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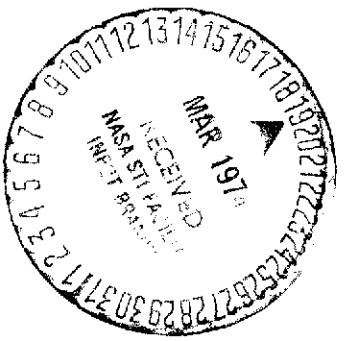
Alfred University Research Foundation Report

CRYSTALLOGRAPHIC AND GENERAL USE PROGRAMS FOR THE XDS Σ 5 COMPUTER

by

Robert L. Snyder
NYS College of Ceramics



This work was supported in part by the National Aeronautics and Space Administration Cooperative Agreement NCAw 33-187-002 and a grant from the Alfred University Research Foundation.

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INTRODUCTION

The programs described here are all written in basic FORTRAN IV and fall into three catagories: (1) Interactive programs to be executed under time sharing (BTM), (2) Non interactive programs which are executed in batch processing Mode (BPM), and (3) Large non interactive programs which require more memory than is available in the normal BPM/BTM operating system and must be run overnight on a special system called XRAY which releases about 45,000 words of memory to the user.

Programs in catagories (1) and (2) are stored as FORTRAN source files in the account FSNYDER under the name by which the program is referred to in this write up. Programs in catagory (3) are stored in the XRAY system as load modules. The type of file in account FSNYDER is identified by the first two letters in the name: SO_____ means a FORTRAN source file, SU_____ is a FORTRAN source Set Up program (i.e., one which sets up an input file for a BPM or XRAY system run), LM_____ is a load module, BO_____ is a binary output file from the compiler and FN_____ is a BCD data file required by logical unit number N of the program named.

Interactive programs are executed from teletype by assigning the source file to the system data control block called M:SI as follows: ASSIGN M:SI, (FILE, SO_____, FSNYDER). The FORTRAN compiler and loader are then called in sequence. The only additional information needed is the number and name of any input or output files used by the program. When needed these will be described in the program description. All additional information and instructions will be supplied by the program.

Programs in the second catagory (BPM) may be executed in two ways: (1) Punch the control cards given in program write up along with any input data on cards and submit the deck at the computer center, or (2) Build an input file containing the control cards and data and submit this file to the batch job stream from terminal by assigning it to M:SI and calling the BPM subsystem. A third way exists for a number of batch programs and that is to execute a type 1 interactive program from terminal which sets up an input file for the BPM program. These set up programs eliminate the need to follow these written instructions, and will ask for all data required.

STANDARD COORDINATE FILE

Numerous programs described here use the standard coordinate file. Instructions for preparing such a file follow:

Record 1: cols. 1-80 Title information identifying data (80A1)

Record 2: Cell parameter information (6F7.4)

cols. 1-7 $\overline{a}$ (Å) cols. 8-14 $\overline{b}$ (Å) cols. 15-21 $\overline{c}$ (Å)

cols. 22-28 cos α cols. 29-35 cos β cols. 36-42 cos γ

Record 3: Atomic coordinates in standard ORFLS format (A4,A2,3X5F9.6)

NOTE: All programs except the crystallographic least squares ignore cols. 10-27.

cols. 1-6 any characters identifying the atoms
cols. 10-18 atomic scattering factor identifier
cols. 19-27 site occupancy multiplier (usually 1.0)
cols. 28-36 X coordinate
cols. 37-45 Y coordinate
cols. 26-54 Z coordinate

Record 4: May either be the second atomic coordinate card or the temperature parameter card for the previously read atom. All programs except the least squares program will ignore the interspersed temperature cards if present. (6F9.6)

cols. 1-9 Isotropic B or β_{11} cols. 10-18 β_{22} cols. 19-27 β_{33}

cols. 28-36 β_{12} cols. 37-45 β_{13} cols. 46-54 β_{23}

Record 4+N (or 2N): Coordinate card terminator

cols. 28-36 = 999.

