRE-ACRS+1)>128)  THEN DO;                          PRSU0130
               PUT EDIT ('***** FW IS TOO LARGE FOR THE NUMBER OF GRID',PRSU0140
                         ' POINTS ACROSS THE PAGE * TERMINATING *****') PRSU0150
                        (SKIP(4),COL(20),A,A);                         PRSU0160
               GO TO TERM;                                 END;        PRSU0170
          IF (FW=2) THEN I=1;                              ELSE I=2;   PRSU0180
          PMIN = MN(I);                                                PRSU0190
          PMAX = MX(I);                                                PRSU0200
          IF ((PMIN<MN(I)) | (PMAX>MX(I)))  THEN DO;                   PRSU0210
               PUT EDIT ('***** PMIN OR PMAX OUT OF RANGE * DEFAULTS ', PRSU0220
                         'ASSUMED *****')                              PRSU0230
                        (SKIP(4),COL(20),A,A);                         PRSU0240
               IF (PMIN<MN(I))  THEN PMIN = MN(I);                     PRSU0250
               IF (PMAX>MX(I))  THEN PMAX = MX(I);         END;        PRSU0260
          IF (PMIN>0)  THEN PMIN=0;                                    PRSU0270
          ALLOCATE  NUMS (PMIN-1:PMAX+1) CHAR(FW);                     PRSU0280
 /*                                                                    PRSU0290
          NUMS ARRAY CONTAINS CHAR REPRESENTATION OF ALL NUMBERS FROM  PRSU0300
          PMIN TO PMAX.  HEAD IS THE HEADING FOR EACH LAYER            PRSU0310
                                                                 */    PRSU0320
 BL:      DO J = 1 TO 132 BY 1;                                        PRSU0330
          SUBSTR(HEAD,J,1) = ' ';                          END BL;     PRSU0340
 NM:      DO I = PMIN TO PMAX;                                         PRSU0350
          XXX = I;                                                     PRSU0360
          NUMS(I) = SUBSTR(XXX,10-FW,FW);                  END NM;     PRSU0370
          PMN = PMIN - 1;                                              PRSU0380
          PMX = PMAX + 1;                                              PRSU0390
          NUMS(PMN) = SUBSTR('      ',6-FW,FW);                        PRSU0400
          NUMS(PMX) = SUBSTR('******',6-FW,FW);                        PRSU0410
          J = 5 - FW;                                                  PRSU0420
 HD:      DO I = ACRS TO ACRE;                                         PRSU0430
```

```
          J = J + FW;
          SUBSTR(HEAD,J,FW) = NUMS(I);                          END HD;     PRSU0440
          ISTP = 0;                                                         PRSU0450
RTN:      RETURN;                                                           PRSU0460
TERM:     ISTP = 1;                                                         PRSU0470
          GO TO RTN;                                                        PRSU0480
          END PRSETUP;                                                      PRSU0490
                                                                            PRSU0500



                                                                            LYRS0010
/*   PICK PEAKS FROM EACH LAYER AND WRITE OUT THE REVISED LAYERS    */      LYRS0020
LAYERS:   PROCEDURE (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX);                  LYRS0030
          DECLARE   (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX)                   LYRS0040
                                        FIXED BINARY (15);                  LYRS0050
          DECLARE   MPOUT           FILE ENVIRONMENT (REGIONAL(1)) KEYED;   LYRS0060
          DECLARE  (LNACR(0:IACR), LNDWN(0:IDWN), LAYER(0:IACR,0:IDWN))     LYRS0070
                                        CONTROLLED FIXED BINARY;            LYRS0080
          OPEN FILE (MPOUT) UPDATE RECORD DIRECT;                           LYRS0090
          ALLOCATE  LAYER, LNDWN, LNACR;                                    LYRS0100
          PUT PAGE;                                                         LYRS0110
/*                                                                          LYRS0120
          FIND THE PEAKS LAYER BY LAYER                                     LYRS0130
                                                                    */      LYRS0140
LAYLP:    DO L = 0 TO ILAY-1 BY 1;                                          LYRS0150
          READ FILE (MPOUT) INTO (LAYER) KEY (L);                           LYRS0160
/*                                                                          LYRS0170
          GO THROUGH THE LAYERS ROW BY ROW                                  LYRS0180
                                                                    */      LYRS0190
LINLP:    DO K = 0 TO IDWN BY 1;                                            LYRS0200
          LNACR(*) = LAYER (*,K);                                           LYRS0210
          CALL PICKER (LNACR,IACR);                                         LYRS0220
          LAYER(*,K) = LNACR;                                               LYRS0230
          END LINLP;                                                        LYRS0240
/*                                                                          LYRS0250
          GO THROUGH THE LAYERS COLUMN BY COLUMN                            LYRS0260
                                                                    */      LYRS0270
COLUP:    DO J = 0 TO IACR BY 1;                                            LYRS0280
          LNDWN = LAYER (J,*);                                              LYRS0290
          CALL PICKER (LNDWN,IDWN);                                         LYRS0300
          LAYER(J,*) = LNDWN;                                               LYRS0310
          END COLUP;                                                        LYRS0320
/*                                                                          LYRS0330
          CHECK DIAGONAL ELEMENTS                                           LYRS0340
                                                                    */      LYRS0350
KLUP:     DO K = 0 TO IDWN BY 1;                                            LYRS0360
          IF (K=0)   THEN IDM = IDWN - 1;                                   LYRS0370
                     ELSE IDM = K - 1;                                      LYRS0380
          IF (K=IDWN)  THEN IDP = 1;                                        LYRS0390
```

```
                    ELSE IDP = K + 1;                                          LYRS0400
JLUP:     DO J = 0 TO IACR BY 1;                                               LYRS0410
          IF (LAYER(J,K) = 0)  THEN GO TO NDJL;                    ELSE;       LYRS0420
          IF (J=0)  THEN IAM = IACR - 1;                                       LYRS0430
                    ELSE IAM = J - 1;                                          LYRS0440
          IF (J=IACR)  THEN IAP = 1;                                           LYRS0450
                    ELSE IAP = J + 1;                                          LYRS0460
          LJK = LAYER(J,K);                                                    LYRS0470
          LAJK = ABS(LAYER(J,K));                                              LYRS0480
          IF (ABS(LAYER(IAP,IDP)) > LAJK)  THEN LJK = -LAJK;                   LYRS0490
                    ELSE LAYER(IAP,IDP) = -ABS(LAYER(IAP,IDP));                LYRS0500
          IF (ABS(LAYER(IAP,IDM)) > LAJK)  THEN LJK = -LAJK;                   LYRS0510
                    ELSE LAYER(IAP,IDM) = -ABS(LAYER(IAP,IDM));                LYRS0520
          IF (ABS(LAYER(IAM,IDP)) > LAJK)  THEN LJK = -LAJK;                   LYRS0530
                    ELSE LAYER(IAM,IDP) = -ABS(LAYER(IAM,IDP));                LYRS0540
          IF (ABS(LAYER(IAM,IDM)) > LAJK)  THEN LJK = -LAJK;                   LYRS0550
                    ELSE LAYER(IAM,IDM) = -ABS(LAYER(IAM,IDM));                LYRS0560
          LAYER(J,K) = LJK;                                                    LYRS0570
NDJL:     END JLUP;                                                            LYRS0580
          END KLUP;                                                            LYRS0590
          /*                                                                   LYRS0600
          OUTPUT THE CONTOURED MAP LAYER                                       LYRS0610
                                                                        */     LYRS0620
          REWRITE FILE (MPOUT) FROM (LAYER) KEY (L);                           LYRS0630
          PUT EDIT ('PEAK-PICKED LAYER ',L,' HAS BEEN REWRITTEN.')             LYRS0640
                   (SKIP,A,F(3),A);                                            LYRS0650
          END LAYLP;                                                           LYRS0660
          RETURN;                                                              LYRS0670
          END LAYERS;                                                          LYRS0680


* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                          PIKR0010
 /*  PROCEDURE TO CONTOUR A LINE                                      */      PIKR0020
 PICKER:  PROCEDURE (LINE,IACR);                                              PIKR0030
          DECLARE   LINE (*)              FIXED BINARY (15);                  PIKR0040
          DECLARE  (IACR,IA,IB,I,LIK)     FIXED BINARY (15);                  PIKR0050
          DECLARE  (OK, MK)               BIT (1);                            PIKR0060
          IA = ABS (LINE(IACR-1));                                            PIKR0070
          IB = IACR - 1;                                                      PIKR0080
          OK = '1'B;                                                          PIKR0090
          I = 0;                                                              PIKR0100
          MK = '0'B;                                                          PIKR0110
 SGD:     LIK = ABS (LINE(I));                                                PIKR0120
          IF (LIK > IA)  THEN GO TO OK1;                              ELSE    PIKR0130
          IF (OK)  THEN GO TO OK0;                    ELSE GO TO RST;         PIKR0140
 OK0:     OK = '0'B;                                                          PIKR0150
          GO TO INC;                                                          PIKR0160
 OK1:     OK = '1'B;                                                          PIKR0170
```

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RST:    IF (¬MK)  THEN LINE(IB) = -IA;                                  ELSE;   PIKR0180
INC:    IA = LIK;                                                               PIKR0190
        IB = I;                                                                 PIKR0200
        I = I + 1;                                                              PIKR0210
        IF (MK)  THEN GO TO NDL;                                        ELSE;   PIKR0220
        IF (I = IACR+1)  THEN GO TO FLS;        ELSE GO TO SGD;                 PIKR0230
FLS:    I = 0;                                                                  PIKR0240
        MK = '1'B;                                                              PIKR0250
        GO TO SGD;                                                              PIKR0260
NDL:    RETURN;                                                                 PIKR0270
        END PICKER;                                                             PIKR0280


* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                           NRLY0010
 /*    PICK PEAKS BETWEEN LAYERS AND OUTPUT THEIR POSITION AND HEIGHT */       NRLY0020
 NTRLAY:  PROCEDURE (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX,#PEAK,IPRT);          NRLY0030
          DECLARE   (IACR,IDWN,ILAY,FW,SP,IACS,PMIN,PMAX,#PEAK,IPRT)          NRLY0040
                                    FIXED BINARY (15);                        NRLY0050
          DECLARE  (LAYER(0:IACR,0:IDWN), LYRB4(0:IACR,0:IDWN))               NRLY0060
                                    CONTROLLED FIXED BINARY (15);             NRLY0070
          DECLARE   HEAD            CHARACTER (132) STATIC EXT;               NRLY0080
          DECLARE 1 PEAK,                                                     NRLY0090
                    2 (U,V,W,VALU)  FIXED BINARY (31);                        NRLY0100
          DECLARE   MPOUT           FILE ENVIRONMENT(REGIONAL(1)) KEYED,      NRLY0110
                    PEAKS           FILE RECORD SEQUENTIAL;                   NRLY0120
          DECLARE   LNACR(0:IACR)   CONTROLLED FIXED BINARY(15);              NRLY0130
          ALLOCATE  LNACR;                                                    NRLY0140
          #PEAK = 0;                                                          NRLY0150
          PUT PAGE;                                                           NRLY0160
          OPEN FILE (MPOUT) UPDATE RECORD DIRECT;                             NRLY0170
          ALLOCATE  LAYER, LYRB4;                                             NRLY0180
          READ FILE (MPOUT) INTO (LYRB4) KEY (ILAY-1);                        NRLY0190
 /*                                                                           NRLY0200
          GO THROUGH THE MAP LAYER BY LAYER                                   NRLY0210
                                                                        */    NRLY0220
 LAYLUP:  DO L = 0 TO ILAY-1 BY 1;                                            NRLY0230
          READ FILE (MPOUT) INTO (LAYER) KEY(L);                              NRLY0240
          IF (L=0)  THEN LB4 = ILAY - 1;                                      NRLY0250
                    ELSE LB4 = L - 1;                                         NRLY0260
 /*                                                                           NRLY0270
          GO THROUGH EACH LAYER LINE BY LINE                                  NRLY0280
                                                                        */    NRLY0290
 DWNLUP:  DO K = 0 TO IDWN BY 1;                                              NRLY0300
          IF (K=0)  THEN IDM = IDWN - 1;                                      NRLY0310
                    ELSE IDM = K - 1;                                         NRLY0320
          IF (K=IDWN)  THEN IDP = 1;                                          NRLY0330
                       ELSE IDP = K + 1;                                      NRLY0340
 /*                                                                           NRLY0350
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          GO THROUGH EACH LINE POINT BY POINT                                    NRLY0360
                                                                              */ NRLY0370
ACRLUP:   DO J = 0 TO IACR BY 1;                                                 NRLY0380
          IF (LAYER(J,K) = 0)  THEN GO TO NDAL;                          ELSE;   NRLY0390
          IF (J=0)  THEN IAM = IACR - 1;                                         NRLY0400
                    ELSE IAM = J - 1;                                            NRLY0410
          IF (J=IACR)  THEN IAP = 1;                                             NRLY0420
                       ELSE IAP = J + 1;                                         NRLY0430
          LJK = LAYER(J,K);                                                      NRLY0440
          LAJK = ABS(LAYER(J,K));                                                NRLY0450
/*                                                                               NRLY0460
          DETERMINE IF THE PEAK SHOULD BE KEPT                                   NRLY0470
                                                                              */ NRLY0480
          IF (ABS(LYRB4(IAP,IDP)) > LAJK)  THEN LJK = -LAJK;                     NRLY0490
                    ELSE LYRB4(IAP,IDP) = -ABS(LYRB4(IAP,IDP));                  NRLY0500
          IF (ABS(LYRB4(IAP,  K)) > LAJK)  THEN LJK = -LAJK;                     NRLY0510
                    ELSE LYRB4(IAP,  K) = -ABS(LYRB4(IAP,  K));                  NRLY0520
          IF (ABS(LYRB4(IAP,IDM)) > LAJK)  THEN LJK = -LAJK;                     NRLY0530
                    ELSE LYRB4(IAP,IDM) = -ABS(LYRB4(IAP,IDM));                  NRLY0540
          IF (ABS(LYRB4(  J,IDP)) > LAJK)  THEN LJK = -LAJK;                     NRLY0550
                    ELSE LYRB4(  J,IDP) = -ABS(LYRB4(  J,IDP));                  NRLY0560
          IF (ABS(LYRB4(  J,  K)) > LAJK)  THEN LJK = -LAJK;                     NRLY0570
                    ELSE LYRB4(  J,  K) = -ABS(LYRB4(  J,  K));                  NRLY0580
          IF (ABS(LYRB4(  J,IDM)) > LAJK)  THEN LJK = -LAJK;                     NRLY0590
                    ELSE LYRB4(  J,IDM) = -ABS(LYRB4(  J,IDM));                  NRLY0600
          IF (ABS(LYRB4(IAM,IDP)) > LAJK)  THEN LJK = -LAJK;                     NRLY0610
                    ELSE LYRB4(IAM,IDP) = -ABS(LYRB4(IAM,IDP));                  NRLY0620
          IF (ABS(LYRB4(IAM,  K)) > LAJK)  THEN LJK = -LAJK;                     NRLY0630
                    ELSE LYRB4(IAM,  K) = -ABS(LYRB4(IAM,  K));                  NRLY0640
          IF (ABS(LYRB4(IAM,IDM)) > LAJK)  THEN LJK = -LAJK;                     NRLY0650
                    ELSE LYRB4(IAM,IDM) = -ABS(LYRB4(IAM,IDM));                  NRLY0660
          LAYER(J,K) = LJK;                                                      NRLY0670
NDAL:     END ACRLUP;                                                            NRLY0680
          END DWNLUP;                                                            NRLY0690
          REWRITE FILE (MPOUT) FROM (LYRB4) KEY (LB4);                           NRLY0700
          IF (IPRT=1)  THEN CALL OUTP;                                   ELSE;   NRLY0710
          PUT EDIT ('MAP LAYER ',L,' HAS BEEN REWRITTEN')                        NRLY0720
                   (SKIP,A,F(3),A);                                              NRLY0730
          LYRB4 = LAYER;                                                         NRLY0740
          END LAYLUP;                                                            NRLY0750
          REWRITE FILE (MPOUT) FROM (LAYER) KEY (ILAY-1);                        NRLY0760
          FREE LYRB4;                                                            NRLY0770
          PUT PAGE;                                                              NRLY0780
          OPEN FILE (PEAKS) OUTPUT;                                              NRLY0790
/*                                                                               NRLY0800
          FIND AND WRITE OUT ALL THE PEAKS                                       NRLY0810
                                                                              */ NRLY0820
LUPLAY:   DO L = 0 TO ILAY-1 BY 1;                                               NRLY0830
          READ FILE (MPOUT) INTO (LAYER) KEY (L);                                NRLY0840
          W = L;                                                                 NRLY0850
```

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/*                                                                      NRLY0860
          LOOP THROUGH LINES AND GRID POINTS                            NRLY0870
                                                                     */ NRLY0880
LUPDWN:   DO K = 0 TO IDWN-1 BY 1;                                      NRLY0890
          V = K;                                                        NRLY0900
LUPACR:   DO J = 0 TO IACR-1 BY 1;                                      NRLY0910
          IF (LAYER(J,K) <= 0)  THEN GO TO NDA;                 ELSE;   NRLY0920
          U = J;                                                        NRLY0930
          VALU = LAYER(J,K);                                            NRLY0940
          PUT EDIT ('PEAK FOUND AT:  U=',U,'V =',V,'W =',W,'HEIGHT =',  NRLY0950
                    VALU,' ') (4 (A,F(4),X(4)),X(1),A);                 NRLY0960
          WRITE FILE (PEAKS) FROM (PEAK);                               NRLY0970
          #PEAK = #PEAK + 1;                                            NRLY0980
NDA:      END LUPACR;                                                   NRLY0990
          END LUPDWN;                                                   NRLY1000
          PUT SKIP(2);                                                  NRLY1010
          END LUPLAY;                                                   NRLY1020
          CLOSE FILE (MPOUT), FILE (PEAKS);                             NRLY1030
          FREE LAYER;                                                   NRLY1040
          PUT EDIT ('#PEAKS FOUND =',#PEAK)     (SKIP(3),A,F(6));       NRLY1050
/*                                                                      NRLY1060
          PROCEDURE TO OUTPUT A MAP LAYER                               NRLY1070
                                                                     */ NRLY1080
OUTP:     PROCEDURE;                                                    NRLY1090
          PUT EDIT ('LAYER NUMBER ',L,' OF ',ILAY,HEAD,' ')             NRLY1100
                   (PAGE,2 (A,F(4)),SKIP(2),A(132),SKIP,A);             NRLY1110
LOOP:     DO LUPI = 0 TO IDWN BY 1;                                     NRLY1120
          LNACR(*) = LAYER(*,LUPI);                                     NRLY1130
          CALL PLINE (FW,SP,PMIN,PMAX,LUPI,IACS,IACR,LNACR);            NRLY1140
          END LOOP;                                                     NRLY1150
          PUT EDIT (HEAD) (SKIP(3),A(132));                             NRLY1160
          RETURN;                                                       NRLY1170
          END OUTP;                                                     NRLY1180
          RETURN;                                                       NRLY1190
          END NTRLAY;                                                   NRLY1200
```

```
* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                   PKST0010
 /*   SORT THE PEAKS INTO DESCENDING ORDER BY HEIGHT                */ PKST0020
 PKSORT:  PROCEDURE (#PEAK);                                           PKST0030
 /* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * PKST0040
 METHOD:                                                               PKST0050
          A MEDIAN VALUE IS PICKED FROM THE LIST.  THE LIST IS DIVIDED PKST0060
          INTO TWO PARTS, WITH ALL THE VALUES LARGER THAN THE MEDIAN IN PKST0070
          THE UPPER PART AND ALL THE SMALLER VALUES IN THE LOWER PART. PKST0080
          EACH PART IS FURTHER DIVIDED IN THE SAME MANNER UNTIL ALL     PKST0090
          PARTS ARE OF LENGTH ONE, WHEREUPON THE SORT IS COMPLETE.      PKST0100
          THE ARRAYS IL AND IU STORE POINTERS TO EACH OF THE PARTS.     PKST0110
```