Record 4+N+1: Symmetry cards (3(F11.6,2F2.0))

Include one for each general position listed in the International Tables for your space group. The format is the same for all programs requiring symmetry information. However, all symmetry relations, including those related by a center of symmetry or a non-primitive Bravais lattice, should be included here. A number of programs do not require symmetry cards and for those programs this section may be skipped.

Symmetry	Code to be Used
0	blank
X	1
-X	-1
Y	2
-Y	-2
Z	3
-Z	-3

cols. 1-11	translation for X (e.g. 0.5)
cols. 12-13	symmetry code for X
cols. 14-15	second symmetry code for X (if needed-usually left blank)
cols. 16-26	translation for Y
cols. 27-28	symmetry code for Y
cols. 29-30	second symmetry code for Y (if needed)
cols. 38-41	translation for Z
cols. 42-43	symmetry code for Z
cols. 44-45	second symmetry code for Z (if needed)

Last Record: Symmetry card terminator

cols. 1-11 = 999.

SOLLS

I. Program language and type: FORTRAN IV - interactive

II. Function: To carry out a linear least squares analysis and, if desired, plot the results on the teletype.

III. Source: original program by R. Snyder

IV. Procedure: a normal least squares analysis is performed including a statistical analysis of the best straight line. If you wish the data will be plotted on the teletype.

V. Data required: X and Y values.

VI. BTM execution: Assign SOLLS. FSNYDER to M:SI, call the compiler, load and execute. All instructions will be supplied by the program.

SODATAV

I. Program language and type: FORTRAN IV - interactive.

II. Function: To find the mean, standard deviation and mean deviation for any data set - weighted averages and statistical rejection criteria can be applied.

III. Source: Revised from an original program by R. Snyder for the IBM 1620.

IV. Procedure: If a weighted average is desired the standard deviation of each datum must be input. The weights will be computed as $1/\sigma^2$. Either of two tests may be applied to test if any piece of data can be rejected as containing a non-random error. The first is a three sigma test -- any datum that falls outside of the mean plus or minus 3σ(mean)will be rejected and a new mean and deviation will be computed without the rejected data. Since this criterion is not very severe a second option based on a technique described by Kolthoff and Sandell in their "Textbook of Quantitative Analysis," p. 276 may be chosen. This technique first applies the critical ratio test (i.e., that the deviation from the mean/average deviation is larger than 2.5). The mean is then recomputed without any data that fail this test. Then any value whose deviation from the new mean/new average deviation is greater than 4.0 is permanently rejected. Those data which fail the critical ratio test but pass the second are reaccepted and a final mean and deviation are calculated.

V. Data required: Any set of numbers and, if a weighted average is desired, standard deviations.

VI. BTM execution: Assign SODATAV, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be supplied by the program.

SULINUS

I. Program language and type: FORTRAN IV - interactive, requires an output file.

II. Function: To set up a batch run to perform a linear least squares and plot the results on both the CALCOMP plotter and line printer.

III. Source: This and the associated batch program SOLINUS are original programs by R. Snyder.

IV. Procedure: The program allows the user to manipulate the X and/or Y values so as to carry out the linear least squares procedure on the values multiplied by a constant and/or raised to any power or have base 10 logarithms taken. The original data and the best straight line are plotted on the CALCOMP plotter while a line printer plot of the data only is produced.

V. Data required: X and Y values and titles for the plots.

VI. BTM execution: Assign SULINUS, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = ANYNAME, OUT

then execute. All instructions will be supplied by the program.

SUGENPLOT

I. Program language and type: FORTRAN IV - interactive, requires two output files.

II. Function: To set up a batch run to plot any set of data on the CALCOMP plotter.

III. Source: Original program by R. Snyder using SOGENPLOT written by P. Prideaux.

IV. Procedure: The program at the user's instruction will take base 10 log or reciprocals of the X and/or Y values read. The data will then be set up to be plotted on the CALCOMP plotter with the option to leave the pen up or down between points.

V. Data required: X and Y values.

VI. BTM execution: Assign SUGENPLOT, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = ANYNAME, OUT
F:20 = ANYNAME, OUT

then execute. All instructions will be supplied by the program.

SOCALL

I. Program language and type: FORTRAN IV - terminals or batch.

II. Function: To find and print all the CALL statements made by any program or subroutine. Generally used to obtain the information necessary to construct an overlay tree.

III. Source: Adopted from an original program by R. Snyder for the IBM 360.

IV. Procedure: FORTRAN source statements are analyzed for the occurrence of any CALL statements which are printed for each main program, subroutine or function encountered.

V. Date required: A FORTRAN source file.

VI. BTM execution: Assign SOCALL, FSNYDER to M:SI. call the compiler and loader. When the loader prompts F: reply as follows:

F: 105 = NAME OF FORTAN SOURCE FILE, IN

then execute.

SOØ26Ø29

I. Program language and type: FORTRAN IV - terminal or batch.

II. Function: To convert files or cards wirtten in the old IBM Ø 26 code (BCD) to the new Ø 29 code (EBCDIC).

III. Source: Original program by R. Borst.

IV. Procedure: Equal signs in the old code now interpret as # therefore all occurrences of # are replaced by =. Further all @ are replaced by ", all & are replaced by +, all < are replaced by) and all % are replaced by (.

V. Data required: A file of Ø 26 characters.

VI. BTM execution: Assign file SOØ26Ø29, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: the user should type F: 106 = OUTPUT FILE NAME, OUT, then execute. After execution the file assigned to Unit 106 will contain the converted copy.

SOCHEM

I. Program language and type: FORTRAN IV - interactive.

II. Function: To calculate the amount of chemicals needed to run any chemical reaction, specifying the quantity of any one product desired or reactant to start with.

III. Source: Original program by Eric Ross.

IV. Procedure: A general chemical equation of the type

$$n_1A + n_2B + n_3C + \ldots = n_4E + n_5F + \ldots n_mX$$

the values for n_1 to n_m, where m = the total number of chemicals appearing in the equation, must be input along with the chemical symbols for A to X . Chemicals may be in any state (solid, liquid, solution or gas) and specified in any units. Specification of any n_mX will determine how much of the other chemicals are needed.

V. Data required: A balanced chemical equation.

VI: BTM execution: Assign SOCHEM, FSNYDER to M:SI, compile, load and execute. All instructions will be supplied by the program.

a. SOSORT - This is an extremely efficient in-core sorting routine based on the shellsort alogarithm to sort from the lowest to highest values of an array.

Source: Written by R. Snyder from an article in some forgotten journal, ca. 1968.

Call: CALL SORT(LIM, MOVE)

Parameters: LIM - the number of data in the array to be sorted.
MOVE - this is the name of a user supplied subroutine. which must be supplied with SORT. Whatever name is chosen, for example CHANGE, must be declared external to the calling routine with the statement EXTERNAL CHANGE. There is a sample of this subroutine (called NJKL) on the file SOSORT. All arrays to be sorted or carried along must be declared in common or added to the called parameters. A simple example of a MOVE routine to sort an array called F and carry along values in an array called S follows:

```
Main calling routine
COMMON F (200), S (200)
N is the number of data in the arrays F and S
EXTERNAL CHANGE
CALL SORT (N, CHANGE)
:
END
SUBROUTINE SORT (LIM, MOVE)
:  exactly as on file SOSORT
END
SUBROUTINE CHANGE (M4, M1)
COMMON F(200), S(200)

 10 M5 = M4 + M1
(user supplied IF statement-substitutes name of array to be sorted for F)
    IF(F(M4)-F(M5))30, 30, 20
 20 HOLD = F(M4)                    user supplied
    F(M4) = F(M5)                   interchange statements
    F(M5) = HOLD
    HOLD = S(M4)
    S(M4) = S(M5)
    S(M5) = HOLD
    M4 = M4 - M1
    IF(M4-1)30, 10, 10
 30 RETURN
    END
```

b. SORANDU - this subroutine will generate a fixed and floating point random number each time called.