```
                                                                        PKST0120
        A SORT IN  ASCENDING ORDER IS ACCOMPLISHED BY REVERSING THE     PKST0130
        COMPARISONS ON THE SEVEN CARDS INVOLVING LOGICAL COMPARISONS    PKST0140
        WITH THE EG ELEMENT IN THE B STRUCTURAL ARRAY.  THESE           PKST0150
        COMPARISONS ARE THE STATEMENTS LABELED: REV1, REV2, REV3,       PKST0160
        REV4, REV5, REV6, REV7.     THEY ARE REVERSED IN THE FOLLOWING  PKST0170
        MANNER:  >=  -->  <=   AND  <=  -->  >= .                       PKST0180
                                                                        PKST0190
*,* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */ PKST0200
        DECLARE  (IU(16), IL(16))     FIXED BINARY;                     PKST0210
        DECLARE   #PEAK               FIXED BINARY (15);                PKST0220
        DECLARE 1 PEAK,                                                 PKST0230
                  2 (U,V,W,VALU)      FIXED BINARY (31);                PKST0240
        DECLARE   PEAKS               FILE RECORD SEQUENTIAL;           PKST0250
        DECLARE 1 T,                                                    PKST0260
                  2 (U,V,W,EG)        FIXED BINARY (15);                PKST0270
        DECLARE 1 B (#PEAK)           CONTROLLED,                       PKST0280
                  2 (U,V,W,EG)        FIXED BINARY (15);                PKST0290
        DECLARE 1 TT LIKE T;                                            PKST0300
        ALLOCATE B;                                                     PKST0310
        OPEN FILE (PEAKS);                                              PKST0320
/*                                                                      PKST0330
        READ IN THE PEAKS PICKED FROM THE MAP                           PKST0340
                                                                    */  PKST0350
ILUP:   DO I = 1 TO #PEAK BY 1;                                         PKST0360
        READ FILE (PEAKS) INTO (PEAK);                                  PKST0370
        B.U(I) = PEAK.U;                                                PKST0380
        B.V(I) = PEAK.V;                                                PKST0390
        B.W(I) = PEAK.W;                                                PKST0400
        B.EG(I) = PEAK.VALU;                                            PKST0410
        END ILUP;                                                       PKST0420
        CLOSE FILE (PEAKS);                                            PKST0430
/*                                                                      PKST0440
        DO THE ACTUAL SORT                                              PKST0450
                                                                    */  PKST0460
        M = 1;                                                          PKST0470
        II, I = 1;                                                      PKST0480
        J = #PEAK;                                                      PKST0490
L05:    IF (I >= J) THEN              GO TO L70;              ELSE;     PKST0500
L10:    K = I;                                                          PKST0510
        IJ = (J+I)/2;                                                   PKST0520
        T = B(IJ);                                                      PKST0530
REV1:   IF (B.EG(I) >= T.EG) THEN     GO TO L20;              ELSE;     PKST0540
        B(IJ) = B(I);                                                   PKST0550
        B(I) = T;                                                       PKST0560
        T = B(IJ);                                                      PKST0570
L20:    L=J;                                                            PKST0580
REV2:   IF (B.EG(J) <= T.EG) THEN     GO TO L40;              ELSE;     PKST0590
        B(IJ) = B(J);                                                   PKST0600
        B(J) = T;                                                       PKST0610
```

```
          T = B(IJ);                                                          PKST0620
REV3:     IF (B.EG(I) >= T.EG) THEN     GO TO L40;              ELSE;       PKST0630
          B(IJ) = B(I);                                                       PKST0640
          B(I) = T;                                                           PKST0650
          T = B(IJ);                    GO TO L40;                            PKST0660
L30:      B(L) = B(K);                                                        PKST0670
          B(K) = TT;                                                          PKST0680
L40:      L = L-1;                                                            PKST0690
REV4:     IF (B.EG(L) < T.EG) THEN      GO TO L40;              ELSE;       PKST0700
          TT = B(L);                                                          PKST0710
L50:      K = K+1;                                                            PKST0720
REV5:     IF (B.EG(K) > T.EG) THEN      GO TO L50;              ELSE;       PKST0730
          IF (K <= L) THEN              GO TO L30;              ELSE;       PKST0740
          IF (L-I <= J-K) THEN          GO TO L60;              ELSE;       PKST0750
          IL(M) = I;                                                          PKST0760
          IU(M) = L;                                                          PKST0770
          I = K;                                                              PKST0780
          M = M+1;                      GO TO L80;                            PKST0790
L60:      IL(M) = K;                                                          PKST0800
          IU(M) = J;                                                          PKST0810
          J = L;                                                              PKST0820
0.615661  M = M+1;                      GO TO L80;                            PKST0830
L70:      M = M-1;                                                            PKST0840
          IF (M = 0)  THEN GO TO NDSRT;                         ELSE;       PKST0850
          I = IL(M);                                                          PKST0860
          J = IU(M);                                                          PKST0870
L80:      IF (J-I >= II) THEN           GO TO L10;              ELSE;       PKST0880
          IF (I = II) THEN              GO TO L05;              ELSE;       PKST0890
          I = I-1;                                                            PKST0900
L90:      I = I+1;                                                            PKST0910
          IF (I = J) THEN               GO TO L70;              ELSE;       PKST0920
          T = B(I+1);                                                         PKST0930
REV6:     IF (B.EG(I) >= T.EG) THEN     GO TO L90;              ELSE;       PKST0940
          K = I;                                                              PKST0950
L95:      B(K+1) = B(K);                                                      PKST0960
          K = K-1;                                                            PKST0970
REV7:     IF (T.EG > B.EG(K)) THEN      GO TO L95;              ELSE;       PKST0980
          B(K+1) = T;                   GO TO L90;                            PKST0990
/*                                                                            PKST1000
          WRITE OUT THE SORTED PEAKS                                          PKST1010
                                                                    */        PKST1020
NDSRT:    PUT EDIT ('LIST OF SORTED PEAKS',                                   PKST1030
                    '       IU        IV        IW   IHEIGHT    ',          PKST1040
                    '       IU        IV        IW   IHEIGHT    ',          PKST1050
                    '       IU        IV        IW   IHEIGHT    ')          PKST1060
                   (PAGE,A,SKIP,3 A);                                         PKST1070
          PUT SKIP;                                                           PKST1080
          OPEN FILE (PEAKS) OUTPUT;                                           PKST1090
LUPI:     DO I = 1 TO #PEAK BY 1;                                             PKST1100
          PEAK.U = B.U(I);                                                    PKST1110
```

```
          PEAK.V = B.V(I);                                                    PKST1120
          PEAK.W = B.W(I);                                                    PKST1130
          PEAK.VALU = B.EG(I);                                                PKST1140
          WRITE FILE (PEAKS) FROM (PEAK);                                     PKST1150
          PUT EDIT (PEAK,' ') (4 F(10),X(3),A);                               PKST1160
          PUT FILE (PUNCH) EDIT (PEAK) (4 F(5));                              PKST1170
          END LUPI;                                                           PKST1180
          CLOSE FILE (PEAKS);                                                 PKST1190
          FREE B;                                                             PKST1200
          PUT EDIT ('THE SORTED PEAKS HAVE BEEN WRITTEN OUT')                 PKST1210
                   (SKIP(4),A);                                               PKST1220
          RETURN;                                                             PKST1230
          END PKSORT;                                                         PKST1240


* PROCESS('ATR,XREF');                                                       PLIN0010
 /*   PROCEDURE TO PRINT A LINE OF THE MAP                                */ PLIN0020
 (SUBRG,STRG):                                                              PLIN0030
 PLINE:   PROCEDURE (FW, SP, PMN, PMX, LN, ACRS, ACRE, LIN);                PLIN0040
          DECLARE   NUMS(*)          CHAR(*) EXTERNAL CONTROLLED,           PLIN0050
                    HEAD             CHAR (132) STATIC EXTERNAL,            PLIN0060
                    LINE             CHAR (132) STATIC,                     PLIN0070
                    LIN(*)           CONTROLLED FIXED BINARY,               PLIN0080
                   (FW, SP, PMN, PMX, LN, ACRS, ACRE, LL)                   PLIN0090
                                     FIXED BINARY;                          PLIN0200
          LINE = HEAD;                                                      PLIN0210
          SUBSTR(LINE,1,2) = SUBSTR(NUMS(LN),FW-1,2);                       PLIN0220
          J = 5 - FW;                                                       PLIN0230
 LOOP:    DO I = ACRS TO ACRE;                                              PLIN0240
          J = J + FW;                                                       PLIN0250
          LL = LIN(I);                                                      PLIN0260
          IF (LL<PMN)  THEN LL=PMN - 1;                                     PLIN0270
          IF (LL>PMX)  THEN LL=PMX + 1;                                     PLIN0280
          SUBSTR(LINE,J,FW) = NUMS(LL);                    END LOOP;        PLIN0290
          J = J + FW + 2;                                                   PLIN0300
          IF (J>130)  THEN GO TO PRINT;                                     PLIN0310
          SUBSTR(LINE,J,2) = SUBSTR(NUMS(LN),FW-1,2);                       PLIN0320
 PRINT:   PUT SKIP(SP+1) EDIT (LINE) (A(132));                              PLIN0330
          RETURN;                                                           PLIN0340
          END PLINE;                                                        PLIN0350


//LKED.SYSLMOD  DD  DSNAME=PROG.CRYST,                                      JCL-0060
//    UNIT=DISK,VOLUME=SER=PROGPK,DISP=(OLD,KEEP)                           JCL-0070
//LKED.SYSIN  DD  *                                                         JCL-0080
  OVERLAY ALPHA                                                             OVLY0010
```

```
INSERT SETUP                                    OVLY0020
OVERLAY BETA                                    OVLY0030
INSERT TM_DT                                    OVLY0040
OVERLAY BETA                                    OVLY0050
INSERT PRSETUP                                  OVLY0060
OVERLAY ALPHA                                   OVLY0070
INSERT LAYERS                                   OVLY0080
INSERT PICKER                                   OVLY0090
OVERLAY ALPHA                                   OVLY0100
INSERT NTRLAY                                   OVLY0110
INSERT PLINE                                    OVLY0120
OVERLAY ALPHA                                   OVLY0130
INSERT PKSORT                                   OVLY0140
NAME  ALPP(R)                                   JCL-0090
```

APPENDIX B

PROGRAM LISTING OF ALOP

```
//A375ALOP  JOB  'A0310,RE=128K,TI=04,LI=5',WISMER,MSGLEVEL=(1,1)          JCL-0010
//PATTERSN  EXEC   PL1LFCL,PARM.PL1L='ATR,XREF,NOSTMT,OPT=02',             JCL-0020
//     TIME.PL1L=(2,40),REGION.PL1L=128K,                                  JCL-0030
//     PARM.LKED='LIST,LET,OVLY',TIME.LKED=(0,50)                          JCL-0040
//PL1L.SYSIN  DD  *                                                       JCL-0050
 /*    FIND THE BEST SET OF PATTERSON PEAKS                          */ ALP00010
 ALOP:    PROCEDURE (SDBG) OPTIONS (MAIN);                              ALP00020
 /* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * ALP00030
        THIS PROGRAM IS DESIGNED TO PICK A LIKELY HEAVY ATOM PEAK       ALP00040
      FROM A LIST OF PATTERSON PEAKS, PREFERABLY NOT ON A HARKER LINE   ALP00050
      OR PLANE, WITH COORDINATES UH, VH, WH.  IT THEN SEARCHES THE REST  ALP00060
      OF THE LIST.  FOR EACH PEAK IN THE LIST, WITH COORDINATES U, V, W,ALP00070
      THERE MUST ALSO BE A PEAK AT (U-UH,V-VH,W-WH) OR, IF NOT, AT MOST ALP00080
      1 GRID POINT AWAY IN ANY DIRECTION.  IF THERE IS SUCH A PEAK,     ALP00090
      U,V,W, IS RETAINED AND GIVEN THE VALUE SQRT(P(U,V,W)*P(U-UH,V-VH, ALP00100
      W-WH)),  WEIGHTED IF THE PEAK IS NOT RIGHT ON.                    ALP00110
          THE SECOND PART OF THE PROGRAM MAKES USE OF THE LIST OF PEAKS ALP00120
      RETAINED BY PART ONE.  FOR EVERY PEAK IN ELECTRON-DENSITY SPACE   ALP00130
      AT (X,Y,Z) THERE SHOULD ALSO BE A PEAK AT (PX*X+QX, PY*Y+QY,      ALP00140
      PZ*Z+QZ) WHERE PX,PY,PZ = 1,-1 AND QX,QY,QZ = 0,1/2,  THE COORDIN-ALP00150
      ATES OF PATTERSON SPACE (U,V,W) ARE RELATED TO THOSE OF ELECTRON- ALP00160
      DENSITY SPACE (X,Y,Z) BY THE RELATION: (X,Y,Z)=(U-TX,V-TY,W-TZ).  ALP00170
      THE ELECTRON-DENSITY COORDINATE OF THE SYMMETRY-RELATED PEAK IS   ALP00180
      THUS GIVEN BY: (PX(U-TX)+QX,PY(V-TY)+QY,PZ(W-TZ)+QZ) AND THE      ALP00190
      PATTERSON COORDINATES OF THIS PEAK ARE: U'=PX*U+QX+(1-PX)*TX,      ALP00200
      V'=PY*V+QY+(1-PY)*TY, W'=PZ*W+QZ+(1-PZ)*TZ.  PART TWO SEARCHES    ALP00210
      THE LIST OF RETAINED PEAKS FOR THOSE PEAKS WHICH OCCUR BOTH AT    ALP00220
      U,V,W, AND AT U',V',W' FOR VARIOUS VALUES OF TX,TY,TZ, EXCLUDING  ALP00230
      TX,TY,TZ=0.  FOR EACH VALUE OF TX,TY,TZ BOTH THE NUMBER OF        ALP00240
      COINCIDENCES AND THE AVERAGE PEAK HEIGHT IS COMPUTED, AND THOSE   ALP00250
      TEN SETS OF TX,TY,TZ GIVING THE LARGEST VALUE FOR EACH OF THESE   ALP00260
      TWO QUANTITIES ARE OUTPUT.                                        ALP00270
          THIS PROGRAM WAS WRITTEN IN FEBRUARY, 1972 BY R.K.WISMER.     ALP00280
                                                                        ALP00290
  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * ALP00300
 CARD COLUMN FORMAT VARIABLE  EXPLANATION                               ALP00310
   1     1-80  A(80)  TITLE    ANY ALPHANUMERIC TITLE.                   ALP00320
   2     1- 4  F(4)   #PEAKS   NUMBER OF PEAKS TO BE INPUT.              ALP00330
         5- 8  F(4)   IACR     NUMBER OF GRIDS ACROSS A FULL LINE.       ALP00340
         9-12  F(4)   IDWN     NUMBER OF LINES DOWN A FULL LAYER.        ALP00350
        13-16  F(4)   ILAY     NUMBER OF LAYERS IN A FULL MAP.           ALP00360
        17-20  F(4)   #SYMM    NUMBER OF SYMMETRY CARDS TO FOLLOW.       ALP00370
 3,ETC. 1- 4  F(4)   PX       =1,-1                                     ALP00380
         5- 8  F(4)   XQ       =0,1. QX = XQ/2                           ALP00390
         9-12  F(4)   PY       =1,-1                                     ALP00400
        13-16  F(4)   YQ       =0,1. QY = YQ/2                           ALP00410
        17-20  F(4)   PZ       =1,-1                                     ALP00420
        21-24  F(4)   ZQ       =0,1. QZ = ZQ/2                           ALP00430
  * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */ALP00440
          DECLARE   TITLE              CHARACTER (80);                   ALP00450
```

```
          DECLARE   STAMP                 CHARACTER (54) EXTERNAL;          ALP00460
          DECLARE 1 SYMMPQ (#SYMM)        CONTROLLED EXTERNAL,              ALP00470
                    2 (PX,QX,PY,QY,PZ,QZ)    FIXED BINARY (15);             ALP00480
          DECLARE  (#PEAKS,#SYMM,#RTND,IACR,IDWN,ILAY)                       ALP00490
                                          FIXED BINARY (15);                ALP00500
          DECLARE  (SGNL, NCNT)           BIT (1) EXTERNAL;                 ALP00510
/*                                                                          ALP00520
          SGNL='1'B IF THERE IS A SYMMETRY ELEMENT WITH PX=PY=PZ=-1.        ALP00530
          NCNT='1'B IF THERE ARE SYMMETRY ELEMENTS WITH ONLY:   PX=-1,      ALP00540
                    PY=-1, PZ=-1, PX=PY=-1, PY=PZ=-1, PZ=PX=-1.             ALP00550
                                                                      */    ALP00560
          DECLARE  (ITXYZ,LNG,IERR)       FIXED BINARY (31);                ALP00570
          DECLARE   IHESRTA    ENTRY      (CHAR(53), CHAR(39),              ALP00580
                                           FIXED BIN(31), FIXED BIN(31));   ALP00590
          DECLARE   SFLD                  CHARACTER (53),                   ALP00600
                    RFLD                  CHARACTER (39);                   ALP00610
          DECLARE   SORTIN                FILE RECORD SEQUENTIAL;           ALP00620
          DECLARE   SDBG                  CHARACTER (100) VARYING;          ALP00630
          DECLARE   DBG                   EXTERNAL BIT (1);                 ALP00640
          DECLARE   DNV                   BIT (1) EXTERNAL;                 ALP00650
          IF (LENGTH(SDBG) > 1)  THEN DNV = '1'B;       ELSE DNV = '0'B;    ALP00660
          IF (LENGTH(SDBG) = 0)  THEN DBG = '0'B;       ELSE DBG = '1'B;    ALP00670
          CALL TM_DT;                                                       ALP00680
          LNG = 24000;                                                      ALP00690
          RFLD=' RECORD TYPE=V,LENGTH=(24,24,24,24,24) ';                   ALP00700
          ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA (I);  EXIT;  END;          ALP00710
/*                                                                          ALP00720
          READ AND INTERPRET THE CONTROL CARDS                              ALP00730
                                                                      */    ALP00740
          IF (DBG)  THEN PUT EDIT ('DEBUGGING OUTPUT WILL BE PRINTED.')     ALP00750
                                  (SKIP(4),A);                      ELSE;   ALP00760
          GET EDIT (TITLE,#PEAKS,IACR,IDWN,ILAY,#SYMM)                      ALP00770
                   (A(80),5 F(4));                                          ALP00780
          PUT EDIT (TITLE, STAMP,                                           ALP00790
                    'NUMBER OF POINTS ACROSS A FULL LINE =',IACR,           ALP00800
                    'NUMBER OF LINES DOWN A FULL LAYER =',IDWN,             ALP00810
                    'NUMBER OF LAYERS IN A FULL MAP =',ILAY,                ALP00820
                    'NUMBER OF PEAKS IN INPUT DATA SET =',#PEAKS,           ALP00830
                    'NUMBER OF SYMMETRY CARDS TO BE READ =',#SYMM)          ALP00840
                   (A(80),SKIP(3),A(54),5 (SKIP(3),X(20),A,F(4)));          ALP00850
          ALLOCATE SYMMPQ;                                                  ALP00860
SLUP:     DO I = 1 TO #SYMM BY 1;                                           ALP00870
          GET EDIT (PX(I),QX(I),PY(I),QY(I),PZ(I),QZ(I))                    ALP00880
                   (SKIP,6 F(4));                                           ALP00890
          PUT EDIT ('SYMMETRY OPERATION',I,PX(I),'*X +',QX(I),'/2',         ALP00900
                    PY(I),'*Y +',QY(I),'/2',PZ(I),'*Z +',QZ(I),'/2')        ALP00910
                   (SKIP(2),X(25),A,F(3),3 (F(7),A,F(2),A));                ALP00920
          END SLUP;                                                         ALP00930
          GET SKIP;                                                         ALP00940
/*                                                                          ALP00950
```

```
            CLOSE FILE (SYSIN);                                              ALP00960
            PICK AN APPROPRIATE HEAVY-ATOM PEAK & TEST ALL OTHER PEAKS       ALP00970
                                                                    */       ALP00980
            CALL PART1 (#PEAKS,IACR,IDWN,ILAY,#RTND);                        ALP00990
/*                                                                           ALP01000
            USING SYMMETRY, FIND ALL POSSIBLE VALUES OF TX, TY, TZ           ALP01010
                                                                    */       ALP01020
            CALL PART2 (#RTND,IACR,IDWN,ILAY,#SYMM);                         ALP01030
            IF (¬SGNL)  THEN GO TO PT4;                          ELSE;       ALP01040
/*                                                                           ALP01050
/*                                                                           ALP01060
            GROUP ALL TX, TY, TZ AND OUTPUT THOSE WITH FREQUENCY > 5         ALP01070
                                                                    */       ALP01080
PT3:        OPEN FILE (SORTIN) OUTPUT;                                       ALP01090
            CALL PART3 (IACR,IDWN,ILAY,#RTND);                               ALP01100
            IF (¬NCNT)  THEN GO TO SRT;                          ELSE;       ALP01110
/*                                                                           ALP01120
            PICK ALL NON-INVERSION TX,TY,TZ > 5 IN # AND OUTPUT W/ SYM#      ALP01130
                                                                    */       ALP01140
PT4:        CALL PART4 (IACR, IDWN, ILAY);                                   ALP01150
/*                                                                           ALP01160
            SORT THE FILE OF TX,TY,TZ BY TX, TY, TZ & SYM#                   ALP01170
                                                                    */       ALP01180
SRT:        CLOSE FILE (SORTIN);                                             ALP01190
            SFLD=' SORT FIELDS=(11,02,FI,D,21,4,FL,D),SIZE=E7000         ';  ALP01200
            CALL IHESRTA (SFLD,RFLD,LNG,IERR);                               ALP01210
            IF (IERR=0)  THEN GO TO PT5;                         ELSE;       ALP01220
            PUT EDIT ('THE SECOND SORT WAS UNSUCCESSFUL -- RETRY')           ALP01230
                     (SKIP(2),A);                                            ALP01240
            EXIT;                                                            ALP01250
/*                                                                           ALP01260
            MAP THE SYMMETRY ELEMENTS INTO EACH OTHER                        ALP01270
                                                                    */       ALP01280
PT5:        CALL PART5 (IACR, IDWN, ILAY);                                   ALP01290
/*                                                                           ALP01300
            CHOOSE THE MOST FREQUENT VALUE OF TX, TY, AND TZ                 ALP01310
                                                                    */       ALP01320
            CALL PART6 (IACR, IDWN, ILAY);                                   ALP01330
/*                                                                           ALP01340
            DETERMINE WHICH PEAKS ARE TO BE KEPT                             ALP01350
                                                                    */       ALP01360
            CALL PART7 (IACR, IDWN, ILAY, #RTND, #SYMM);                     ALP01370
            END ALOP;                                                        ALP01380