Source: IBM scientific subroutine package.

Call: Call RANDU(IX, IY, YFL)

Parameters: IX - is a user initiated random number which should be set before calling the subroutine and changed before any subsequent call. The usual way of changing it is to set it equal to IY immediately after the call statement.

IY - a fixed point random number
YFL - a floating point random number.

Example of use:

```
   IX = 26
10 CALL RANDU (IX, IY,  YFL)
   IX = IY
     .
     .
     .
     .
   GO TO 10.
```

c. SOTTPLOT - a general subroutine for plotting on the teletype.

Source: Original program by G. M. Linko

Call: CALL TTPLOT(X, Y, XTITLE, YTITLE, GRAPH, NPTS)

Parameters: X - name of the X array
Y - name of the Y array
XTITLE - label for the X axis must be dimensioned to 20 and contain one character per word (read in A1 format)
YTITLE - label for Y axis - same restrictions as above.
GRAPH - label for graph - same restrictions as above.
NPTS - number of points to be plotted must be less than 101 as presently dimensioned.

The program will automatically scale and plot the X and Y arrays on the teletype. NOTE - numbers along the X and Y axis are printed with two significant figures and an exponent, if the entire range of X (or Y) is between .5025 and .5099 then each segment along the axis will be labeled .50 EOO. This is a minor matter in that the data is known and can be printed by the user from the calling program, the plot will always be correct.

SOBRAGG

I. Program language and type: FORTRAN IV - interactive.

II. Function: To calculate d and I/I_o values from x-ray diffraction data (2θ and intensity values).

III. Source: Original program by R. Snyder.

IV. Procedure: Bragg's law ($\lambda = 2d_{hkl} \sin \theta$) is applied to each entry and all intensity values are divided by the maximum value read and multiplied by 100.

V. Data required: λ, 2θ and I values on any arbitrary scale.

VI. BTM execution: Assign SOBRAGG, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be provided by the program.

SUPOWDER

I. Program language and type: FORTRAN IV - interactive, requires two output files.

II. Function: This program sets up and gives instructions on how to punch and submit an input deck to calculate a powder pattern using the program POWDER on the large XRAY system (described in part IVof this writeup).

III. Source: Original program by R. Snyder.

IV. Procedure: This program simply contains the instructions on how to calculate a powder diffraction pattern using POWDER in the larger XRAY system. It was written to facilitate usage of POWDER for those not familiar with the notation used in the description of POWDER.

V. Data required: Crystal structure data for the material whose powder pattern is to be calculated. (i. e., The atomic coordinates, the number of the space group as given in the international tables and the site occupancy of each atom.) I suggest that anyone executing this program have Vol. I of the International Table available at execution time.

VI. BTM execution: Assign SUPOWDER, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = ANYNAME, OUT
F:20 = JUNK, OUT

then execute. Instructions as to what to do with the two output files will be given by the program.

NOTE -- the name chosen for file 10 may not have more than 8 characters in it.

SUSEARCH

I. Program language and type: FORTRAN IV - interactive, requires two output files.

II. Function: This program sets up and gives instructions on how to punch and submit an input deck to search the JCPDS x-ray powder diffraction file and match it against an experimental pattern.

III. Source: Original program by R. Snyder.

IV. Procedure: This program contains the instructions necessary to prepare the deck necessary to run program SEARCH on the larger XRAY system.

V. Data required: The elements known to be present, absent or undetermined in your sample. The diffraction file number of any patterns you wish to have printed whether or not they match (preconceived possibilities).