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                         TMDT0010
 /* CREATES A TIME - DATE STAMP FOR FUTURE USE                      */       TMDT0020
 (SUBRG,STRG):  TM_DT:  PROCEDURE;                                           TMDT0030
```

```
DECLARE STAMP CHARACTER(54) EXTERNAL,  AMPM CHARACTER(4);                    TMDT0040
DECLARE MOS(12) CHARACTER(9) VARYING INITIAL ('JANUARY','FEBRUARY',          TMDT0050
        'MARCH','APRIL','MAY','JUNE','JULY','AUGUST','SEPTEMBER',           TMDT0060
        'OCTOBER','NOVEMBER','DECEMBER');                                    TMDT0070
DECLARE TM CHARACTER(9), TMS(2) CHARACTER(2) DEFINED TM;  TM = TIME;         TMDT0080
DECLARE DT CHARACTER(6), DS (3) CHARACTER(2) DEFINED DT;  DT = DATE;         TMDT0090
IF (TMS(1) > 11)  THEN AMPM = 'P.M.';   ELSE AMPM = 'A.M.';                 TMDT0100
STAMP = 'RUN ON ' || MOS(DS(2)) || ' ' || DS(3) || ', 19' || DS(1) ||       TMDT0110
    ', AT ' || TMS(1) || ' HOURS ' || TMS(2)  || ' MINUTES ' || AMPM;        TMDT0120
END TM_DT;                                                                   TMDT0130
```

```
* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                        -P1-0010
 /*   PICK AN APPROPRIATE HEAVY-ATOM PEAK & TEST ALL OTHER PEAKS      */ -P1-0020
 /*   IN-CORE HEAVY-ATOM SINGLE SUPERPOSITION                         */ -P1-0030
 PART1:   PROCEDURE (#PEAKS,IACR,IDWN,ILAY,#RTND);                         -P1-0040
          DECLARE  (#PEAKS,IACR,IDWN,ILAY,#RTND)  FIXED BINARY (15);       -P1-0050
          DECLARE 1 PEAKS (#PEAKS)        CONTROLLED,                      -P1-0060
                    2 (U,V,W,VALU,MEAN) FIXED BINARY (15);                 -P1-0070
          DECLARE   PKFILE                FILE RECORD INPUT SEQUENTIAL;    -P1-0080
          DECLARE   RETAIN                FILE RECORD SEQUENTIAL;          -P1-0090
          DECLARE 1 PEAKR,                                                 -P1-0100
                    2 (RU,RV,RW,VAL,AVG)      FIXED BINARY (31);           -P1-0110
          DECLARE 1 SPEAK,                                                 -P1-0120
                    2 (SU,SV,SW,VLU)    FIXED BINARY (31);                 -P1-0130
          DECLARE   DIF                 LABEL;                           -P1-0140
          DECLARE  (BU, BV, BW)         BIT (1);                         -P1-0150
          DECLARE  (DELU,DELV,DELW)     FIXED BINARY (15);               -P1-0160
          DECLARE  (P1, P2, P3)         FLOAT BINARY;                    -P1-0170
          DECLARE  (IDU,IDV,IDW)        FIXED BINARY (15);               -P1-0180
          DECLARE   DBG                 EXTERNAL BIT (1);                -P1-0190
          ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA (I,J,K,L); EXIT; END;   -P1-0200
 /*                                                                       -P1-0210
          SET UP CONSTANTS FOR CHECKING                                    -P1-0220
                                                                        */ -P1-0230
          IA2 = IACR / 2;                                                  -P1-0240
          ID2 = IDWN / 2;                                                  -P1-0250
          IL2 = ILAY / 2;                                                  -P1-0260
          P1 = 0.800;                                                      -P1-0270
          P2 = 0.650;                                                      -P1-0280
          P3 = 0.500;                                                      -P1-0290
 /*                                                                       -P1-0300
          READ IN THE PEAKS PICKED FROM THE MAP BY ALPPKR                  -P1-0310
                                                                        */ -P1-0320
          ALLOCATE PEAKS;                                                  -P1-0330
 PLUP:    DO I = 1 TO #PEAKS BY 1;                                         -P1-0340
          GET EDIT (SPEAK) (4 F(5));                                       -P1-0350
          U(I) = SU;                                                       -P1-0360
```

```
          V(I) = SV;                                                          -P1-0370
          W(I) = SW;                                                          -P1-0380
          VALU(I) = VLU;                                                      -P1-0390
          MEAN(I) = 0;                                                        -P1-0400
          END PLUP;                                                           -P1-0410
/*                                                                            -P1-0420
          FIND THE LIKELY HEAVY ATOM PEAK FROM THE FIRST 20%                  -P1-0430
                                                                        */    -P1-0440
          IF (#PEAKS<100)  THEN ITOP = MIN(20,#PEAKS);                        -P1-0450
                           ELSE ITOP = #PEAKS / 5;                            -P1-0460
          IA2 = IACR / 2;                                                     -P1-0470
          ID2 = IDWN / 2;                                                     -P1-0480
          IL2 = ILAY / 2;                                                     -P1-0490
          DIF = HARD;                                                         -P1-0500
          ITIME = 1;                                                          -P1-0510
          JTIME = 0;                                                          -P1-0520
TLUP:     DO I = 1 TO ITOP BY 1;                                              -P1-0530
          IU = U(I);                                                          -P1-0540
          IV = V(I);                                                          -P1-0550
          IW = W(I);                                                          -P1-0560
          KVAL = VALU(I);                                                     -P1-0570
          GO TO DIF;                                                          -P1-0580
/*                                                                            -P1-0590
          LARGEST PEAK ACCEPTED AS HEAVY ATOM WHICH HASN'T U,V,W=0,1/2        -P1-0600
                                                                        */    -P1-0610
HARD:     IF ((IU=0)|(IU=IACR)|(IU=IA2)|(IV=0)|(IV=IDWN)|(IV=ID2)|            -P1-0620
              (IW=0)|(IW=ILAY)|(IW=IL2))  THEN GO TO NOPE;                    -P1-0630
                                          ELSE GO TO YEP;                     -P1-0640
/*                                                                            -P1-0650
          LARGEST ACCEPTED AS HEAVY ATOM HAVING ONLY ONE OF U,V,W=0,1/2       -P1-0660
                                                                        */    -P1-0670
MEDM:     BU = ¬((IU=0)|(IU=IACR)|(IU=IA2));                                  -P1-0680
          BV = ¬((IV=0)|(IV=IDWN)|(IV=ID2));                                  -P1-0690
          BW = ¬((IW=0)|(IW=ILAY)|(IW=IL2));                                  -P1-0700
          IF ((BU&BV) | (BU&BW) | (BV&BW))  THEN GO TO YEP;                   -P1-0710
                                            ELSE GO TO NOPE;                  -P1-0720
/*                                                                            -P1-0730
          LARGEST ACCEPTED AS HEAVY ATOM HAVING TWO ONLY OF U,V,W=0,1/2       -P1-0740
                                                                        */    -P1-0750
EASY:     BU = ¬((IU=0)|(IU=IACR)|(IU=IA2));                                  -P1-0760
          BV = ¬((IV=0)|(IV=IDWN)|(IV=ID2));                                  -P1-0770
          BW = ¬((IW=0)|(IW=ILAY)|(IW=IL2));                                  -P1-0780
          IF (BU | BV | BW)  THEN GO TO YEP;                                  -P1-0790
                             ELSE GO TO NOPE;                                 -P1-0800
NOPE:     END TLUP;                                                           -P1-0810
          IF (ITIME=1)  THEN GO TO FIRST;                                     -P1-0820
                        ELSE IF (ITIME=2)  THEN GO TO SCND;                   -P1-0830
                                           ELSE GO TO FAIL;                   -P1-0840
FIRST:    DIF = MEDM;                                                         -P1-0850
          ITIME = 2;                                                          -P1-0860
```

```
          GO TO TLUP;                                                          -P1-0870
SCND:     DIF = EASY;                                                          -P1-0880
          ITIME = 3;                                                           -P1-0890
          GO TO TLUP;                                                          -P1-0900
/*                                                                             -P1-0910
          UNABLE TO FIND A SUITABLE HEAVY ATOM                                 -P1-0920
                                                                          */   -P1-0930
FAIL:     PUT EDIT ('***** UNABLE TO PICK A HEAVY-ATOM PEAK *****')            -P1-0940
                   (SKIP(4),A);                                                -P1-0950
          EXIT;                                                                -P1-0960
/*                                                                             -P1-0970
          SUITABLE HEAVY ATOM PEAK FOUND                                       -P1-0980
                                                                          */   -P1-0990
YEP:      KU = IU;                                                             -P1-1000
          KV = IV;                                                             -P1-1010
          KW = IW;                                                             -P1-1020
          KP = I;                                                              -P1-1030
          PUT EDIT ('HEAVY ATOM PEAK FOUND AT U =',KU,'V =',KV,'W =',          -P1-1040
                    KW,'VALUE =',KVAL)                                         -P1-1050
                   (SKIP(3),X(20), 4 (A,F(4),X(3)));                           -P1-1060
/*                                                                             -P1-1070
          DECIDE ON WHETHER TO USE A HARKER OR A GENERAL PEAK                  -P1-1080
                                                                          */   -P1-1090
          IF ((ITIME=1) & (JTIME=0))  THEN GO TO TAGN;              ELSE;      -P1-1100
          IF ((ITIME¬=1) & (JTIME=1))  THEN GO TO COMPR;            ELSE;      -P1-1110
          GO TO RSTR;                                                          -P1-1120
TAGN:     GKP = KP;          GKVL = KVAL;          JTIME = 1;                  -P1-1130
          GKU = KU;          GKV = KV;             GKW = KW;                   -P1-1140
          GO TO FIRST;                                                         -P1-1150
COMPR:    GNRL = FLOAT (GKVL);                                                 -P1-1160
          HRKR = FLOAT (KVAL) / 2.2000;                                        -P1-1170
          IF (HRKR > GNRL)  THEN GO TO TYPE;                        ELSE;      -P1-1180
          KU = GKU;          KV = GKV;             KW = GKW;                   -P1-1190
          KP = GKP;          KVAL = GKVL;                                      -P1-1200
TYPE:     PUT EDIT ('##### PEAK FINALLY CHOSEN AT:   #####',                   -P1-1210
                    'U =',KU,'V =',KV,'W =',KW,'VALUE =',KVAL,                 -P1-1220
                   'INDEX =',KP) (SKIP(2),X(10),A,SKIP,3 (X(20),A,F(5)),       -P1-1230
                    SKIP,2 (X(20),A,F(5)));                                    -P1-1240
/*                                                                             -P1-1250
          USING THIS PEAK, DETERMINE WHICH PEAKS TO RETAIN                     -P1-1260
                                                                          */   -P1-1270
RSTR:     PUT EDIT ('PEAKS FOUND, USING HEAVY-ATOM PEAK',                      -P1-1280
                    '    U    V    W   HEIGHT     MEAN',                      -P1-1290
                    '    U    V    W   HEIGHT     MEAN',                      -P1-1300
                    '    U    V    W   HEIGHT     MEAN',                      -P1-1310
                    '    U    V    W   HEIGHT     MEAN',' ')                  -P1-1320
                   (PAGE,A,SKIP,A,A,A,A,SKIP,A);                               -P1-1330
          PUT SKIP;                                                            -P1-1340
ILUP:     DO I = 1 TO #PEAKS BY 1;                                             -P1-1350
/*                                                                             -P1-1360
```

```
          CALCULATE THE PEAK POSITION TO LOOK FOR                                  -P1-1370
                                                                                 */ -P1-1380
          K = I;                                                                   -P1-1390
          IDU = KU + U(I);                                                         -P1-1400
          IDV = KV + V(I);                                                         -P1-1410
          IDW = KW + W(I);                                                         -P1-1420
          IF (IDU<0)   THEN IDU = IDU + IACR;                                      -P1-1430
                       ELSE IF (IDU>IACR)  THEN IDU = IDU - IACR; ELSE;            -P1-1440
          IF (IDU<0)   THEN IDU = IDU + IACR;                                      -P1-1450
                       ELSE IF (IDU>IACR)  THEN IDU = IDU - IACR; ELSE;            -P1-1460
          IF (IDV<0)   THEN IDV = IDV + IDWN;                                      -P1-1470
                       ELSE IF (IDV>IDWN)  THEN IDV = IDV - IDWN; ELSE;            -P1-1480
          IF (IDV<0)   THEN IDV = IDV + IDWN;                                      -P1-1490
                       ELSE IF (IDV>IDWN)  THEN IDV = IDV - IDWN; ELSE;            -P1-1500
          IF (IDW<0)   THEN IDW = IDW + ILAY;                                      -P1-1510
                       ELSE IF (IDW>ILAY)  THEN IDW = IDW - ILAY; ELSE;            -P1-1520
          IF (IDW<0)   THEN IDW = IDW + ILAY;                                      -P1-1530
                       ELSE IF (IDW>ILAY)  THEN IDW = IDW - ILAY; ELSE;            -P1-1540
/*                                                                                 -P1-1550
          DETERMINE IF ANY OF THE OTHER PEAKS FITS EXACTLY                         -P1-1560
          TO THIS CALCULATED POSITION, OR IF IT IS OFF ONLY SLIGHTLY               -P1-1570
                                                                                 */ -P1-1580
JLUP:     DO J = 1 TO #PEAKS BY 1;                                                 -P1-1590
          L = J;                                                                   -P1-1600
          DELU = U(J) - IDU;                                                       -P1-1610
          DELV = V(J) - IDV;                                                       -P1-1620
          DELW = W(J) - IDW;                                                       -P1-1630
          IF (DELU >  IA2)  THEN DELU = DELU - IACR;              ELSE;            -P1-1640
          IF (DELU >  IA2)  THEN DELU = DELU - IACR;              ELSE;            -P1-1650
          IF (DELU < -IA2)  THEN DELU = DELU + IACR;              ELSE;            -P1-1660
          IF (DELU < -IA2)  THEN DELU = DELU + IACR;              ELSE;            -P1-1670
          IF (DELV >  ID2)  THEN DELV = DELV - IDWN;              ELSE;            -P1-1680
          IF (DELV >  ID2)  THEN DELV = DELV - IDWN;              ELSE;            -P1-1690
          IF (DELV < -ID2)  THEN DELV = DELV + IDWN;              ELSE;            -P1-1700
          IF (DELV < -ID2)  THEN DELV = DELV + IDWN;              ELSE;            -P1-1710
          IF (DELW >  IL2)  THEN DELW = DELW - ILAY;              ELSE;            -P1-1720
          IF (DELW >  IL2)  THEN DELW = DELW - ILAY;              ELSE;            -P1-1730
          IF (DELW < -IL2)  THEN DELW = DELW + ILAY;              ELSE;            -P1-1740
          IF (DELW < -IL2)  THEN DELW = DELW + ILAY;              ELSE;            -P1-1750
          IF ((DELU=0) & (DELV=0) & (DELW=0))  THEN GO TO OFF0;   ELSE;            -P1-1760
          DELU = ABS (DELU);                                                       -P1-1770
          DELV = ABS (DELV);                                                       -P1-1780
          DELW = ABS (DELW);                                                       -P1-1790
          IF(((DELU=1) & (DELV=0) & (DELW=0)) |                                    -P1-1800
             ((DELU=0) & (DELV=1) & (DELW=0)) |                                    -P1-1810
             ((DELU=0) & (DELV=0) & (DELW=1)))  THEN GO TO OFF1; ELSE;             -P1-1820
          IF(((DELU=1) & (DELV=1) & (DELW=0)) |                                    -P1-1830
             ((DELU=0) & (DELV=1) & (DELW=1)) |                                    -P1-1840
             ((DELU=1) & (DELV=0) & (DELW=1)))  THEN GO TO OFF2; ELSE;             -P1-1850
          IF ((DELU=1) & (DELV=1) & (DELW=1))  THEN GO TO OFF3;  ELSE;            -P1-1860
```

```
          END JLUP;                                                          -P1-1870
          GO TO NDI;                                                         -P1-1880
/*                                                                           -P1-1890
          PEAK IS RIGHT ON                                                   -P1-1900
                                                                          */ -P1-1910
OFF0:     MEAN(J) = SQRT (FLOAT (VALU(I) * VALU(J)));                        -P1-1920
          PUT EDIT (U(J),V(J),W(J),VALU(J),MEAN(J)) (3 F(5),2 F(9));         -P1-1930
          GO TO NDI;                                                         -P1-1940
/*                                                                           -P1-1950
          PEAK IS OFF 1 GRID IN ONE DIRECTION                                -P1-1960
                                                                          */ -P1-1970
OFF1:     MEAN(J) = P1 * SQRT (FLOAT (VALU(I) * VALU(J)));                   -P1-1980
          PUT EDIT (U(J),V(J),W(J),VALU(J),MEAN(J)) (3 F(5),2 F(9));         -P1-1990
          GO TO NDI;                                                         -P1-2000
/*                                                                           -P1-2010
          THE PEAK IS OFF 1 GRID POINT IN EACH OF TWO DIRECTIONS             -P1-2020
                                                                          */ -P1-2030
OFF2:     MEAN(J) = P2 * SQRT (FLOAT (VALU(I) * VALU(J)));                   -P1-2040
          PUT EDIT (U(J),V(J),W(J),VALU(J),MEAN(J)) (3 F(5),2 F(9));         -P1-2050
          GO TO NDI;                                                         -P1-2060
/*                                                                           -P1-2070
          THE PEAK IS OFF 1 GRID POINT IN ALL THREE DIRECTIONS               -P1-2080
                                                                          */ -P1-2090
OFF3:     MEAN(J) = P3 * SQRT (FLOAT (VALU(I) * VALU(J)));                   -P1-2100
          PUT EDIT (U(J),V(J),W(J),VALU(J),MEAN(J)) (3 F(5),2 F(9));         -P1-2110
NDI:      END ILUP;                                                          -P1-2120
/*                                                                           -P1-2130
          WRITE OUT THE PEAKS WHICH WERE FOUND                               -P1-2140
                                                                          */ -P1-2150
          OPEN FILE (RETAIN) OUTPUT;                                         -P1-2160
          #RTND = 0;                                                         -P1-2170
LUPI:     DO I = 1 TO #PEAKS BY 1;                                           -P1-2180
          IF (MEAN(I)=0)  THEN GO TO FNLI;                          ELSE;    -P1-2190
          RU = U(I);                                                         -P1-2200
          RV = V(I);                                                         -P1-2210
          RW = W(I);                                                         -P1-2220
          VAL = VALU(I);                                                     -P1-2230
          AVG = MEAN(I);                                                     -P1-2240
          #RTND = #RTND + 1;                                                 -P1-2250
          WRITE FILE (RETAIN) FROM (PEAKR);                                  -P1-2260
FNLI:     END LUPI;                                                          -P1-2270
          CLOSE FILE (RETAIN);                                               -P1-2280
          FREE PEAKS;                                                        -P1-2290
          RETURN;                                                            -P1-2300
          END PART1;                                                         -P1-2310


* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                        -P2-0010
```

```
/*    USING SYMMETRY, FIND ALL THE VALUES OF TX, TY, TZ                */ -P2-0020
/*    FROM THE PEAKS OBTAINED FROM THE SUPERPOSITION OF PART 1         */ -P2-0030
PART2:    PROCEDURE (#RTND,IACR,IDWN,ILAY,#SYMM);                       -P2-0040
/*                                                                      -P2-0050
          THIS SECTION COMPUTES ALL OF THE POSSIBLE VALUES OF TX,TY, &  -P2-0060
          TZ FROM THE PEAKS LEFT BY THE SUPERPOSITION AS FOLLOWS:       -P2-0070
          LET U,V,W & U',V',W' REPRESENT THE TWO PEAKS.  IF THESE PEAKS -P2-0080
          ARE SYMMETRY RELATED BUT THE SUPERPOSITION ORIGIN IS OFF      -P2-0090
          BY TX,TY,TZ, THEN U = X+TX, V = Y+TY, AND W = Z+TZ.  DEPENDING-P2-0100
          ON THE VALUES OF PX,PY,PZ THERE ARE THEN 18 DIFFERENT COMBINA--P2-0110
          TIONS OF THE TWO PEAKS (DESIGNATED AS P1 AND P2):             -P2-0120
                                                                        -P2-0130
 QUANTITY      U OF QUANTITY          V OF QUANTITY          W OF QUANTITY   -P2-0140
 --------  ---------------------  ---------------------  ---------------------  -P2-0150
     P1          X + TX                 Y + TY                 Z + TZ          -P2-0160
     P2(0)  ---  QX + X + TX            QY + Y + TY            QZ + Z + TZ     -P2-0170
 P2(0)+P1        QX + 2X + 2TX          QY + 2Y + 2TY          QZ + 2Z + TZ    -P2-0180
 P2(0)-P1        QX                     QY                     QZ              -P2-0190
     P2(1)  ---  QX - X + TX            QY + Y + TY            QZ + Z + TZ     -P2-0200
 P2(1)+P1    *   QX + 2TX               QY + 2Y + 2TY          QZ + 2Z + TZ    -P2-0210
 P2(1)-P1        QX - 2X            #   QY                 #   QZ              -P2-0220
     P2(2)  ---  QX + X + TX            QY - Y + TY            QZ + Z + TZ     -P2-0230
 P2(2)+P1        QX + 2X + 2TX      *   QY + 2TY               QZ + 2Z + 2TZ   -P2-0240
 P2(2)-P1    #   QX                     QY - 2Y            #   QZ              -P2-0250
     P2(3)  ---  QX - X + TX            QY - Y + TY            QZ + Z + TZ     -P2-0260
 P2(3)+P1    *   QX + 2TX           *   QY + 2TY               QZ + 2Z + 2TZ   -P2-0270
 P2(3)-P1        QX - 2X                QY - 2Y            #   QZ              -P2-0280
     P2(4)  ---  QX + X + TX            QY + Y + TY            QZ - Z + TZ     -P2-0290
 P2(4)+P1        QX + 2X + 2TX          QY + 2Y + 2TY      *   QZ + 2TZ        -P2-0300
 P2(4)-P1    #   QX                 #   QY                     QZ - 2Z         -P2-0310
     P2(5)  ---  QX - X + TX            QY + Y + TY            QZ - Z + TZ     -P2-0320
 P2(5)+P1    *   QX + 2TX               QY + 2Y + 2TY      *   QZ + 2TZ        -P2-0330
 P2(5)-P1        QX - 2X            #   QY                     QZ - 2Z         -P2-0340
     P2(6)  ---  QX + X + TX            QY - Y + TY            QZ - Z + TZ     -P2-0350
 P2(6)+P1        QX + 2X + 2TX      *   QY + 2TY           *   QZ + 2TZ        -P2-0360
 P2(6)-P1    #   QX                     QY - 2Y                QZ - 2Z         -P2-0370
     P2(7)  ---  QX - X + TX            QY - Y + TY            QZ - Z + TZ     -P2-0380
 P2(7)+P1    *   QX + 2TX           *   QY + 2TY           *   QZ + 2TZ        -P2-0390
 P2(7)-P1        QX - 2X                QY - 2Y                QZ - 2Z         -P2-0400
                                                                        -P2-0410
          AS QX,QY,QZ ARE EITHER 0 OR 1/2 FOR ANY SYMMETRY ELEMENT AND  -P2-0420
          ARE KNOWN, VALUES OF  TX; TY; TX,TY; TZ; TX,TZ; TY,TZ OR      -P2-0430
          TX,TY,TZ ARE THEN COMPUTED.  FOR ALL BUT THE INVERSION, THE   -P2-0440
          FREQUENCY OF OCCURRENCE OF THESE VALUES IS STORED IN CORE.    -P2-0450
          FOR THE INVERSION, THE TX,TY,TZ TRIPLES ARE WRITTEN OUT,      -P2-0460
          SORTED INTO ORDER, AND THEN GROUPED TOGETHER ON REAPING IN    -P2-0470
          PART 3.  A LATITUDE OF ONE GRID POINT IN EACH DIRECTION IS    -P2-0480
          ALLOWED FOR THE VALUES OF TX, TY, TZ AND APPROPRIATE WEIGHTS  -P2-0490
          ASSIGNED.  THE ASTERISKED (*) RELATIONS ABOVE GIVE VALUES     -P2-0500
          OF TX,TY,TZ, PROVIDED THE NUMBERED (#) RELATIONS ARE OBEYED.  -P2-0510
```

```
                                                                    */ -P2-0520
     DECLARE (#RTND,IACR,IDWN,ILAY,#SYMM)     FIXED BINARY (15);     -P2-0530
     DECLARE   IS (#SYMM)                     FIXED BINARY (15) CONTROLLED;  -P2-0540
     DECLARE 1 PEAKS (#RTND)                  CONTROLLED EXTERNAL,   -P2-0550
               2 (U,V,W,VALU,MEAN)            FIXED BINARY (15);     -P2-0560
     DECLARE 1 SYMMPQ (#SYMM)                 CONTROLLED EXTERNAL,   -P2-0570
               2 (PX,QX,PY,QY,PZ,QZ)          FIXED BINARY (15);     -P2-0580
     DECLARE   RETAIN                         FILE RECORD SEQUENTIAL;-P2-0590
     DECLARE 1 PEAKR,                                                -P2-0600
               2 (RU,RV,RW,VAL,AVG)           FIXED BINARY (31);     -P2-0610
     DECLARE 1 TXYZ,                                                 -P2-0620
               2 (TX, TY, TZ, KS)             FIXED BINARY (15),     -P2-0630
               2 (VIJ, MIJ, FREQ)             FLOAT BINARY;          -P2-0640
     DECLARE   SYM(7)                         LABEL;                 -P2-0650
     DECLARE   ITXYZ                          FIXED BINARY (31);     -P2-0660
     DECLARE  (XLINE#(0:IACR), YLINE#(0:IDWN), ZLINE#(0:ILAY),       -P2-0670
          XYLAY#(0:IA,0:ID), YZLAY#(0:ID,0:IL), ZXLAY#(0:IL,0:IA))   -P2-0680
                                   EXTERNAL CONTROLLED FLOAT BINARY;  -P2-0690
/*   THE SEVEN-MEMBERED BIT(1) ARRAY "ION" SHOWS THE TYPE OF SYMMETRY  -P2-0700
     ELEMENTS BEING USED.  THE BIT IS SET IF THE SYMMETRY ELEMENT IS   -P2-0710
     PRESENT.                                                          -P2-0720
     ELEMENT                  NO    PX    PY    PZ   DETERMINE TX,TY,TZ?  -P2-0730
     PLANE PERP. TO X          1    -1     1     1   TX                -P2-0740
     PLANE PERP. TO Y          2     1    -1     1   TY                -P2-0750
     AXIS IN Z                 3    -1    -1     1   TX, TY            -P2-0760
     PLANE PERP. TO Z          4     1     1    -1   TZ                -P2-0770
     AXIS IN Y                 5    -1     1    -1   TX, TZ            -P2-0780
     AXIS IN X                 6     1    -1    -1   TY, TZ            -P2-0790
     INVERSION                 7    -1    -1    -1   TX, TY, TZ        -P2-0800
     SGNL='1'B IF THERE IS AN INVERSION;  NCNT='1'B IF THERE ARE OTHERS -P2-0810
                                                                    */ -P2-0820
     DECLARE  (ION(7),SGNL,NCNT)   BIT (1) EXTERNAL;                 -P2-0830
     DECLARE   AL(7)               LABEL;                            -P2-0840
     DECLARE   DBG                 EXTERNAL BIT (1);                 -P2-0850
     DECLARE  (IA2,ID2,IL2,I4A,I4D,I4L,JPIU,JPIV,JPIW,JMIU,JMIV,     -P2-0860
               JMIW,JMIUP,JMIVP,JMIWP,JMIUM,JMIVM,JMIWM)             -P2-0870
                                   FIXED BINARY (15);                -P2-0880
     DECLARE   LAY# (0:ILAY)       EXTERNAL CTL BIT(1);              -P2-0890
     DECLARE  (XQ, YQ, ZQ)         EXTERNAL FIXED BIN;               -P2-0900
     IA2 = IACR / 2;                                                 -P2-0910
     ID2 = IDWN / 2;                                                 -P2-0920
     IL2 = ILAY / 2;                                                 -P2-0930
     I4A = IACR * 4;                                                 -P2-0940
     I4D = IDWN * 4;                                                 -P2-0950
     I4L = ILAY * 4;                                                 -P2-0960
/*                                                                   -P2-0970
     I1 : MIRRORS AND PLANES RIGHT ON (TX|TY|TZ).                    -P2-0980
     I2 : TWO-FOLDS OR SCREWS RIGHT ON (TX,TY|TY,TZ|TX,TZ).          -P2-0990
     I3 : MIRRORS AND PLANES OFF ONE GRID POINT.                     -P2-1000
     I4 : TWO-FOLDS OR SCREWS OFF ONE IN ONE DIRECTION.              -P2-1010
```

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          I6 : TWO-FOLDS OR SCREWS OFF ONE IN BOTH DIRECTIONS.                  -P2-1020
                                                                          */    -P2-1030
          DECLARE  (I1,I2,I3,I4,I5,I6,TH)          FLOAT BINARY;               -P2-1040
          DECLARE  (J1,J2,J3,J4,J5,J6,MEANIJ)      FLOAT BINARY;               -P2-1050
          TH = 10.000;                    J1 = 18;                            -P2-1060
          J2 = 10;                        J3 = 9;                             -P2-1070
          J4 = 6;                         J5 = 4;                             -P2-1080
          J6 = 2;                                                             -P2-1090
          ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA                              -P2-1100
                    (I,KS,J,K,TX,TY,TZ);          EXIT;          END;         -P2-1110
/*                                                                            -P2-1120
          READ IN THE PEAKS, SORTED BY LAYER                                  -P2-1130
                                                                          */    -P2-1140
          OPEN FILE (RETAIN) INPUT;                                           -P2-1150
          ALLOCATE  PEAKS, IS;                                                -P2-1160
ILUP:     DO I = 1 TO #RTND BY 1;                                             -P2-1170
          READ FILE (RETAIN) INTO (PEAKR);                                    -P2-1180
          U(I) = RU;                                                          -P2-1190
          V(I) = RV;                                                          -P2-1200
          W(I) = RW;                                                          -P2-1210
          VALU(I) = VAL;                                                      -P2-1220
          MEAN(I) = AVG;                                                      -P2-1230
          END ILUP;                                                           -P2-1240
          CLOSE FILE (RETAIN);                                                -P2-1250
          ION = '0'B;                                                         -P2-1260
          NCNT = '0'B;                                                        -P2-1270
          IA = IACR;                                                          -P2-1280
          ID = IDWN;                                                          -P2-1290
          IL = ILAY;                                                          -P2-1300
/*                                                                            -P2-1310
          TRANSFORM THE SYMMETRY ELEMENTS INTO MORE USEABLE FORM              -P2-1320
                                                                          */    -P2-1330
SLUP:     DO I = 1 TO #SYMM BY 1;                                             -P2-1340
          IS(I) = 0;                                                          -P2-1350
          IF (PX(I) = -1)  THEN IS(I) = IS(I) + 1;              ELSE;         -P2-1360
          IF (PY(I) = -1)  THEN IS(I) = IS(I) + 2;              ELSE;         -P2-1370
          IF (PZ(I) = -1)  THEN IS(I) = IS(I) + 4;              ELSE;         -P2-1380
          IF (QX(I) = 1)  THEN QX(I) = IACR / 2;                ELSE;         -P2-1390
          IF (QY(I) = 1)  THEN QY(I) = IDWN / 2;                ELSE;         -P2-1400
          IF (QZ(I) = 1)  THEN QZ(I) = ILAY / 2;                ELSE;         -P2-1410
          KS = IS(I);                                                         -P2-1420
          IF (KS = 7)  THEN DO;                                               -P2-1430
          XQ = QX(I);                                                         -P2-1440
          YQ = QY(I);                                                         -P2-1450
          ZQ = QZ(I);                                   END;    ELSE;         -P2-1460
          ION(KS) = '1'B;                                                     -P2-1470
          END SLUP;                                                           -P2-1480
          PUT EDIT (#RTND,' PEAKS WERE RETAINED') (SKIP(2),F(5),A);           -P2-1490
          IF (DBG)  THEN PUT EDIT('ION =',ION) (SKIP,A,7 (B(1),X(1)));       -P2-1500
                    ELSE;                                                     -P2-1510
```

```
          IF (DBG)  THEN PUT PAGE;                                    ELSE;  -P2-1520
/*                                                                           -P2-1530
          ALLOCATE ARRAYS FOR MIRRORS, GLIDES, TWO-FOLDS, AND SCREWS       -P2-1540
                                                                      */ -P2-1550
ALLOC:    DO I = 1 TO 7;                                                   -P2-1560
          IF (ION(I))  THEN GO TO AL(I);          ELSE GO TO NDA;          -P2-1570
AL(1):    ALLOCATE XLINE#;                                                 -P2-1580
          XLINE# = 0.000;                                                  -P2-1590
          NCNT = '1'B;                                                     -P2-1600
          GO TO NDA;                                                       -P2-1610
AL(2):    ALLOCATE YLINE#;                                                 -P2-1620
          YLINE# = 0.000;                                                  -P2-1630
          NCNT = '1'B;                                                     -P2-1640
          GO TO NDA;                                                       -P2-1650
AL(3):    ALLOCATE XYLAY#;                                                 -P2-1660
          XYLAY# = 0.000;                                                  -P2-1670
          NCNT = '1'B;                                                     -P2-1680
          GO TO NDA;                                                       -P2-1690
AL(4):    ALLOCATE ZLINE#;                                                 -P2-1700
          ZLINE# = 0.000;                                                  -P2-1710
          NCNT = '1'B;                                                     -P2-1720
          GO TO NDA;                                                       -P2-1730
AL(5):    ALLOCATE ZXLAY#;                                                 -P2-1740
          ZXLAY# = 0.000;                                                  -P2-1750
          NCNT = '1'B;                                                     -P2-1760
          GO TO NDA;                                                       -P2-1770
AL(6):    ALLOCATE YZLAY#;                                                 -P2-1780
          YZLAY# = 0.000;                                                  -P2-1790
          NCNT = '1'B;                                                     -P2-1800
          GO TO NDA;                                                       -P2-1810
AL(7):    ALLOCATE  LAY#;                                                  -P2-1820
          LAY# = '0'B;                                                     -P2-1830
NDA:      END ALLOC;                                                       -P2-1840
          SGNL = ION(7);                                                   -P2-1850
/*                                                                         -P2-1860
          SEARCH THROUGH ALL PEAKS                                         -P2-1870
                                                                      */ -P2-1880
OUTER:    DO J = 1 TO #RTND BY 1;                                          -P2-1890
          JU = U(J);                                                       -P2-1900
          JV = V(J);                                                       -P2-1910
          JW = W(J);                        MEANJ = MEAN(J);               -P2-1920
INNER:    DO I = J TO #RTND BY 1;           MEANIJ=FLOAT(MEANJ+MEAN(I))/TH; -P2-1930
          IU = U(I);          I1 = J1 * MEANIJ;   I2 = J2 * MEANIJ;        -P2-1940
          IV = V(I);          I3 = J3 * MEANIJ;   I4 = J4 * MEANIJ;        -P2-1950
          IW = W(I);          I5 = J5 * MEANIJ;   I6 = J6 * MEANIJ;        -P2-1960
/*                                                                         -P2-1970
          COMPUTE THE SUM (P) AND THE DIFFERENCE (M) BETWEEN PEAKS         -P2-1980
          JU,JV,JW AND IU,IV,IW ALLOWING ONE GRID POINT POSITIVE (P)       -P2-1990
          AND NEGATIVE (M) ERROR                                           -P2-2000
                                                                      */ -P2-2010
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```
          JPIU = JU + IU;                                                    -P2-2020
          JPIV = JV + IV;                                                    -P2-2030
          JPIW = JW + IW;                                                    -P2-2040
          JMIU = MOD (JU - IU + I4A, IACR);                                  -P2-2050
          JMIV = MOD (JV - IV + I4D, IDWN);                                  -P2-2060
          JMIW = MOD (JW - IW + I4L, ILAY);                                  -P2-2070
          JMIUP = MOD (JMIU + 1 + I4A,  IACR);                               -P2-2080
          JMIUM = MOD (JMIU - 1 + I4A,  IACR);                               -P2-2090
          JMIVP = MOD (JMIV + 1 + I4D,  IDWN);                               -P2-2100
          JMIVM = MOD (JMIV - 1 + I4D,  IDWN);                               -P2-2110
          JMIWP = MOD (JMIW + 1 + I4L,  ILAY);                               -P2-2120
          JMIWM = MOD (JMIW - 1 + I4L,  ILAY);                               -P2-2130
/*                                                                           -P2-2140
          LOOP THROUGH ALL SYMMETRY ELEMENTS                                 -P2-2150
                                                                        */   -P2-2160
SYML:     DO K = 1 TO #SYMM BY 1;                                            -P2-2170
          KS = IS (K);                                                       -P2-2180
          GO TO SYM(KS);                                                     -P2-2190
/*                                                                           -P2-2200
          MIRROR OR GLIDE PLANE PERPENDICULAR TO X; DETERMINE TX             -P2-2210
          NOTE P2(1) ABOVE THAT V2-V1 = QY+/-1 AND W2-W1 = QZ+/-1            -P2-2220
          BEFORE U2+U1 = QX+2TX HOLDS.                                       -P2-2230
                                                                        */   -P2-2240
SYM(1):   IF ((JMIVP ¬= QY(K)) & (JMIV ¬= QY(K)) & (JMIVM ¬= QY(K)))         -P2-2250
                    THEN GO TO NDSY;                                ELSE;    -P2-2260
          IF ((JMIWP ¬= QZ(K)) & (JMIW ¬= QZ(K)) & (JMIWM ¬= QZ(K)))         -P2-2270
                    THEN GO TO NDSY;                                ELSE;    -P2-2280
          TX = MOD (((JPIU - QX(K)) / 2) + I4A,  IACR);                      -P2-2290
          XLINE#(TX) = XLINE#(TX) + I1;                                      -P2-2300
          TX = MOD (TX + 1,  IACR);                                          -P2-2310
          XLINE#(TX) = XLINE#(TX) + I3;                                      -P2-2320
          TX = MOD (TX - 2 + IACR,  IACR);                                   -P2-2330
          XLINE#(TX) = XLINE#(TX) + I3;                                      -P2-2340
          GO TO NDSY;                                                        -P2-2350
/*                                                                           -P2-2360
          MIRROR OR GLIDE PLANE PERPENDICULAR TO Y; DETERMINE TY             -P2-2370
          NOTE P2(2) ABOVE THAT U2-U1 = QX+/-1 AND W2-W1 = QZ+/-1            -P2-2380
          BEFORE V2+V1 = GY+2TY HOLDS.                                       -P2-2390
                                                                        */   -P2-2400
SYM(2):   IF ((JMIUP ¬= QX(K)) & (JMIU ¬= QX(K)) & (JMIUM ¬= QX(K)))         -P2-2410
                    THEN GO TO NDSY;                                ELSE;    -P2-2420
          IF ((JMIWP ¬= QZ(K)) & (JMIW ¬= QZ(K)) & (JMIWM ¬= QZ(K)))         -P2-2430
                    THEN GO TO NDSY;                                ELSE;    -P2-2440
          TY = MOD (((JPIV - QY(K)) / 2) + I4D,  IDWN);                      -P2-2450
          YLINE#(TY) = YLINE#(TY) + I1;                                      -P2-2460
          TY = MOD (TY + 1,  IDWN);                                          -P2-2470
          YLINE#(TY) = YLINE#(TY) + I3;                                      -P2-2480
          TY = MOD (TY - 2 + IDWN,  IDWN);                                   -P2-2490
          YLINE#(TY) = YLINE#(TY) + I3;                                      -P2-2500
          GO TO NDSY;                                                        -P2-2510
```