VI. BTM execution: Assign file SUSEARCH, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply with

F:10 = ANYNAME, OUT
F:20 = JUNK, OUT

then execute. Instructions as to what to do with the two output files will be given by the program. NOTE: the name chosen for file 10 may not contain more than 8 characters.

SUINDEX1

I. Program language and type: FORTRAN IV - interactive, requires and output file.

II. Function: To set up a batch run of the Battelle indexing program.

III. Source: Original program by R. Snyder.

IV. Procedure: For information on the calculation see writeup for LMINDEX1 (section III. B1).

V. Data required: $\lambda_{K\alpha 1}$, $\lambda_{K\alpha 2}$ and 2θ values.

VI. BTM execution: Assign SUINDEX1, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = ANYNAME, OUT

then execute. All instructions will be supplied by the program.

SOINDEXC

I. Program language and type: FORTRAN IV - interactive.

II. Function: Index cubic powder patterns from d or 2θ values.

III. Source: Original program by R. Snyder.

IV. Procedure: The program is based on the fact that the difference between adjacent d^{*2} values must be an integral multiple of a^{*2}. d^{*2} values and the differences between them are computed for all reflections and the smallest Δd^{*2} is used to compute a value for $\bar{a}$, which is used to index. If the indexing fails three further attempts are made using the minimum Δd^{*2}/ 2, 3 and 4.

V. Data required: λ and d(or 2θ) values.

VI. BTM execution: Assign file SOINDEXC, FSNYDER to M:SI then call the compiler and loader and execute. All instructions will be provided by the program.

SOCELL

I. Program language and type: FORTRAN IV - interactive.

II. Function: Least squares refinement of lattice parameters from h,k., l and 2θ (or sin θ) values.

III. Source: Original program for the IBM 1620 by R. Shiono revised and made interactive for the XDS Σ5 by R. Snyder.

IV. Procedure: Given a set of observed data (i. e., h, k, l indices and 2θ (or sin(θ) values) this program refines the starting approximate lattice constants by an iterative least squares procedure for any crystal class. Then program automatically cycles until the least squares errors are less than ϵ, an input constant. *

V. Data required: Starting crude values for the lattice parameters, h, k,l, and 2θ and optionally weights for a number of reflections and ϵ.

VI. BTM execution: Assign SOCELL, FSNYDER to M:SI, compile, load and execute. All instructions will be supplied by the program.

*The mathematical procedure use is taken from Main and Woolfson, Acta. Cryst., 16, 731 (1963).

SOCELLC

I. Program language and type: FORTRAN IV - interactive.

II. Funtion: To determine a precise lattice parameter for cubic space group from hkl and 2θ values.

III. Source: Original program by R. Snyder.

IV. Procedure: A value for the lattice parameter $\bar{a}$ is calculated from each input reflection from the relation

$$a^{*2} = d^{*2}/(h^2 + k^2 + l^2) \qquad \bar{a} = 1/\sqrt{a^{*2}}$$

A linear least squares is then carried out for the values of a vs. $\cos^2\theta$. The extrapolated Y intercept yields a value for a , free of absorption and all of the other systematic errors associated with the Debye-Scherrer camera (and many of those associated with the diffractometer). Because other systematic errors may be present a plot on the teletype is produced to allow the user to verify the expected linear relationship.

V. Data required: λ and the hkl and 2θ values for a series of preferably high order reflections.

VI. BTM execution: Assign SOCELLC, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be provided by the program.

LMCELLTH

I. Program language and type: FORTRAN IV - interactive, instructional.

II. Function: To determine precision lattice parameters for tetragonal and hexagonal systems.

III. Source: Original program by R. Snyder.

IV. Procedure: The method begins by solving two equations of the type $d^{*2} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2a^*b^*hk \cos \gamma^*$. The user supplies hkl and d (or 2θ) values. Simultaneous solution gives starting crude values for $\bar{a}$ and $\bar{c}$ and the c/a ratio. Using these values and the known hkl and d for a number of high order reflections we can solve the following pseudo-independent equations for values of $\bar{a}_o$ and $\bar{c}_o$:

Tetragonal:

$$a_o = \frac{\lambda}{2 \sin \theta} \left[(h^2 + k^2) + \frac{l^2}{(c/a)^2} \right]^{1/2}$$

$$c_o = \frac{\lambda}{2 \sin \theta} \left[\left(\frac{c}{a} \right) (h^2 + k^2) + l^2 \right]^{1/2}$$

Hexagonal:

$$a_o = \frac{\lambda}{2 \sin \theta} \left[\frac{4}{3} (h^2 + hk + k^2) + (a/c)^2 l^2 \right]^{1/2}$$

$$c_o = \frac{\lambda}{2 \sin \theta} \left[\frac{4}{3} (c/a)^2 (h^2 + hk + k^2) + l^2 \right]^{1/2}$$

Extrapolation of the $\bar{a}_o$ or $\bar{c}_o$ values vs. $\cos^2 \theta$ to $\cos^2 \theta = 0$ gives an improved value for $\bar{a}_o$ and $\bar{c}_o$. The program plots these extrapolations on the teletype and repeats the procedure, starting with the improved values, on user command.

V. Data requires: A series of hkl and 2θ values.

IV. BTM execution: This program is too large to execute in the normal manner so the RUN subsystem is used on the stored load module. To execute type the underlined letters !RUN LOAD MOD FID: LMCELLTH (FSNYDER). Then type ;G and hit return. The program will supply all needed instructions (and some that aren't needed).

SOQUANT

I. Program language and type: FORTRAN IV - interactive.

II. Function: To perform a quantitative analysis using x-ray powder diffraction internal standard method.

III. Source: Original program by R. Snyder.

IV. Procedure: To eliminate the non-linear effects of absorption on a plot of the integrated intensity of a diffraction peak vs. the weight percent of the material causing the peak, we must add a constant weight fraction of an internal standard to a series of samples of known composition. In reference to a particular fully resolved peak of both the material we wish to analyze and the internal standard the ratio of the integrated intensities will be a linear function of composition. Thus the program accepts integrated peak intensities and background measurements in counts/sec. for both an internal standard peak and a peak of the material we wish to analyze,for as many different compositions as you have measured. The intensities are corrected for background and a linear regression is performed on the intensity ratios vs. composition to obtain a standard curve. The standard curve is plotted on the teletype. Then similar information is supplied for your unknown samples and their compositions are computed from the standard curve.

V. Data required: B1, B2, I, T and C for each of the standards. Where B1 and B 2 are the backgrounds in counts per second on each side of the diffraction peak, I is the total number of counts accumulated on scanning through the peak in time T,and C is the concentration of the material of interest in this sample before adding the internal standard. Corresponding B1, B2, I and T values for the internal standard peaks in the standard samples. Finally B1, B2, I and T values for both the material of interest and internal standard peaks in unknown samples.

VI. BTM execution: Assign SOQUANT, FSNYDER to M:SI, call the compiler, laoder and execute. All instructions will be provided by the program.

SOXRAY1

I. Program language and type: FORTRAN IV - interactive.

II. Function: To calculate Miller indices, d^*, d and 2θ for all possible reflections for any crystal system. A list of these quantities is produced for all reflections with indices ranging between user specified maximum and minimum limits on h, k and l.