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/*                                                                      -P2-2520
      TWO-FOLD OR TWO-FOLD SCREW AXIS IN Z; DETERMINE TX & TY           -P2-2530
      NOTE P2(3) ABOVE THAT W2-W1 = QZ+/-1 BEFORE U2+U1 = QX+2TX        -P2-2540
      AND V2+V1 = QY+2TY HOLDS.                                         -P2-2550
                                                                    */  -P2-2560
SYM(3):  IF ((JMIWP ¬= QZ(K)) & (JMIW ¬= QZ(K)) & (JMIWM ¬= QZ(K)))     -P2-2570
                  THEN GO TO NDSY;                              ELSE;   -P2-2580
         TX = MOD ((((JPIU - QX(K)) / 2) + I4A,  IACR);                 -P2-2590
         TY = MOD ((((JPIV - QY(K)) / 2) + I4D,  IDWN);                 -P2-2600
         XYLAY#(TX,TY) = XYLAY#(TX,TY) + I2;                            -P2-2610
         TXP = MOD (TX + 1, IACR);                                      -P2-2620
         TYP = MOD (TY + 1, IDWN);                                      -P2-2630
         TXM = MOD (TX - 1 + IACR, IACR);                               -P2-2640
         TYM = MOD (TY - 1 + IDWN, IDWN);                               -P2-2650
         XYLAY#(TX,TYP) = XYLAY#(TX,TYP) + I4;                          -P2-2660
         XYLAY#(TX,TYM) = XYLAY#(TX,TYM) + I4;                          -P2-2670
         XYLAY#(TXP,TY) = XYLAY#(TXP,TY) + I4;                          -P2-2680
         XYLAY#(TXM,TY) = XYLAY#(TXM,TY) + I4;                          -P2-2690
         XYLAY#(TXM,TYP) = XYLAY#(TXM,TYP) + I6;                        -P2-2700
         XYLAY#(TXM,TYM) = XYLAY#(TXM,TYM) + I6;                        -P2-2710
         XYLAY#(TXP,TYM) = XYLAY#(TXP,TYM) + I6;                        -P2-2720
         XYLAY#(TXP,TYP) = XYLAY#(TXP,TYP) + I6;                        -P2-2730
         GO TO NDSY;                                                    -P2-2740
/*                                                                      -P2-2750
         MIRROR OR GLIDE PLANE PERPENDICULAR TO Z; DETERMINE TZ         -P2-2760
         NOTE P2(4) ABOVE THAT U2-U1 = QX+/-1 AND V2-V1 = QY+/-1        -P2-2770
         BEFORE W2+W1 = QZ+2TZ HOLDS                                    -P2-2780
                                                                    */  -P2-2790
SYM(4):  IF ((JMIUP ¬= QX(K)) & (JMIU ¬= QX(K)) & (JMIUM ¬= QX(K)))     -P2-2800
                  THEN GO TO NDSY;                              ELSE;   -P2-2810
         IF ((JMIVP ¬= QY(K)) & (JMIV ¬= QY(K)) & (JMIVM ¬= QY(K)))     -P2-2820
                  THEN GO TO NDSY;                              ELSE;   -P2-2830
         TZ = MOD ((((JPIW - QZ(K)) / 2) + I4L,  ILAY);                 -P2-2840
         ZLINE#(TZ) = ZLINE#(TZ) + I1;                                  -P2-2850
         TZ = MOD (TZ + 1,  ILAY);                                      -P2-2860
         ZLINE#(TZ) = ZLINE#(TZ) + I3;                                  -P2-2870
         TZ = MOD (TZ - 2 + ILAY,  ILAY);                               -P2-2880
         ZLINE#(TZ) = ZLINE#(TZ) + I3;                                  -P2-2890
         GO TO NDSY;                                                    -P2-2900
/*                                                                      -P2-2910
         TWO-FOLD OR TWO-FOLD SCREW AXIS IN Y; DETERMINE TX & TZ        -P2-2920
         NOTE P2(5) ABOVE THAT V2-V1 = QY+/-1 BEFORE U2+U1 = QX+2TX     -P2-2930
         AND W2+W1 = QZ+2TZ HOLDS.                                      -P2-2940
                                                                    */  -P2-2950
SYM(5):  IF ((JMIVP ¬= QY(K)) & (JMIV ¬= QY(K)) & (JMIVM ¬= QY(K)))     -P2-2960
                  THEN GO TO NDSY;                              ELSE;   -P2-2970
         TX = MOD ((((JPIU - QX(K)) / 2) + I4A,  IACR);                 -P2-2980
         TZ = MOD ((((JPIW - QZ(K)) / 2) + I4L,  ILAY);                 -P2-2990
         ZXLAY#(TZ,TX) = ZXLAY#(TZ,TX) + I2;                            -P2-3000
         TZP = MOD (TZ + 1, ILAY);                                      -P2-3010
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            TXP = MOD (TX + 1, IACR);                                          -P2-3020
            TZM = MOD (TZ - 1 + ILAY, ILAY);                                   -P2-3030
            TXM = MOD (TX - 1 + IACR, IACR);                                   -P2-3040
            ZXLAY#(TZ,TXP) = ZXLAY#(TZ,TXP) + I4;                              -P2-3050
            ZXLAY#(TZ,TXM) = ZXLAY#(TZ,TXM) + I4;                              -P2-3060
            ZXLAY#(TZP,TX) = ZXLAY#(TZP,TX) + I4;                              -P2-3070
            ZXLAY#(TZM,TX) = ZXLAY#(TZM,TX) + I4;                              -P2-3080
            ZXLAY#(TZM,TXP) = ZXLAY#(TZM,TXP) + I6;                            -P2-3090
            ZXLAY#(TZM,TXM) = ZXLAY#(TZM,TXM) + I6;                            -P2-3100
            ZXLAY#(TZP,TXM) = ZXLAY#(TZP,TXM) + I6;                            -P2-3110
            ZXLAY#(TZP,TXP) = ZXLAY#(TZP,TXP) + I6;                            -P2-3120
            GO TO NDSY;                                                        -P2-3130
/*                                                                             -P2-3140
            TWO-FOLD OR TWO-FOLD SCREW AXIS IN X; DETERMINE TY & TZ            -P2-3150
            NOTE P2(6) ABOVE THAT U2-U1 = QX+/-1 BEFORE V2+V1 = QY+2TY         -P2-3160
            AND W2+W1 = QZ+2TZ                                                 -P2-3170
                                                                          */   -P2-3180
SYM(6):     IF ((JMIUP ¬= QX(K)) & (JMIU ¬= QX(K)) & (JMIUM ¬= QX(K)))         -P2-3190
                        THEN GO TO NDSY;                              ELSE;    -P2-3200
            TZ = MOD ((((JPIW - QZ(K)) / 2) + I4L,  ILAY);                     -P2-3210
            TY = MOD ((((JPIV - QY(K)) / 2) + I4D,  IDWN);                     -P2-3220
            YZLAY#(TY,TZ) = YZLAY#(TY,TZ) + I2;                                -P2-3230
            TYP = MOD (TY + 1, IDWN);                                          -P2-3240
            TZP = MOD (TZ + 1, ILAY);                                          -P2-3250
            TYM = MOD (TY - 1 + IDWN, IDWN);                                   -P2-3260
            TZM = MOD (TZ - 1 + ILAY, ILAY);                                   -P2-3270
            YZLAY#(TY,TZP) = YZLAY#(TY,TZP) + I4;                              -P2-3280
            YZLAY#(TY,TZM) = YZLAY#(TY,TZM) + I4;                              -P2-3290
            YZLAY#(TYP,TZ) = YZLAY#(TYP,TZ) + I4;                              -P2-3300
            YZLAY#(TYM,TZ) = YZLAY#(TYM,TZ) + I4;                              -P2-3310
            YZLAY#(TYM,TZP) = YZLAY#(TYM,TZP) + I6;                            -P2-3320
            YZLAY#(TYM,TZM) = YZLAY#(TYM,TZM) + I6;                            -P2-3330
            YZLAY#(TYP,TZM) = YZLAY#(TYP,TZM) + I6;                            -P2-3340
            YZLAY#(TYP,TZP) = YZLAY#(TYP,TZP) + I6;                            -P2-3350
            GO TO NDSY;                                                        -P2-3360
/*                                                                             -P2-3370
            CENTER OF INVERSION; DETERMINE TX, TY, & TZ                        -P2-3380
                                                                          */   -P2-3390
SYM(7):     TZ = MOD ((((JPIW -  ZQ  ) / 2) + I4L,  ILAY);                     -P2-3400
/*                                                                             -P2-3410
            DETERMINE THE LAYERS WITH TX.TY.TZ                                 -P2-3420
                                                                          */   -P2-3430
OUTP:       DO IZ = -1 TO 1 BY 1;                                              -P2-3440
            JZ = MOD (TZ + IZ + ILAY, ILAY);                                   -P2-3450
            LAY#(JZ) = '1'B;                                                   -P2-3460
            END OUTP;                                                          -P2-3470
NDSY:       END SYML;                                                          -P2-3480
            END INNER;                                                         -P2-3490
            IF (DBG)  THEN PUT EDIT (' PEAK# =',J) (A,F(4));       ELSE;       -P2-3500
            END CUTER;                                                         -P2-3510
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          RETURN;                                                          -P2-3520
          END PART2;                                                       -P2-3530



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                       -P3-0010
 /*   OUTPUT ALL VALUES OF TX.TY.TZ WITH FREQUENCY > 5 TO BE SORTED  */    -P3-0020
 PART3:   PROCEDURE (IACR,IDWN,ILAY,#RTND);                                -P3-0030
 /*                                                                        -P3-0040
          IN PART2, ALL OF THE POSSIBLE VALUES OF TZ WERE FLAGGED AS       -P3-0050
      TO WHETHER OR NOT THEY OCCURRED.  IN THIS SUBROUTINE, A LAYER OF     -P3-0060
      TX.TY IS FILLED FOR EACH VALUE OF TZ, WITH THE FREQUENCY OF          -P3-0070
      OCCURRENCE OF EACH VALUE OF TX.TY.TZ.  AFTER THE LAYER HAS BEEN      -P3-0080
      CREATED, ALL OF THE TX.TY.TZ TRIPLES WITH FREQUENCY > 5 ARE OUTPUT-P3-0090
                                                                    */     -P3-0100
          DECLARE   LAYER (0:IACR,0:IDWN)    FLOAT BIN CTL;                -P3-0110
          DECLARE   LAY#(0:ILAY)             EXTERNAL BIT(1) CTL;          -P3-0120
          DECLARE  (IACR,IDWN,ILAY,#RTND)    FIXED BINARY (15);            -P3-0130
          DECLARE   SORTIN                   FILE RECORD SEQUENTIAL;       -P3-0140
          DECLARE  (DBG, DNV)                EXTERNAL BIT (1);             -P3-0150
          DECLARE 1 PEAKS (#RTND)            CONTROLLED EXTERNAL,          -P3-0160
                    2 (U,V,W,VALU,MEAN)      FIXED BINARY (15);            -P3-0170
          DECLARE 1 SXYZ,                                                  -P3-0180
                    2 (SX, SY, SZ, SK)       FIXED BINARY (15),            -P3-0190
                    2 (VAL, AVG, FREQ)       FLOAT BINARY;                 -P3-0200
          DECLARE  (02,03,04,05,M1,M2,M3,TH) FLOAT BINARY;                 -P3-0210
          DECLARE  (XQ, YQ, ZQ)              EXTERNAL FIXED BIN;           -P3-0220
          DECLARE   #INV                     FIXED BIN;                    -P3-0230
          #INV = 0;                    TH = 50.000;                        -P3-0240
          02 = 2.00;                                                       -P3-0250
          03 = 3.00;                                                       -P3-0260
          04 = 4.00;                                                       -P3-0270
          05 = 5.00;                                                       -P3-0280
          X5 = 05 * 5.0000;                                                -P3-0290
          VAL, AVG = 0.0000;                                               -P3-0300
          SK = 7;                                                          -P3-0310
          I4A = IACR * 4;                                                  -P3-0320
          I4D = IDWN * 4;                                                  -P3-0330
          I4L = ILAY * 4;                                                  -P3-0340
          ON ERROR SNAP EXIT;                                              -P3-0350
          IF (DBG)  THEN PUT EDIT ('XQ =',XQ,'YQ =',YQ,'ZQ =',ZQ)          -P3-0360
                    (SKIP(4),3 (A,F(5),X(2)));                  ELSE;      -P3-0370
          IF (DBG)  THEN PUT EDIT ('LAY# =  ',LAY#)                        -P3-0380
                    (SKIP(2),A,(ILAY+1) (X(2),B(1)));           ELSE;      -P3-0390
          IF (DNV)  THEN DO;                                               -P3-0400
          PUT EDIT ('THE TX, TY, TZ PAIRS THAT HAVE MORE THAN 5',          -P3-0410
                    ' TX TY TZ SY   VALU   MEAN   FREQ',                   -P3-0420
                    ' TX TY TZ SY   VALU   MEAN   FREQ',                   -P3-0430
                    ' TX TY TZ SY   VALU   MEAN   FREQ',                   -P3-0440
```

```
                    ' TX TY TZ SY   VALU   MEAN   FREQ')                          -P3-0450
                   (PAGE,A,SKIP,A,A,A,A);   PUT SKIP;      END; ELSE;   -P3-0460
          OPEN FILE (SORTIN) OUTPUT;                                              -P3-0470
          ALLOCATE LAYER;                                                         -P3-0480
/*                                                                                -P3-0490
          LOOP THROUGH THE LAYERS, ONE AT A TIME                                  -P3-0500
          IF (¬LAY#( LAY))  THEN GO TO NDLAY;                        ELSE;        -P3-0510
                                                                        */ -P3-0520
LAYLUP:   DO LAY = 0 TO ILAY BY 1;                                                -P3-0530
          LAYER = 0.000;                                                          -P3-0540
/*                                                                                -P3-0550
          OUTER LOOP THROUGH ALL THE PEAKS                                        -P3-0560
                                                                        */ -P3-0570
OUTER:    DO J = 1 TO #RTND BY 1;        MEANJ = MEAN(J);                         -P3-0580
          K = J + 1;                                                              -P3-0590
          IF (K > #RTND)  THEN GO TO NDOTR;                          ELSE;        -P3-0600
          JU = U(J);                                                              -P3-0610
          JV = V(J);                                                              -P3-0620
          JW = W(J);                                                              -P3-0630
/*                                                                                -P3-0640
          INNER LOOP THROUGH THE REMAINDER OF THE PEAKS                           -P3-0650
                                                                        */ -P3-0660
INNER:    DO I = K TO #RTND BY 1;        MEANIJ=FLOAT(MEANJ+MEAN(I))/TH;          -P3-0670
          JPIW = MOD (((JW + W(I) - ZQ) / 2) + I4L, ILAY);                        -P3-0680
          JPIWP = MOD (JPIW + 1, ILAY);                                           -P3-0690
          JPIWM = MOD (JPIW - 1 + ILAY, ILAY);                                    -P3-0700
          IF (JPIW =  LAY)  THEN GO TO RTON;                         ELSE;        -P3-0710
          IF ((JPIWP =  LAY)|(JPIWM =  LAY))  THEN GO TO ZOFF1;                   -P3-0720
                                              ELSE GO TO NDINR;                   -P3-0730
/*                                                                                -P3-0740
          THE VALUE OF ILAY = TZ                                                  -P3-0750
                                                                        */ -P3-0760
RTON:     M1 = 05 * MEANIJ;                                                      -P3-0770
          M2 = 04 * MEANIJ;                                                       -P3-0780
          M3 = 03 * MEANIJ;                                                       -P3-0790
          GO TO OK;                                                               -P3-0800
/*                                                                                -P3-0810
          THE VALUE OF ILAY = TZ+1 OR TZ-1                                        -P3-0820
                                                                        */ -P3-0830
ZOFF1:    M1 = 04 * MEANIJ;                                                      -P3-0840
          M2 = 03 * MEANIJ;                                                       -P3-0850
          M3 = 02 * MEANIJ;                                                       -P3-0860
/*                                                                                -P3-0870
          SET UP THE VALUES OF TX AND TY OFF ONE GRID POINT                       -P3-0880
                                                                        */ -P3-0890
OK:       JPIU = MOD (((JU + U(I) - XQ) / 2) + I4A, IACR);                        -P3-0900
          JPIV = MOD (((JV + V(I) - YQ) / 2) + I4D, IDWN);                        -P3-0910
          JPIUP = MOD (JPIU + 1, IACR);                                           -P3-0920
          JPIVP = MOD (JPIV + 1, IDWN);                                           -P3-0930
          JPIUM = MOD (JPIU - 1 + IACR, IACR);                                    -P3-0940
```

```
          JPIVM = MOD (JPIV - 1 + IDWN, IDWN);                                  -P3-0950
/*                                                                              -P3-0960
          FILL THE ARRAY WITH THE FREQUENCIES                                   -P3-0970
                                                                          */    -P3-0980
FILL:     LAYER (JPIU ,JPIV )  =  LAYER (JPIU ,JPIV ) + M1;                     -P3-0990
          LAYER (JPIU ,JPIVP)  =  LAYER (JPIU ,JPIVP) + M2;                     -P3-1000
          LAYER (JPIU ,JPIVM)  =  LAYER (JPIU ,JPIVM) + M2;                     -P3-1010
          LAYER (JPIUP,JPIV )  =  LAYER (JPIUP,JPIV ) + M2;                     -P3-1020
          LAYER (JPIUP,JPIVP)  =  LAYER (JPIUP,JPIVP) + M3;                     -P3-1030
          LAYER (JPIUP,JPIVM)  =  LAYER (JPIUP,JPIVM) + M3;                     -P3-1040
          LAYER (JPIUM,JPIV )  =  LAYER (JPIUM,JPIV ) + M2;                     -P3-1050
          LAYER (JPIUM,JPIVP)  =  LAYER (JPIUM,JPIVP) + M3;                     -P3-1060
          LAYER (JPIUM,JPIVM)  =  LAYER (JPIUM,JPIVM) + M3;                     -P3-1070
NDINR:    END INNER;                                                            -P3-1080
NDOTR:    END OUTER;                                                            -P3-1090
/*                                                                              -P3-1100
          WRITE OUT THE TX.TY.TZ TRIPLES FROM THE LAYER                         -P3-1110
                                                                          */    -P3-1120
          SZ = LAY;                                                             -P3-1130
SYLP:     DO SY = 0 TO IDWN BY 1;                                               -P3-1140
SXLP:     DO SX = 0 TO IACR BY 1;                                               -P3-1150
          FREQ = LAYER (SX,SY);                                                 -P3-1160
          IF (FREQ > X5)  THEN GO TO OUTP;          ELSE GO TO NDSX;            -P3-1170
OUTP:     WRITE FILE (SORTIN) FROM (SXYZ);                                      -P3-1180
          #INV = #INV + 1;                                                      -P3-1190
          IF (ONV)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7));          ELSE;        -P3-1200
NDSX:     END SXLP;                                                             -P3-1210
          END SYLP;                                                             -P3-1220
NDLAY:    END LAYLUP;                                                           -P3-1230
          FREE LAYER, LAY#, PEAKS;                                              -P3-1240
          PUT EDIT('THERE ARE',#INV,'TX.TY.TZ TRIPLES FROM INVERSIONS.')-P3-1250
               (SKIP(2),A,F(10),X(1),A);                                        -P3-1260
          PUT EDIT ('***** ALL INVERSIONS HAVE BEEN OUTPUT *****')              -P3-1270
                (SKIP(2),A);                                                    -P3-1280
          RETURN;                                                               -P3-1290
          END PART3;                                                            -P3-1300
```

```
* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                           -P4-0010
 /*   OUTPUT TX, TY, TZ, TX.TY, TY.TZ, TZ.TX WITH FREQUENCY > 10          */    -P4-0020
 PART4:   PROCEDURE (IACR, IDWN, ILAY);                                         -P4-0030
 /*                                                                             -P4-0040
          IN PART2 THE TX,TY,TZ,TX.TY,TY.TZ,TX.TZ GROUP(S) ARE PRODUCED -P4-0050
          FROM THE NON-INVERSION SYMMETRY ELEMENTS.  THESE VALUES OF    -P4-0060
          THE TRANSLATIONS ARE STORED IN THE EXTERNAL ARRAYS XLINE#,    -P4-0070
          YLINE#, ZLINE#, XYLAY#, YZLAY#, ZXLAY#.  THESE VALUES ARE     -P4-0080
          WRITTEN OUT ON THE FILE "SORTIN", WITH THE UNDETERMINED VALUES-P4-0090
          SET EQUAL TO -1.                                                      -P4-0100
```

```
                                                                    */ -P4-0110
        DECLARE  (IACR,IA,IDWN,ID,ILAY,IL) FIXED BINARY (15);         -P4-0120
        DECLARE   ION(7)                   BIT (1) EXTERNAL;          -P4-0130
        DECLARE   SORTIN                   FILE RECORD SEQUENTIAL;    -P4-0140
        DECLARE   SLB(6)                   LABEL;                     -P4-0150
        DECLARE  (XLINE#(0:IACR), YLINE#(0:IDWN), ZLINE#(0:ILAY),     -P4-0160
             XYLAY#(0:IA,0:ID), YZLAY#(0:ID,0:IL), ZXLAY#(0:IL,0:IA)) -P4-0170
                                EXTERNAL CONTROLLED FLOAT BINARY;     -P4-0180
        DECLARE 1 SXYZ,                                               -P4-0190
                  2 (SX, SY, SZ, SK)  FIXED BINARY (15),              -P4-0200
                  2 (VALU,MEAN,FREQ)  FLOAT BINARY;                   -P4-0210
        DECLARE   TEN                 FLOAT BINARY;                   -P4-0220
        DECLARE   DBG                 EXTERNAL BIT (1);               -P4-0230
        TEN = 10.000;                                                 -P4-0240
        IA = IACR;                                                    -P4-0250
        ID = IDWN;                                                    -P4-0260
        IL = ILAY;                                                    -P4-0270
        VALU, MEAN = 1.000;                                           -P4-0280
        ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA                        -P4-0290
                  (SK,SX,SY,SZ);                  EXIT;       END;    -P4-0300
        IF (DBG)  THEN DO;                                            -P4-0310
        PUT EDIT ('PEAKS FROM MIRRORS, GLIDES, TWO-FOLDS, & SCREWS',  -P4-0320
                  '  SX SY SZ TY   VALUE    MEAN    FREQ',           -P4-0330
                  '  SX SY SZ TY   VALUE    MEAN    FREQ',           -P4-0340
                  '  SX SY SZ TY   VALUE    MEAN    FREQ',           -P4-0350
                  '  SX SY SZ TY   VALUE    MEAN    FREQ')           -P4-0360
                 (PAGE,A,SKIP,A,A,A,A);                               -P4-0370
        PUT SKIP;                       END;            ELSE;       -P4-0380
/*                                                                    -P4-0390
        GO THROUGH ALL OF THE SIX NON-INVERSION SYMMETRY TYPES        -P4-0400
                                                                    */ -P4-0410
STYP:   DO SK = 1 TO 6 BY 1;                                          -P4-0420
        IF (ION(SK))  THEN GO TO SLB(SK);          ELSE GO TO NDS;    -P4-0430
/*                                                                    -P4-0440
        OUTPUT ALL TX WITH # > 10 FOR A PLANE NORMAL TO X             -P4-0450
                                                                    */ -P4-0460
SLB(1): SY, SZ = -1;                                                  -P4-0470
XLUP:   DO SX = 0 TO IACR BY 1;                                       -P4-0480
        IF (XLINE#(SX) < TEN)  THEN GO TO NDX;             ELSE;      -P4-0490
        FREQ = XLINE#(SX);                                            -P4-0500
        IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));  ELSE;      -P4-0510
        WRITE FILE (SORTIN) FROM (SXYZ);                              -P4-0520
NDX:    END XLUP;                                                     -P4-0530
        FREE XLINE#;                                                  -P4-0540
        GO TO NDS;                                                    -P4-0550
/*                                                                    -P4-0560
        OUTPUT ALL TY WITH # > 10 FOR A PLANE NORMAL TO Y             -P4-0570
                                                                    */ -P4-0580
SLB(2): SX, SZ = -1;                                                  -P4-0590
YLUP:   DO SY = 0 TO IDWN BY 1;                                       -P4-0600
```

```
          IF (YLINE#(SY) < TEN)  THEN GO TO NDY;                    ELSE;   -P4-0610
          FREQ = YLINE#(SY);                                                -P4-0620
          IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));         ELSE;   -P4-0630
          WRITE FILE (SORTIN) FROM (SXYZ);                                  -P4-0640
NDY:      END YLUP;                                                         -P4-0650
          FREE YLINE#;                                                      -P4-0660
          GO TO NDS;                                                        -P4-0670
/*                                                                          -P4-0680
          OUTPUT ALL TX.TY WITH # > 10 FOR AN AXIS IN Z                     -P4-0690
                                                                      */    -P4-0700
SLB(3):   SZ = -1;                                                          -P4-0710
XLXY:     DO SX = 0 TO IACR BY 1;                                           -P4-0720
YLXY:     DO SY = 0 TO IDWN BY 1;                                           -P4-0730
          IF (XYLAY#(SX,SY) < TEN)  THEN GO TO NDXY;                ELSE;   -P4-0740
          FREQ = XYLAY#(SX,SY);                                             -P4-0750
          IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));         ELSE;   -P4-0760
          WRITE FILE (SORTIN) FROM (SXYZ);                                  -P4-0770
NDXY:     END YLXY;                                                         -P4-0780
          END XLXY;                                                         -P4-0790
          FREE XYLAY#;                                                      -P4-0800
          GO TO NDS;                                                        -P4-0810
/*                                                                          -P4-0820
          OUTPUT ALL TZ WITH # > 10 FOR A PLANE NORMAL TO Z                 -P4-0830
                                                                      */    -P4-0840
SLB(4):   SX, SY = -1;                                                      -P4-0850
ZLUP:     DO SZ = 0 TO ILAY BY 1;                                           -P4-0860
          IF (ZLINE#(SZ) < TEN)  THEN GO TO NDZ;                    ELSE;   -P4-0870
          FREQ = ZLINE#(SZ);                                                -P4-0880
          IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));         ELSE;   -P4-0890
          WRITE FILE (SORTIN) FROM (SXYZ);                                  -P4-0900
NDZ:      END ZLUP;                                                         -P4-0910
          FREE ZLINE#;                                                      -P4-0920
          GO TO NDS;                                                        -P4-0930
/*                                                                          -P4-0940
          OUTPUT ALL TZ.TX WITH # > 10 FOR AN AXIS IN Y                     -P4-0950
                                                                      */    -P4-0960
SLB(5):   SY = -1;                                                          -P4-0970
ZLZX:     DO SZ = 0 TO ILAY BY 1;                                           -P4-0980
XLZX:     DO SX = 0 TO IACR BY 1;                                           -P4-0990
          IF (ZXLAY#(SZ,SX) < TEN)  THEN GO TO NDZX;                ELSE;   -P4-1000
          FREQ = ZXLAY#(SZ,SX);                                             -P4-1010
          IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));         ELSE;   -P4-1020
          WRITE FILE (SORTIN) FROM (SXYZ);                                  -P4-1030
NDZX:     END XLZX;                                                         -P4-1040
          END ZLZX;                                                         -P4-1050
          FREE ZXLAY#;                                                      -P4-1060
          GO TO NDS;                                                        -P4-1070
/*                                                                          -P4-1080
          OUTPUT ALL TY.TZ WITH # > 10 FOR AN AXIS IN X                     -P4-1090
                                                                      */    -P4-1100
```

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SLB(6):   SX = -1;                                                          -P4-1110
YLYZ:     DO SY = 0 TO IDWN BY 1;                                           -P4-1120
ZLYZ:     DO SZ = 0 TO ILAY BY 1;                                           -P4-1130
          IF (YZLAY#(SY,SZ) < TEN)  THEN GO TO NDYZ;            ELSE;       -P4-1140
          FREQ = YZLAY#(SY,SZ);                                             -P4-1150
          IF (DBG)  THEN PUT EDIT (SXYZ) (4 F(3),3 F(7,0));     ELSE;       -P4-1160
          WRITE FILE (SORTIN) FROM (SXYZ);                                  -P4-1170
NDYZ:     END ZLYZ;                                                         -P4-1180
          END YLYZ;                                                         -P4-1190
          FREE YZLAY#;                                                      -P4-1200
NDS:      END STYP;                                                         -P4-1210
          RETURN;                                                           -P4-1220
          END PART4;                                                        -P4-1230



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                        -P5-0010
 /*   MAP THE SYMMETRY ELEMENTS INTO EACH OTHER                      */     -P5-0020
 PART5:   PROCEDURE (IACR, IDWN, ILAY);                                     -P5-0030
 /*                                                                         -P5-0040
          BEFORE THIS PART, THE VALUE OF TX,TY,TZ,TX.TY,TX.TZ,TY.TZ. &      -P5-0050
          TX.TY.TZ WRITTEN OUT BY PART3 AND PART4, WERE SORTED BY           -P5-0060
          DECREASING FREQUENCY (SO THAT THE MOST FREQUENT ARE FIRST) &      -P5-0070
          BY DECREASING SYMMETRY (SO THAT THE INVERSIONS ARE FIRST).        -P5-0080
          A NUMBER OF EACH OF THESE, PROPORTIONAL TO THE SIZE OF THE        -P5-0090
          MAP AND TO THE TOTAL NUMBER OF EACH SYMMETRY ELEMENT POSSIBLE,    -P5-0100
          IS NOW READ AND STORED.  AT THIS POINT, THE SYMMETRY ELEMENTS     -P5-0110
          ARE MAPPED INTO EACH OTHER, AS SHOWN BELOW, WITH A LATITUDE       -P5-0120
          OF ONE GRID POINT ALLOWED IN EACH DIRECTION:                      -P5-0130
                                                                            -P5-0140
           SYMMETRY ELEMENT        SYMMETRY ELEMENT MAPPED INTO             -P5-0150
                 TX                TX.TY, TX.TZ, TX.TY.TZ                   -P5-0160
                 TY                TX.TY, TY.TZ, TX.TY.TZ                   -P5-0170
                 TZ                TX.TZ, TY.TZ, TX.TY.TZ                   -P5-0180
               TX.TY               TY.TZ, TX.TZ, TX.TY.TZ                   -P5-0190
               TX.TZ               TX.TY, TY.TZ, TX.TY.TZ                   -P5-0200
               TY.TZ               TX.TY, TX.TZ, TX.TY.TZ                   -P5-0210
                                                                            -P5-0220
          A RECORD IS KEPT AS EACH MAPPING IS DONE.  ALSO, THE SUMS OF      -P5-0230
          THE FREQUENCIES ENCOUNTERED BY EACH MAPPING ARE COMPUTED AND      -P5-0240
          STORED.                                                           -P5-0250
                                                                     */     -P5-0260
          DECLARE   (IACR, IDWN, ILAY)  FIXED BINARY (15);                  -P5-0270
          DECLARE   (IA8,ID8,IL8,#XYZ)  FIXED BINARY (15) EXTERNAL;         -P5-0280
          DECLARE 1 TXYZ,                                                   -P5-0290
                    2 (TX, TY, TZ, SK)  FIXED BINARY (15),                  -P5-0300
                    2 (VALU,MEAN,FRQ)   FLOAT BINARY;                       -P5-0310
          DECLARE   SORTOUT             FILE RECORD SEQUENTIAL;           -P5-0320
          DECLARE  (ION(7),SGNL,NCNT)   BIT (1) EXTERNAL;                   -P5-0330
```

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          DECLARE 1 STORE (#XYZ)          CONTROLLED,                              -P5-0340
                    2 (SX, SY, SZ, KS)    FIXED BINARY (15),                       -P5-0350
                    2 FREQ                FLOAT BINARY;                            -P5-0360
          DECLARE  (CST(7), TST(7))       FIXED BINARY (15);                       -P5-0370
          DECLARE 1 RESULT (#XYZ)         CONTROLLED EXTERNAL,                     -P5-0380
                    2 (RX, RY, RZ, RS)    FIXED BINARY (15),                       -P5-0390
                   2 (BX, BY, BXY, BZ, BXZ, BYZ)  BIT (1),                        -P5-0400
                    2 OK                  FLOAT BINARY;                            -P5-0410
          DECLARE  (FREQI, P1, P2, P0)    FLOAT BINARY;                            -P5-0420
          DECLARE   CK(7)                 LABEL;                                   -P5-0430
          DECLARE   DBG                   EXTERNAL BIT (1);                        -P5-0440
          ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA                                   -P5-0450
                   (SK,I,J,KSI,IS,KSJ);           EXIT;          END;             -P5-0460
          /*                                                                       -P5-0470
          P0:  RIGHT ON                                                            -P5-0480
          P1:  OFF ONE GRID POINT IN ONE DIRECTION                                 -P5-0490
          P2:  OFF ONE GRID POINT IN EACH OF TWO DIRECTIONS                        -P5-0500
                                                                              */   -P5-0510
          P1 = 0.8500;                                                             -P5-0520
          P2 = 0.7000;                                                             -P5-0530
          P0 = 1.0000;                                                             -P5-0540
          /*                                                                       -P5-0550
          ALLOCATE ARRAY TO HOLD THE LARGEST TX, TY, TZ / SYMM TYPE                -P5-0560
                                                                              */   -P5-0570
          IA8 = IACR / 4;                                                          -P5-0580
          ID8 = IDWN / 4;                                                          -P5-0590
          IL8 = ILAY / 4;                                                          -P5-0600
          TST(1) = ION(1) * IA8 * 2;                                               -P5-0610
          TST(2) = ION(2) * ID8 * 2;                                               -P5-0620
          TST(4) = ION(4) * IL8 * 2;                                               -P5-0630
          TST(3) = ION(3) * IA8 * ID8 * 2;                                         -P5-0640
          TST(5) = ION(5) * IL8 * IA8 * 2;                                         -P5-0650
          TST(6) = ION(6) * ID8 * IL8 * 2;                                         -P5-0660
          TST(7) = ION(7) * IA8 * ID8 * IL8 * 2;                                   -P5-0670
          #XYZ = TST(1)+TST(2)+TST(3)+TST(4)+TST(5)+TST(6)+TST(7);                 -P5-0680
          IF (IDBG)  THEN PUT EDIT ('TST =',TST,'ION =',ION)                       -P5-0690
                                  (SKIP,A,7 F(4),X(5),A,7 B(1)); ELSE;             -P5-0700
          ALLOCATE  STORE;                                                         -P5-0710
          FREQ = 0.000;                                                            -P5-0720
          CST = 0;                                                                 -P5-0730
          /*                                                                       -P5-0740
          READ IN THE HIGHEST VALUES OF TX, TY, TZ                                 -P5-0750
                                                                              */   -P5-0760
          ON ENDFILE (SORTOUT) GO TO FIND;                                         -P5-0770
          I = 0;                                                                   -P5-0780
RRD:      READ FILE (SORTOUT) INTO (TXYZ);                                         -P5-0790
          IF (CST(SK) >= TST(SK))  THEN GO TO RRD;                         ELSE;   -P5-0800
          CST(SK) = CST(SK) + 1;                                                   -P5-0810
          I = I + 1;                                                               -P5-0820
          SX(I) = TX;                                                              -P5-0830
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          SY(I) = TY;                                                          -P5-0840
          SZ(I) = TZ;                                                          -P5-0850
          KS(I) = SK;                                                          -P5-0860
          FREQ(I) = FREQ(I) + FRQ;                                             -P5-0870
          IF (I < #XYZ)  THEN GO TO RRD;                              ELSE;    -P5-0880
/*                                                                             -P5-0890
          MERGE THE LOWER SYMMETRY ELEMENTS INTO THE HIGHER                    -P5-0900
                                                                          */   -P5-0910
FIND:     CLOSE FILE (SORTOUT);                                                -P5-0920
          ALLOCATE  RESULT;                                                    -P5-0930
          BX, BY, BXY, BZ, BXZ, BYZ = '0'B;                                    -P5-0940
          RX = SX;                                                             -P5-0950
          RY = SY;                                                             -P5-0960
          RZ = SZ;                                                             -P5-0970
          RS = KS;                                                             -P5-0980
          OK = 0.000;                                                          -P5-0990
          IF (DBG)  THEN DO;                                                   -P5-1000
          PUT EDIT ('SAVED TX, TY, TZ -- BEFORE MAPPING')(PAGE,A);             -P5-1010
          PUT EDIT ('  TX TY TZ SY      FREQ TX TY TZ SY      FREQ',          -P5-1020
                    ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',          -P5-1030
                    ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ')          -P5-1040
                   (SKIP(2),A,A,A);     PUT SKIP(2);                         -P5-1050
          PUT EDIT ((STORE (I) DO I = 1 TO #XYZ)) (4 F(3),E(10,3,4));          -P5-1060
                                        END;                          ELSE;    -P5-1070
ILUP:     DO I = 1 TO #XYZ BY 1;                                               -P5-1080
          IS = KS(I);                                                          -P5-1090
          ISX = SX(I);                                                         -P5-1100
          ISY = SY(I);                                                         -P5-1110
          ISZ = SZ(I);                                                         -P5-1120
          FREQI = FREQ(I);                                                     -P5-1130
JLUP:     DO J = 1 TO #XYZ BY 1;                                               -P5-1140
          KSJ = KS(J);                                                         -P5-1150
          GO TO CK(KSJ);                                                       -P5-1160
/*                                                                             -P5-1170
          MERGE MIRRORS AND GLIDES WITH SCREWS, TWO-FOLDS AND INVERSIONS       -P5-1180
          MERGE TX WITH TX.TY, TX.TZ, OR TX.TY.TZ                              -P5-1190
                                                                          */   -P5-1200
CK(1):    IF ((IS=1)|(IS=2)|(IS=4)|(IS=6))  THEN GO TO NDJ;           ELSE;    -P5-1210
          IDX = ABS (ISX - SX(J));                                             -P5-1220
          IF (IDX < 2)  THEN BX(I),BX(J) = '1'B;                      ELSE;    -P5-1230
CMPX:     IF (IDX=0)  THEN OK(I) = OK(I) + (FREQI * FREQ(J));         ELSE;    -P5-1240
          IF (IDX=1)  THEN OK(I) = OK(I) + (P1 * FREQI*FREQ(J));      ELSE;    -P5-1250
          GO TO NDJ;                                                           -P5-1260
/*                                                                             -P5-1270
          MERGE TY WITH TX.TY, TY.TZ OR TX.TY.TZ                               -P5-1280
                                                                          */   -P5-1290
CK(2):    IF ((IS=1)|(IS=2)|(IS=4)|(IS=5))  THEN GO TO NDJ;           ELSE;    -P5-1300
          IDY = ABS (ISY - SY(J));                                             -P5-1310
          IF (IDY < 2)  THEN BY(I),BY(J) = '1'B;                      ELSE;    -P5-1320
CMPY:     IF (IDY=0)  THEN OK(I) = OK(I) + (FREQI * FREQ(J));         ELSE;    -P5-1330
```

```
          IF (IDY=1)  THEN OK(I) = OK(I) + (P1 * FREQI*FREQ(J)); ELSE;   -P5-1340
          GO TO NDJ;                                                     -P5-1350
/*                                                                       -P5-1360
          MERGE TZ WITH TX.TZ, TY.TZ OR TX.TY.TZ                         -P5-1370
                                                                    */   -P5-1380
CK(4):    IF ((IS=1)|(IS=2)|(IS=3)|(IS=4))  THEN GO TO NDJ;       ELSE;   -P5-1390
          IDZ = ABS (ISZ - SZ(J));                                       -P5-1400
          IF (IDZ < 2)  THEN BZ(I),BZ(J) = '1'B;                 ELSE;   -P5-1410
CMPZ:     IF (IDZ=0)  THEN OK(I) = OK(I) + (FREQI * FREQ(J));    ELSE;   -P5-1420
          IF (IDZ=1)  THEN OK(I) = OK(I) + (P1 * FREQI*FREQ(J)); ELSE;   -P5-1430
          GO TO NDJ;                                                     -P5-1440
/*                                                                       -P5-1450
          MAP MIRRORS & GLIDES INTO INVERSIONS & OTHER MIRRORS & GLIDES  -P5-1460
          MERGE TX.TY WITH TX.TZ, TY.TZ OR TX.TY.TZ                      -P5-1470
                                                                    */   -P5-1480
CK(3):    IF ((IS=1)|(IS=2)|(IS=3)|(IS=4))  THEN GO TO NDJ;       ELSE;   -P5-1490
          IDX = ABS (ISX - SX(J));                                       -P5-1500
          IDY = ABS (ISY - SY(J));                                       -P5-1510
          IF ((IDX<2) & (IDY<2))  THEN BXY(I),BXY(J)='1'B;       ELSE;   -P5-1520
          ID1 = IDX;                                                     -P5-1530
          ID2 = IDY;                                                     -P5-1540
          IF (IS=5)  THEN IF (IDX>1)  THEN GO TO NDJ;                    -P5-1550
                                      ELSE DO;     BXY(I) = '1'B;        -P5-1560
                          BXY(J)='1'B;      GO TO CMPX;      END; ELSE;  -P5-1570
          IF (IS=6)  THEN IF (IDY>1)  THEN GO TO NDJ;                    -P5-1580
                                      ELSE DO;     BXY(I) = '1'B;        -P5-1590
                          BXY(J)='1'B;      GO TO CMPY;      END; ELSE;  -P5-1600
          IF ((IS=7)&(IDY<2)&(IDX<2))  THEN GO TO CMPXYZ;                -P5-1610
                                       ELSE GO TO NDJ;                   -P5-1620
/*                                                                       -P5-1630
          MERGE TX.TZ WITH TX.TY, TY.TZ OR TX.TY.TZ                      -P5-1640
                                                                    */   -P5-1650
CK(5):    IF ((IS=1)|(IS=2)|(IS=4)|(IS=5))  THEN GO TO NDJ;       ELSE;   -P5-1660
          IDZ = ABS (ISZ - SZ(J));                                       -P5-1670
          IDX = ABS (ISX - SX(J));                                       -P5-1680
          IF ((IDX<2) & (IDZ<2))  THEN BXZ(I),BXZ(J)='1'B;       ELSE;   -P5-1690
          ID1 = IDZ;                                                     -P5-1700
          ID2 = IDX;                                                     -P5-1710
          IF (IS=3)  THEN IF (IDX>1)  THEN GO TO NDJ;                    -P5-1720
                                      ELSE DO;     BXZ(I) = '1'B;        -P5-1730
                          BXZ(J)='1'B;      GO TO CMPX;      END; ELSE;  -P5-1740
          IF (IS=6)  THEN IF (IDZ>1)  THEN GO TO NDJ;                    -P5-1750
                                      ELSE DO;     BXZ(I) = '1'B;        -P5-1760
                          BXZ(J)='1'B;      GO TO CMPZ;      END; ELSE;  -P5-1770
          IF ((IS=7)&(IDX<2)&(IDZ<2))  THEN GO TO CMPXYZ;                -P5-1780
                                       ELSE GO TO NDJ;                   -P5-1790
/*                                                                       -P5-1800
          MERGE TY.TZ WITH TX.TY, TX.TZ OR TX.TY.TZ                      -P5-1810
                                                                    */   -P5-1820
CK(6):    IF ((IS=1)|(IS=2)|(IS=4)|(IS=6))  THEN GO TO NDJ;       ELSE;   -P5-1830
```

```
          IDY = ABS (ISY - SY(J));                                              -P5-1840
          IDZ = ABS (ISZ - SZ(J));                                              -P5-1850
          IF ((IDY<2) & (IDZ<2))  THEN BYZ(I),BYZ(J)='1'B;        ELSE;         -P5-1860
          ID1 = IDY;                                                            -P5-1870
          ID2 = IDZ;                                                            -P5-1880
          IF (IS=3)  THEN IF (IDY>1)  THEN GO TO NDJ;                           -P5-1890
                                      ELSE DO;    BYZ(I) = '1'B;              -P5-1900
                          BYZ(J)='1'B;        GO TO CMPY;       END; ELSE;      -P5-1910
          IF (IS=5)  THEN IF (IDZ>1)  THEN GO TO NDJ;                           -P5-1920
                                      ELSE DO;    BYZ(I) = '1'B;              -P5-1930
                          BYZ(J)='1';         GO TO CMPZ;       END; ELSE;      -P5-1940
          IF ((IS=7)&(IDY<2)&(IDZ<2))  THEN GO TO CMPXYZ;                       -P5-1950
                                       ELSE GO TO NDJ;                          -P5-1960
CMPXYZ:   IF (ID1=0)  THEN IF (ID2=0)  THEN P = P0;                             -P5-1970
                                       ELSE P = P1;                             -P5-1980
                      ELSE IF (ID2=0)  THEN P = P1;                             -P5-1990
                                       ELSE P = P2;                             -P5-2000
          OK(J) = OK(J) + (P * FREQI * FREQ(J));                                -P5-2010
CK(7):    NDJ:      END JLUP;                                                   -P5-2020
          END ILUP;                                                             -P5-2030
          OK = OK * ((1000.000 * FLOAT(#XYZ)) / SUM(OK));                       -P5-2040
          IF (DBG)  THEN DO;                                                    -P5-2050
          PUT EDIT ('SAVED TX, TY, TZ --- AFTER MAPPING')(SKIP(3),A);           -P5-2060
          PUT EDIT ('  TX TY TZ SY      FREQ TX TY TZ SY      FREQ',           -P5-2070
                    '  TX TY TZ SY      FREQ TX TY TZ SY      FREQ',           -P5-2080
                    '  TX TY TZ SY      FREQ TX TY TZ SY      FREQ')           -P5-2090
                   (SKIP(2),A,A,A);      PUT SKIP(2);                         -P5-2100
          PUT EDIT ((RESULT(I) DO I = 1 TO #XYZ))(4 F(3),6 B(1),F(4,0));        -P5-2110
                                        END;                      ELSE;       -P5-2120
          FREE STORE;                                                           -P5-2130
          RETURN;                                                               -P5-2140
          END PART5;                                                            -P5-2150


* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                           -P6-0010
 /*    CHOOSE THE MOST FREQUENT VALUE OF TX, TY, AND TZ                  */    -P6-0020
 PART6:    PROCEDURE (IACR, IDWN, ILAY);                                      -P6-0030
 /*                                                                           -P6-0040
      THIS SUBROUTINE CHECKS THROUGH ALL OF THE PEAKS MAPPED INTO EACH       -P6-0050
      OTHER TO FIND THE HIGHEST SYMMETRY ELEMENT INTO WHICH ALL THE          -P6-0060
      LOWER SYMMETRY ELEMENTS HAVE BEEN MAPPED, WHICH HIGHER SYMMETRY        -P6-0070
      ELEMENT ALSO HAS THE HIGHEST FREQUENCY.  IF THIS SYMMETRY ELEMENT      -P6-0080
      IS SUCH THAT ALL OF THE OTHER SYMMETRY ELEMENT TYPES HAVE BEEN         -P6-0090
      MAPPED INTO IT, THE PROGRAM SETS THE APPROPRIATE VALUES OF TX,TY,      -P6-0100
      & TZ AND EXITS.  IF THIS LEAVES ANY ONE OF TX, TY, OR TZ UNDETER-      -P6-0110
      MINED, IT IS SET TO ZERO, AS THE ORIGIN IN THAT DIRECTION MAY BE       -P6-0120
      SET TO ANY VALUE.  IF THE SYMMETRY ELEMENTS DETERMINE ALL THREE        -P6-0130
      OF TX,TY,TZ BUT DO NOT OVERLAP, SUCH AS TX.TZ AND TY, THE HIGHEST      -P6-0140
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FREQUENCY OF EACH IS USED TO DETERMINE THE POSITION OF THE ORIGIN.-P6-0150
IF THE SYMMETRY ELEMENTS OVERLAP, SUCH AS TX.TY, TY.TZ, AND TY.TZ,-P6-0160
THEN THE DIFFERENT SYMMETRY TYPES ARE SEPARATED INTO THREE ARRAYS,-P6-0170
ONE FOR TX.TY, ONE FOR TY.TZ, AND ONE FOR TX.TZ, SORTED BY DECREA--P6-0180
SING FREQUENCY.  THE THREE ARRAYS ARE THEN MERGED, IN THE FOLLOW- -P6-0190
ING MANNER: LET TX1.TY1, TY2.TZ2, & TX3.TZ3 BE THE THREE DOUBLES. -P6-0200
THEN, IF TX1=TX3 & TY1=TY2 & TZ2=TZ3, THE TRIPLE TX1.TY2.TZ3 IS   -P6-0210
THEN SAVED WITH THE SUM OF THE THREE FREQUENCIES.  THE TRIPLE     -P6-0220
WITH THE HIGHEST FREQUENCY SUM IS THEN USED AS THE ORIGIN.        -P6-0230
                                                                  */ -P6-0240
    DECLARE   DBG                    EXTERNAL BIT (1);            -P6-0250
    DECLARE  (ION(7),SGNL,NCNT)      BIT (1) EXTERNAL;            -P6-0260
    DECLARE   (IA8,ID8,IL8,#XYZ)     FIXED BINARY (15) EXTERNAL;  -P6-0270
    DECLARE 1 RESULT (#XYZ)          CONTROLLED EXTERNAL,         -P6-0280
              2 (RX, RY, RZ, RS)     FIXED BINARY (15),           -P6-0290
             2 (BX, BY, BXY, BZ, BXZ, BYZ)  BIT (1),             -P6-0300
              2 OK                   FLOAT BINARY;                -P6-0310
    DECLARE  (CKR (7), CKDB)         BIT (6);                     -P6-0320
    DECLARE   CKOK (7)               FLOAT BINARY;                -P6-0330
    DECLARE   JOK (7)                FIXED BINARY (15);           -P6-0340
    DECLARE 1 S2XY3 (IAD8)           CONTROLLED,                  -P6-0350
              2 (X3, Y3)             FIXED BINARY (15),           -P6-0360
              2 OK3                  FLOAT BINARY;                -P6-0370
    DECLARE 1 S2XZ5 (IAL8)           CONTROLLED,                  -P6-0380
              2 (X5, Z5)             FIXED BINARY (15),           -P6-0390
              2 OK5                  FLOAT BINARY;                -P6-0400
    DECLARE 1 S2YZ6 (IDL8)           CONTROLLED,                  -P6-0410
              2 (Y6, Z6)             FIXED BINARY (15),           -P6-0420
              2 OK6                  FLOAT BINARY;                -P6-0430
    DECLARE  (J3,K3,L5,J5,K6,L6)     FIXED BINARY (15);           -P6-0440
    DECLARE   CHR                    CHARACTER (1);               -P6-0450
    DECLARE  (IFX, IFY, IFZ)         FIXED BINARY (15) EXTERNAL;  -P6-0460
    DECLARE   FOK                    FLOAT BINARY;                -P6-0470
    DECLARE 1 FXYZ (#OK)             CONTROLLED EXTERNAL,         -P6-0480
              2 (XR, YR, ZR, SR)     FIXED BINARY (15),           -P6-0490
              2 BSTRG                BIT (6),                     -P6-0500
              2 GOK                  FLOAT BINARY;                -P6-0510
    DECLARE   #OK                    FIXED BINARY EXTERNAL;       -P6-0520
    ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA                        -P6-0530
 (#OK,INDX,II,J,JRS,IRS,JFNL,I3,I3,I6,J3,J5,J6,I,L,K,I356);       -P6-0540
                                          EXIT;          END;    -P6-0550
/*                                                                -P6-0560
    "CKR" HOLDS BIT STRINGS TO BE CHECKED.  FOR EXAMPLE IF THERE  -P6-0570
    ARE THE FOLLOWING SYMMETRY ELEMENTS TY, TX.TZ, TX.TY.TZ,      -P6-0580
    AS IN P21/C,  THEN ONE WOULD HAVE ION(1),ION(3),ION(4),ION(6) -P6-0590
    =0 AND ION(2),ION(5),ION(7) = 1.  PART5 SHOULD HAVE MAPPED    -P6-0600
    TY INTO TX.TY.TZ AND TX.TZ INTO TX.TY.TZ, AND WOULD HAVE LEFT -P6-0610
    A RECORD OF SUCH MAPPING.  IF, FOR A PARTICULAR TRIPLE OF     -P6-0620
    TX.TY.TZ THERE IS NO INDICATION OF BOTH TY AND TX.TZ BEING    -P6-0630
    MAPPED IN, THEN THAT TRIPLE IS ASSUMED TO BE FALSE.           -P6-0640
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                                                                        */ -P6-0650
        CKR(7) = ION(1) ||ION(2) ||ION(3) ||ION(4) ||ION(5) ||ION(6); -P6-0660
        CKR(6) = '0'B   ||ION(2) ||ION(3) ||ION(4) ||ION(5) ||'1'B;   -P6-0670
        CKR(5) = ION(1) ||'0'B   ||ION(3) ||ION(4) ||'1'B   ||ION(6); -P6-0680
        CKR(3) = ION(1) ||ION(2) ||'1'B   ||'0'B   ||ION(5) ||ION(6); -P6-0690
        CKR(4) = '000'B || ION(4) || '00'B;                             -P6-0700
        CKR(2) = '0'B || ION(2) || '0000'B;                             -P6-0710
        CKR(1) = ION(1) || '00000'B;                                    -P6-0720
        IF (DBG)  THEN PUT EDIT('CKR =',CKR) (SKIP,A,7 (B(7),X(1)));   -P6-0730
                  ELSE;                                                 -P6-0740
        CKOK = 0.000;                                                   -P6-0750
        JOK = 0;                          #OK = 0;                      -P6-0760
        IRS = 0;                          IDL8 = ID8 * IL8 * 2;         -P6-0770
        IAD8 = IA8 * ID8 * 2;             IAL8 = IA8 * IL8 * 2;         -P6-0780
/*                                                                      -P6-0790
        DETERMINE THE HIGHEST SYMMETRY ELEMENT TO BE CONSIDERED         -P6-0800
                                                                        */ -P6-0810
LUPJ:   DO J = 1 TO #XYZ BY 1;                                          -P6-0820
        CKDB = BX(J) || BY(J) || BXY(J) || BZ(J) || BXZ(J) || BYZ(J);   -P6-0830
        JRS = RS(J);                                                    -P6-0840
        IF (CKDB ¬= CKR(JRS))  THEN DO;                                 -P6-0850
             OK(J) = 0.000;                                             -P6-0860
             GO TO NDJL;                  END;                  ELSE;  -P6-0870
        IF (OK(J) > CKOK(JRS))  THEN DO;                                -P6-0880
             CKOK(JRS) = OK(J);                                         -P6-0890
             JOK(JRS) = J;                END;                  ELSE;  -P6-0900
        IF (JRS = 4)  THEN JRS = 3;                             ELSE    -P6-0910
        IF (JRS = 3)  THEN JRS = 4;                             ELSE;   -P6-0920
        IF (JRS >= IRS)  THEN IRS = JRS;                        ELSE;   -P6-0930
NDJL:   IF (OK(J) > 0.0)  THEN #OK = #OK + 1;                   ELSE;   -P6-0940
        END LUPJ;                                                       -P6-0950
        IF (DBG)  THEN DO;                                              -P6-0960
        PUT EDIT ('SAVED TX, TY, TZ --- BEFORE MERGING & SORTING')      -P6-0970
                 (PAGE,A);                                              -P6-0980
        PUT EDIT (' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',       -P6-0990
                  ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',       -P6-1000
                  ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ')       -P6-1010
                 (SKIP(2),A,A,A);     PUT SKIP(2);                      -P6-1020
        PUT EDIT ((RESULT(I) DO I = 1 TO #XYZ))(4 F(3),6 B(1),F(4,0));  -P6-1030
        PUT EDIT ('JOK =',JOK,'CKOK =',CKOK)                            -P6-1040
                 (SKIP,A,7 F(5),X(10),A,7 F(10,2));                     -P6-1050
                                  END;                          ELSE;   -P6-1060
/*                                                                      -P6-1070
        BRANCH, DEPENDING ON THE TYPE OF THE HIGHEST SYMM. ELEMENT      -P6-1080
                                                                        */ -P6-1090
        IF (IRS = 3)  THEN IRS = 4;                             ELSE    -P6-1100
        IF (IRS = 4)  THEN IRS = 3;                             ELSE;   -P6-1110
        JFNL = JOK(IRS);                                                -P6-1120
        IFX = RX(JFNL);                                                 -P6-1130
        IFY = RY(JFNL);                                                 -P6-1140
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          IFZ = RZ(JFNL);                                                    -P6-1150
          FOK = OK(JFNL);                                                    -P6-1160
          IF (IRS=7)  THEN GO TO CMP7;                              ELSE;    -P6-1170
          IF ((IRS=6) & (¬ION(5)) & (¬ION(3))) THEN GO TO CMP6;     ELSE;    -P6-1180
          IF ((IRS=5) & (¬ION(6)) & (¬ION(3))) THEN GO TO CMP5;     ELSE;    -P6-1190
          IF ((IRS=3) & (¬ION(6)) & (¬ION(5))) THEN GO TO CMP3;     ELSE;    -P6-1200
          IF ((IRS=4) | (IRS=2) | (IRS=1))  THEN GO TO CMPL;        ELSE;    -P6-1210
/*                                                                           -P6-1220
          THERE ARE THREE TWO-FOLD AXES OR TWO-FOLD SCREW AXES               -P6-1230
                                                                        */   -P6-1240
          ALLOCATE  S2XY3, S2XZ5, S2YZ6;                                     -P6-1250
          X3, Y3 = 0;                                                        -P6-1260
          OK3 = 0.000;                                                       -P6-1270
          X5, Z5 = 0;                                                        -P6-1280
          OK5 = 0.000;                                                       -P6-1290
          Y6, Z6 = 0;                                                        -P6-1300
          OK6 = 0.000;                                                       -P6-1310
          I3, I5, I6 = 1;                                                    -P6-1320
          J3 = JOK(3);                                                       -P6-1330
          J5 = JOK(5);                                                       -P6-1340
          J6 = JOK(6);                                                       -P6-1350
          I356 = 3;                                                          -P6-1360
          K356, L356 = 0;                                                    -P6-1370
          OK3, OK5, OK6 = 0.000;                                             -P6-1380
A3:       IF (I3 > (IAD8))      THEN GO TO A5;                      ELSE;    -P6-1390
          IF (J3 = 0)  THEN GO TO A5;                               ELSE;    -P6-1400
          X3(I3) = RX(J3);                                                   -P6-1410
          Y3(I3) = RY(J3);                                                   -P6-1420
          OK3(I3) = OK(J3);                                                  -P6-1430
          OK(J3) = 0.000;                                                    -P6-1440
A5:       IF (I5 > (IAL8))      THEN GO TO A6;                      ELSE;    -P6-1450
          IF (J5 = 0)  THEN GO TO A6;                               ELSE;    -P6-1460
          X5(I5) = RX(J5);                                                   -P6-1470
          Z5(I5) = RZ(J5);                                                   -P6-1480
          OK5(I5) = OK(J5);                                                  -P6-1490
          OK(J5) = 0.000;                                                    -P6-1500
A6:       IF (I6 > (IDL8))      THEN GO TO Z356;                    ELSE;    -P6-1510
          IF (J6 = 0)  THEN GO TO Z356;                             ELSE;    -P6-1520
          Y6(I6) = RY(J6);                                                   -P6-1530
          Z6(I6) = RZ(J6);                                                   -P6-1540
          OK6(I6) = OK(J6);                                                  -P6-1550
          OK(J6) = 0.000;                                                    -P6-1560
/*                                                                           -P6-1570
          PLACE ALL OF THE TWO-FOLDS IN ARRAYS IN DESCENDING ORDER           -P6-1580
                                                                        */   -P6-1590
Z356:     K356 = L356;                                                       -P6-1600
          L356 = I356;                                                       -P6-1610
          I356 = I3 + I5 + I6;                                               -P6-1620
          IF (K356=I356)  THEN GO TO PKAL;                          ELSE;    -P6-1630
          IF (DBG)  THEN PUT EDIT (I356) (F(6));                    ELSE;    -P6-1640
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```
          J3, J5, J6 = 0;                                                    -P6-1650
          B3, B5, B6 = 0.001;                                                -P6-1660
          IF (I356 > #XYZ)  THEN GO TO PKAL;                                 -P6-1670
DLUP:     DO I = 1 TO #XYZ BY 1;                                             -P6-1680
          OK356 = OK(I);                                                     -P6-1690
          J356 = RS(I);                                                      -P6-1700
          IF ((OK356 > B3) & (J356 = 3))  THEN DO;                           -P6-1710
               B3 = OK356;                                                   -P6-1720
               J3 = I;                              END;          ELSE;      -P6-1730
          IF ((OK356 > B5) & (J356 = 5))  THEN DO;                           -P6-1740
               B5 = OK356;                                                   -P6-1750
               J5 = I;                              END;          ELSE;      -P6-1760
          IF ((OK356 > B6) & (J356 = 6))  THEN DO;                           -P6-1770
               B6 = OK356;                                                   -P6-1780
               J6 = I;                              END;          ELSE;      -P6-1790
          END DLUP;                                                          -P6-1800
          IF (J3 ¬= 0)  THEN I3 = I3 + 1;                         ELSE;      -P6-1810
          IF (J5 ¬= 0)  THEN I5 = I5 + 1;                                    -P6-1820
          IF (J6 ¬= 0)  THEN I6 = I6 + 1;                                    -P6-1830
          IF ((I3>(IAD8))    & (I5>(IAL8))    & (I6>(IDL8)))                 -P6-1840
                THEN GO TO PKAL;                 ELSE GO TO A3;              -P6-1850
/*                                                                           -P6-1860
          FIND THE MOST FREQUENT AND CONSISTANT TX.TY.TZ                     -P6-1870
                                                                       */    -P6-1880
PKAL:     I356 = 0;                                                          -P6-1890
          OK = 0.000;                                                        -P6-1900
          IF (DBG)  THEN DO;                                                 -P6-1910
          PUT EDIT ('SORTED TX.TY, TY.TZ, TX.TZ -- PART 6')                  -P6-1920
                   (SKIP(4),A);                                              -P6-1930
          PUT EDIT (' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',          -P6-1940
                   ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',          -P6-1950
                   ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ')          -P6-1960
                   (SKIP(2),A,A,A);     PUT SKIP(2);                        -P6-1970
          PUT EDIT ((S2XY3(I) DO I = 1 TO IAD8))                             -P6-1980
                   (2 F(3),X(9),F(7,0));                                     -P6-1990
          PUT EDIT ((S2XZ5(I) DO I = 1 TO IAL8))                             -P6-2000
                   (F(3),X(3),F(3),X(6),F(7,0));                             -P6-2010
          PUT EDIT ((S2YZ6(I) DO I = 1 TO IDL8))                             -P6-2020
                   (X(3),2 F(3),X(6),F(7,0));                                -P6-2030
                                        END;                 ELSE;           -P6-2040
LP6:      DO L = 1 TO IDL8 BY 1;                                             -P6-2050
          IF (OK6(L) = 0.000)  THEN GO TO FNL2S;                 ELSE;       -P6-2060
          K6 = Y6(L);                                                        -P6-2070
          L6 = Z6(L);                                                        -P6-2080
LP5:      DO K = 1 TO IAL8 BY 1;                                             -P6-2090
          IF (OK5(K) = 0.000)  THEN GO TO NDL5;                  ELSE;       -P6-2100
          J5 = X5(K);                                                        -P6-2110
          L5 = Z5(K);                                                        -P6-2120
LP3:      DO J = 1 TO IAD8 BY 1;                                             -P6-2130
          IF (OK3(J) = 0.000)  THEN GO TO NDL3;                  ELSE;       -P6-2140
```

```
          J3 = X3(J);                                                          -P6-2150
          K3 = Y3(J);                                                          -P6-2160
          IF ((J3=J5)&(K3=K6) & (L5=L6))  THEN GOOD: DO;                       -P6-2170
               I356 = I356 + 1;                                                -P6-2180
               IF (I356 > #XYZ)  THEN GO TO FNL2S;              ELSE;          -P6-2190
               RX(I356) = J3;                                                  -P6-2200
               RY(I356) = K3;                                                  -P6-2210
               RZ(I356) = L5;                                                  -P6-2220
               RS(I356) = 7;                                                   -P6-2230
               OK(I356) = OK6(L) + OK5(K) + OK3(J);                            -P6-2240
NDL3:     END LP3;                                                            -P6-2250
NDL5:     END LP5;                                                            -P6-2260
          END LP6;                                                            -P6-2270
FNL2S:    IF (DBG)  THEN DO;                                                  -P6-2280
          PUT EDIT ('MERGED TX.TY, TY.TZ, TX.TZ -- PART 6')                   -P6-2290
                   (SKIP(4),A);                                               -P6-2300
          PUT EDIT (' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',           -P6-2310
                   ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ',           -P6-2320
                   ' TX TY TZ SY      FREQ TX TY TZ SY      FREQ')           -P6-2330
                   (SKIP(2),A,A,A);     PUT SKIP(2);                          -P6-2340
          PUT EDIT ((RX(I),RY(I),RZ(I),RS(I),OK(I) DO I = 1 TO #XYZ))          -P6-2350
                   (3 F(3),F(2),F(11,0));                                     -P6-2360
                                    END;                            ELSE;     -P6-2370
          FOK = 0.000;                                                        -P6-2380
FLUP:     DO M = 1 TO #XYZ BY 1;                                              -P6-2390
          IF (OK(M) > FOK)  THEN DO;                                          -P6-2400
               MF = M;                                                        -P6-2410
               FOK = OK(M);       END;                         ELSE;         -P6-2420
          END FLUP;                                                           -P6-2430
          IFX = RX(MF);                                                       -P6-2440
          IFY = RY(MF);                                                       -P6-2450
          IFZ = RZ(MF);                                                       -P6-2460
          GO TO WXYZ;                                                         -P6-2470
/*                                                                            -P6-2480
          THERE IS AN INVERSION CENTER                                        -P6-2490
                                                                         */   -P6-2500
CMP7:     PUT EDIT ('THE HIGHEST SYMMETRY ELEMENT IS AN INVERSION.')          -P6-2510
                   (SKIP(4),A);                                               -P6-2520
          GO TO WXYZ;                                                         -P6-2530
/*                                                                            -P6-2540
          THE HIGHEST SYMMETRY ELEMENT IS A TWO-FOLD OR SCREW                 -P6-2550
                                                                         */   -P6-2560
CMP6:     CHR = 'X';                                                          -P6-2570
          IF (JOK(1) ¬= 0)  THEN DO;                                          -P6-2580
               IFX = RX(JOK(1));                                              -P6-2590
               FOK = FOK + OK(JOK(1));                                        -P6-2600
               GO TO P2G;         END;                          ELSE;       -P6-2610
          IFX = 0;                                                            -P6-2620
          GO TO P2B;                                                          -P6-2630
CMP5:     CHR = 'Y';                                                          -P6-2640
```

```
          IF (JOK(2) ¬= 0)  THEN DO;                                          -P6-2650
               IFY = RY(JOK(2));                                              -P6-2660
               FCK = FCK + OK(JOK(2));                                        -P6-2670
               GO TO P2G;          END;                                ELSE;  -P6-2680
          IFY = 0;                                                            -P6-2690
          GO TO P2B;                                                          -P6-2700
CMP3:     CHR = 'Z';                                                          -P6-2710
          IF (JOK(4) ¬= 0)  THEN DO;                                          -P6-2720
               IFZ = RZ(JOK(4));                                              -P6-2730
               FCK = FCK + OK(JOK(4));                                        -P6-2740
               GO TO P2G;          END;                                ELSE;  -P6-2750
          IFZ = 0;                                                            -P6-2760
P2B:      PUT EDIT (' THE HIGHEST SYMMETRY ELEMENT IS AN AXIS IN ',CHR,       -P6-2770
                    'UNABLE TO DETERMINE T',CHR,'.  THUS, T',CHR,             -P6-2780
                     ' SET EQUAL TO ZERO.')                                   -P6-2790
                    (SKIP(4),X(10),A,A(1),SKIP(1),X(20),3 (A,A(1)));          -P6-2800
          GO TO WXYZ;                                                         -P6-2810
P2G:      PUT EDIT (' THE HIGHEST SYMMETRY ELEMENT IS AN AXIS IN ',CHR,       -P6-2820
                    'HOWEVER, THERE IS A PLANE NORMAL TO ',CHR)               -P6-2830
                    (SKIP(4),X(10),A,A(1),SKIP(1),X(20),A,A(1));              -P6-2840
          GO TO WXYZ;                                                         -P6-2850
/*                                                                            -P6-2860
          THERE IS ONLY A MIRROR OR GLIDE PLANE NORMAL TO ONE AXIS            -P6-2870
                                                                        */    -P6-2880
CMPL:     PUT EDIT ('THERE IS ONLY A PLANE NORMAL TO ONE AXIS.',              -P6-2890
                    'THE T''S IN THE OTHER DIRECTIONS ARE SET =0.')           -P6-2900
                    (SKIP(4),X(10),A,SKIP(1),X(20),A);                        -P6-2910
          IFX, IFY, IFZ = 0;                                                  -P6-2920
          IF (IRS = 4)  THEN IFZ = RZ(JFNL);                          ELSE;   -P6-2930
          IF (IRS = 2)  THEN IFY = RY(JFNL);                          ELSE;   -P6-2940
          IF (IRS = 1)  THEN IFX = RX(JFNL);                          ELSE;   -P6-2950
WXYZ:     PUT EDIT ('**********  TX =',IFX,'TY =',IFY,'TZ =',IFZ)              -P6-2960
                    (SKIP(2),3 (A,F(5),X(5)));                                -P6-2970
          FREE  S2YZ6, S2XY3, S2XZ5;                                          -P6-2980
          ALLOCATE  FXYZ;                                                     -P6-2990
          INDX = 0;                                                           -P6-3000
          PUT EDIT ('SAVED TRIPLES, DOUBLES, AND SINGLES') (PAGE,A);          -P6-3010
          PUT EDIT ('  TX TY TZ SY      FREQ TX TY TZ SY      FREQ',         -P6-3020
                    '  TX TY TZ SY      FREQ TX TY TZ SY      FREQ',         -P6-3030
                    '  TX TY TZ SY      FREQ TX TY TZ SY      FREQ')         -P6-3040
                    (SKIP(2),A,A,A);      PUT SKIP(2);                        -P6-3050
IILP:     DO II = 1 TO #XYZ BY 1;                                             -P6-3060
          IF (OK(II) > 1)  THEN GD: DO;                                       -P6-3070
          INDX = INDX + 1;                                                    -P6-3080
          XR(INDX) = RX(II);                                                  -P6-3090
          YR(INDX) = RY(II);                                                  -P6-3100
          ZR(INDX) = RZ(II);                                                  -P6-3110
          SR(INDX) = RS(II);                                                  -P6-3120
          GOK(INDX) = OK(II);                                                 -P6-3130
          BSTRG(INDX) = BX(II) || BY(II) || BXY(II) || BZ(II)                 -P6-3140
```

```
                    || BXZ(II) || BYZ(II);                                  -P6-3150
      PUT EDIT (FXYZ(INDX)) (4 F(3),B(6),F(4,0));                           -P6-3160
END GD;                        ELSE;                    END IILP;           -P6-3170
FREE RESULT;                                                                -P6-3180
RETURN;                                                                     -P6-3190
END PART6;                                                                  -P6-3200



* PROCESS('ATR,XREF,NOSTMT,OPT=02');                                        -P7-0010
 /*   DETERMINE WHICH PEAKS ARE TO BE KEPT                              */ -P7-0020
 PART7:   PROCEDURE (IACR, IDWN, ILAY, #RTND, #SYMM);                       -P7-0030
 /*                                                                        -P7-0040
      THIS SUBROUTINE MAKES USE OF THE ORIGIN TRANSLATION TX.TY.TZ AND     -P7-0050
      OF THE SYMMETRY ELEMENTS TO DETERMINE WHICH PEAKS FIT IN E.D.        -P7-0060
      SPACE.  IF AT LEAST HALF OF THE SYMMETRY-RELATED PEAKS ARE PRESENT-P7-0070
      WHEN THE ENTIRE MAP HAS BEEN SHIFTED BY TX.TY.TZ, THEN THAT SET    -P7-0080
      OF PEAKS IS OUTPUT IN THE SHIFTED COORDINATES                      -P7-0090
                                                                      */ -P7-0100
          DECLARE  (IACR,IDWN,ILAY,#RTND,#SYMM)   FIXED BINARY (15);    -P7-0110
          DECLARE  (IFX, IFY, IFZ)       FIXED BINARY (15) EXTERNAL;    -P7-0120
          DECLARE 1 SYMMPQ (#SYMM)       CONTROLLED EXTERNAL,           -P7-0130
                    2 (PX,QX,PY,QY,PZ,QZ)    FIXED BINARY (15);        -P7-0140
          DECLARE   #OK                  FIXED BINARY EXTERNAL;         -P7-0150
          DECLARE 1 FXYZ (#OK)           CONTROLLED EXTERNAL,           -P7-0160
                    2 (XR, YR, ZR, SR)   FIXED BINARY (15),             -P7-0170
                    2 BSTRG              BIT (6),                       -P7-0180
                    2 GOK                FLOAT BINARY;                  -P7-0190
          DECLARE 1 PEAKS (#RTND)        CONTROLLED,                    -P7-0200
                    2 (U,V,W,VLU,X,Y,Z) FIXED BINARY;                   -P7-0210
          DECLARE 1 PEAKR,                                              -P7-0220
                    2 (RU,RV,RW,VAL,AVG)     FIXED BINARY (31);         -P7-0230
          DECLARE  (RETAIN, FINAL)       FILE RECORD SEQUENTIAL;        -P7-0240
          DECLARE  (BX, BY, BZ)          BIT (1);                       -P7-0250
          DECLARE   DBG                  BIT (1) EXTERNAL;              -P7-0260
          ON SUBSCRIPTRANGE SNAP BEGIN; PUT DATA (I,J,K); EXIT;  END;   -P7-0270
          DECLARE   JAVG (#SYMM)         CONTROLLED FIXED BINARY;       -P7-0280
          DECLARE   PVALUE (16)          FIXED BINARY (15);             -P7-0290
          DECLARE  (L,M,N)               FIXED BINARY (15);             -P7-0300
          DECLARE  (KX,KY,KZ,NSY,CL(24)) FIXED BINARY (15);             -P7-0310
          DECLARE 1 FPEAK,                                              -P7-0320
                    2 (HITE,FX,FY,FZ,#) FIXED BINARY (31);              -P7-0330
          DECLARE   ONE                  FLOAT BINARY;                  -P7-0340
          ONE = 1.0000;                                                 -P7-0350
          CL(1), CL( 7), CL(13), CL(19) =  40;                          -P7-0360
          CL(2), CL( 8), CL(14), CL(20) =  56;                          -P7-0370
          CL(3), CL( 9), CL(15), CL(21) =  72;                          -P7-0380
          CL(4), CL(10), CL(16), CL(22) =  88;                          -P7-0390
          CL(5), CL(11), CL(17), CL(23) = 104;                          -P7-0400
```

```
          CL(6), CL(12), CL(18), CL(24) = 120;                                  -P7-0410
          L = ROUND (FLOAT (IACR) / 16.000, 0);                                 -P7-0420
          M = ROUND (FLOAT (IDWN) / 16.000, 0);                                 -P7-0430
          N = ROUND (FLOAT (ILAY) / 16.000, 0);                                 -P7-0440
          ISYM = MAX (#SYMM/2 +1, 1);                                           -P7-0450
          IPEAK = 0;                                                            -P7-0460
          QACR = FLOAT (IACR);                                                  -P7-0470
          QDWN = FLOAT (IDWN);                                                  -P7-0480
          QLAY = FLOAT (ILAY);                                                  -P7-0490
          ALLOCATE PEAKS;                                                       -P7-0500
          ALLOCATE JAVG;                                                        -P7-0510
          IF (DBG)  THEN PUT EDIT ('$$$$ TX =',IFX,'TY =',IFY,'TZ =',           -P7-0520
                    IFZ) (SKIP(4),3 (A,F(5),X(5)));                 ELSE;       -P7-0530
/*                                                                              -P7-0540
          READ AND STORE THE PEAKS, TRANSFORMING THEM TO E.D. COORDS.           -P7-0550
                                                                          */    -P7-0560
          OPEN FILE (RETAIN) INPUT;                                             -P7-0570
RLUP:     DO I = 1 TO #RTND BY 1;                                               -P7-0580
          READ FILE (RETAIN) INTO (PEAKR);                                      -P7-0590
          U(I) = RU;                                                            -P7-0600
          V(I) = RV;                                                            -P7-0610
          W(I) = RW;                                                            -P7-0620
          VLU(I) = AVG;                                                         -P7-0630
          X(I) = MOD (RU - IFX, IACR);                                          -P7-0640
          Y(I) = MOD (RV - IFY, IDWN);                                          -P7-0650
          Z(I) = MOD (RW - IFZ, ILAY);                                          -P7-0660
          END RLUP;                                                             -P7-0670
          CLOSE FILE (RETAIN);                                                  -P7-0680
          OPEN FILE (FINAL) OUTPUT;                                             -P7-0690
          NPEAK = 0;                                                            -P7-0700
          PUT EDIT ('PEAK BEING CHECKED (PART7) -- #, OR',                      -P7-0710
                    'IGINAL (UVW) & TRANSFORMED (XYZ) COORDS., EQUIV. P',       -P7-0720
                    'OSITIONS (EX,EY,EZ), & # OF MATCHING PEAK (#MP)',          -P7-0730
                    '   #    U    V    W VALUE    X    Y    Z    ',            -P7-0740
                    '     EX EY EZ #MP     EX EY EZ #MP     EX EY EZ #MP',     -P7-0750
                    '     EX EY EZ #MP     EX EY EZ #MP     EX EY EZ #MP')     -P7-0760
                    (PAGE,A,A,A,SKIP,A,A,A);                                    -P7-0770
          PUT SKIP;                                                             -P7-0780
/*                                                                              -P7-0790
          LOOP THROUGH ALL RETAINED PEAKS TO DETERMINE WHICH ONES ARE           -P7-0800
          ALLOWED BY SYMMETRY AND OUTPUTTING THE ALLOWED PEAKS.                 -P7-0810
                                                                          */    -P7-0820
ILUP:     DO I = 1 TO #RTND BY 1;                                               -P7-0830
          IF (VLU(I) < 1.00)  THEN GO TO NDIL;                          ELSE;   -P7-0840
          RU = U(I);                                                            -P7-0850
          RV = V(I);                                                            -P7-0860
          RW = W(I);                                                            -P7-0870
          VAL = VLU(I);                                                         -P7-0880
          IVAL = VAL;                                                           -P7-0890
          AVG = 0;                                                              -P7-0900
```

```
          RX = X(I);                                                        -P7-0910
          RY = Y(I);                                                        -P7-0920
          RZ = Z(I);                                                        -P7-0930
          PUT EDIT (I,RU,RV,RW,VAL,RX,RY,RZ)                                -P7-0940
                   (SKIP,F(3),3 F(4),F(6),3 F(4));                          -P7-0950
/*                                                                          -P7-0960
          CREATE EQUIVALENT POSITIONS FROM SYMMETRY ELEMENTS                -P7-0970
                                                                      */    -P7-0980
SLUP:     DO K = 1 TO #SYMM BY 1;                                           -P7-0990
          KX = MOD ((RX * PX(K)) + QX(K), IACR);                            -P7-1000
          KY = MOD ((RY * PY(K)) + QY(K), IDWN);                            -P7-1010
          KZ = MOD ((RZ * PZ(K)) + QZ(K), ILAY);                            -P7-1020
          KXI = KX + IACR;                                                  -P7-1030
          KYI = KY + IDWN;                                                  -P7-1040
          KZI = KZ + ILAY;                                                  -P7-1050
          NSY = CL(K);                                                      -P7-1060
          PUT EDIT (KX,KY,KZ) (COL(NSY), 3 F(3));                           -P7-1070
/*                                                                          -P7-1080
          LOOP THROUGH ALL PEAKS - LOOKING FOR SYMMETRY RELATED PEAKS       -P7-1090
                                                                      */    -P7-1100
JLUP:     DO J = 1 TO #RTND BY 1;                                           -P7-1110
          IF (VLU(J) < 1.00)  THEN GO TO NDJL;                      ELSE;   -P7-1120
          OX = MIN (ABS(KX-X(J)),ABS(KXI-X(J)));                            -P7-1130
          OY = MIN (ABS(KY-Y(J)),ABS(KYI-Y(J)));                            -P7-1140
          OZ = MIN (ABS(KZ-Z(J)),ABS(KZI-Z(J)));                            -P7-1150
          BX = (OX <=L);                                                    -P7-1160
          BY = (OY <=M);                                                    -P7-1170
          BZ = (OZ <=N);                                                    -P7-1180
          IF (BX & BY & BZ)  THEN GO TO PNDS;                       ELSE;   -P7-1190
NDJL:     END JLUP;                                                         -P7-1200
          GO TO NDSL;                                                       -P7-1210
PNDS:     AVG = AVG + 1;                                                    -P7-1220
          JAVG(AVG) = J;                                                    -P7-1230
          PUT EDIT (J) (F(4));                                              -P7-1240
          IVAL = IVAL + VLU(J);                                             -P7-1250
NDSL:     END SLUP;                                                         -P7-1260
/*                                                                          -P7-1270
          OUTPUT THE GOOD PEAKS                                             -P7-1280
                                                                      */    -P7-1290
          IF (AVG < ISYM)  THEN GO TO NDIL;                         ELSE;   -P7-1300
          NPEAK = NPEAK + AVG + 1;                                          -P7-1310
          HITE = IVAL / (AVG + 1);                                          -P7-1320
          # = AVG;                                                          -P7-1330
          FX = RX;                                                          -P7-1340
          FY = RY;                                                          -P7-1350
          FZ = RZ;                                                          -P7-1360
          VLU(I) = 0;                                                       -P7-1370
          WRITE FILE (FINAL) FROM (FPEAK);                                  -P7-1380
          IPEAK = IPEAK + 1;                                                -P7-1390
LUPJ:     DO J = 1 TO AVG BY 1;                                             -P7-1400
```

```
          JS = JAVG(J);                                                    -P7-1410
          VLU(JS) = 0;                                                     -P7-1420
NDLJ:     END LUPJ;                                                        -P7-1430
NDIL:     END ILUP;                                                        -P7-1440
          PUT EDIT ('# PEAKS RETAINED =',NPEAK) (SKIP(2),A,F(5));          -P7-1450
          CLOSE FILE (FINAL);                                              -P7-1460
          OPEN FILE (FINAL) INPUT;                                         -P7-1470
          PUT EDIT ('NUMBER OF INDEPENDENT PEAKS =',IPEAK)                 -P7-1480
                   (SKIP(2),A,F(5));                                       -P7-1490
          PUT EDIT ('INDEPENDENT PEAKS AFTER SYMMETRY CHECK',              -P7-1500
                    '     X     Y     Z (FOUR.)     X          Y          Z',-P7-1510
                    '(FRACT.)      HEIGHT      #SYMM',' ')                -P7-1520
                   (PAGE,A,SKIP,A,A,SKIP(2),A);                            -P7-1530
/*                                                                         -P7-1540
          OUTPUT PEAKS REMAINING AFTER SYMMETRY CHECK ON "ORFLS" CARDS     -P7-1550
          WRITE OUT FOUND PEAKS AND PUNCH LEAST SQUARES CARDS              -P7-1560
                                                                    */     -P7-1570
LUPI:     DO I = 1 TO IPEAK BY 1;                                          -P7-1580
          READ FILE (FINAL) INTO (FPEAK);                                  -P7-1590
          XFR = FLOAT (FX) / QACR;                                         -P7-1600
          YFR = FLOAT (FY) / QDWN;                                         -P7-1610
          ZFR = FLOAT (FZ) / QLAY;                                         -P7-1620
          PUT EDIT (FX,FY,FZ,XFR,YFR,ZFR,HITE,#)                           -P7-1630
                   (SKIP,3 F(5),X(4),3 F(10,5),X(9),2 F(10));              -P7-1640
          PUT FILE (PUNCH) EDIT (HITE,ONE,ONE,XFR,YFR,ZFR)                 -P7-1650
                   (SKIP,F(5),X(4),5 F(9,5));                              -P7-1660
          END LUPI;                                                        -P7-1670
          CLOSE FILE (FINAL), FILE (PUNCH);                                -P7-1680
          RETURN;                                                          -P7-1690
          END PART7;                                                       -P7-1700
```

```
//LKED.SYSLMOD  DD  DSNAME=PROG.CRYST,                                     JCL-0060
//     UNIT=DISK,VOLUME=SER=PROGPK,DISP=(OLD,KEEP)                         JCL-0070
//LKED.SYSIN  DD  *                                                        JCL-0080
  OVERLAY ALPHA                                                            OVLY0010
  INSERT TM_DT                                                             OVLY0020
  OVERLAY ALPHA                                                            OVLY0030
  INSERT PART1                                                             OVLY0040
  OVERLAY ALPHA                                                            OVLY0050
  INSERT PART2                                                             OVLY0060
  OVERLAY ALPHA                                                            OVLY0070
  INSERT IHESRTA                                                           OVLY0080
  OVERLAY ALPHA                                                            OVLY0090
  INSERT PART3                                                             OVLY0100
  OVERLAY ALPHA                                                            OVLY0110
  INSERT PART4                                                             OVLY0120
  OVERLAY ALPHA                                                            OVLY0130
```

```
INSERT PART5                                    OVLY0140
OVERLAY ALPHA                                   OVLY0150
INSERT PART6                                    OVLY0160
OVERLAY ALPHA                                   OVLY0170
INSERT PART7                                    OVLY0180
NAME ALOP2(R)                                   JCL-0090
```

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