III. Source: Original program by R. Snyder.

IV. Procedure: d^*, d and 2θ for any reflection are a simple geometric function of the lattice parameters and radiation. The unit cell volume, reciprocal cell parameters and d, d^* and 2θ are evaluated from the following equations.

$$S = (\alpha + \beta + \gamma)/2$$

$$V = 2abc\sqrt{\sin(S)\sin(S-\alpha)\sin(s-\beta)\sin(S-\gamma)}$$

$$a^* = bc\sin(\alpha)/V$$

$$b^* = ac\sin(\beta)/V$$

$$c^* = ab\sin(\gamma)/V$$

$$d^{*2} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^* + 2hla^*c^*\cos\beta^* + 2klb^*c^*\cos\alpha^*$$

$$d = 1/\sqrt{d^{*2}}$$

$$2\theta = 2\sin^{-1}\left(\frac{\lambda}{2d}\right)$$

V: Data required: λ, lattice parameters ($\bar{a}$, $\bar{b}$, $\bar{c}$, α, β, γ) and minimum and maximum limits for hkl -- warning: choose these limits conservatively or you will be buried in output.

VI: BTM execution: Assign SOXRAY1, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be provided by the program.

SOMUONRO

I. Language and type: FORTRAN IV - interactive.

II. Function: To calculate, for any chemical compound, the molecular weight, percent composition and the x-ray mass absorption coefficients (μ/ρ) for Mo, Cu and Cr radiation.

III. Source: Revised from an original program by R. Snyder for the IBM 1620.

IV. Procedure: The program contains tables of element names, atomic weights and mass absorption coefficients which are used to evaluate the various terms in the expression for μ/ρ.

$$\left(\frac{\mu}{\rho}\right)_{\text{Total}} = \frac{W_A}{W_T}\left(\frac{\mu}{\rho}\right)_A + \frac{W_B}{W_T}\left(\frac{\mu}{\rho}\right)_B + \ldots$$

V. Data required: An empirical formula for any chemical compound.

VI. BTM execution: Assign SOMUONRO, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be provided by the program.

SOHKL

I. Program language and type: FORTRAN IV - interactive

II. Function: Produce h, k and ℓ values from the $(h^2+k^2+\ell^2)$ or (h^2+hk+k^2), ℓ^2 values given by the indexing programs.

III. Source: Original program by J. Blendell.

IV. Procedure: Input values of $h^2+k^2+\ell^2$ for cubic systems or h^2+k^2 and ℓ^2 for tetragonal systems or h^2+hk+k^2 and ℓ^2 for hexagonal systems are solved for the h, k and ℓ indices.

V. Data required: The squared index combination as given by the various indexing programs.

VI. BTM execution: Assign SOHKL, FSNYDER to M:SI and call the compiler, loader and execute. All instructions will be supplied by the program.

SOBUNN

I. Program language and type: FORTRAN IV - interactive, requires an output file

II. Function: This program sets up a batch job to produce a CALCOMP plot of $\log d_{hk\ell}$ to be used in indexing a crystal system with Bunn charts.

III. Source: Original program by J. Blendell.

IV. Procedure: From input 2θ values $\log_{10} d$ values are calculated and output with necessary control cards to run SOBUNN on the batch system. SOBUNN will read the $\log_{10} d$ values and output a CALCOMP plot of them to the scale of a Bunn chart.

V. Data required: λ and 2θ values

VI. BTM execution: Assign SOBUNN, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: reply as follows:

F:10=ANY NAME,OUT

Then execute. All instructions will be given by the program.

SOCELDIM

I. Program language and type: FORTRAN IV - interactive.

II. Function: This program performs most of the routine calculations needed in conjunction with single crystal x-ray investigations including:

1. Cell dimensions from precession camera data.
2. Cell dimensions from cone axis photographs.
3. Calculate upper level settings for the precession camera.
4. Cell dimensions from Weissenburg camera data.
5. Cell dimensions from oscillation photographs.
6. Calculate equi-inclination settings for upper level Weissenburg photography.
7. Calculate $\bar{a}$, $\bar{b}$ and $\bar{c}$ from d or d^* values for any crystal system.
8. Calculate unit cell volume and Z (number of formula units in the unit cell).
9. Calculate the x-ray density.
10. Calculate a weighted average for d_{100}, d_{010} or d_{001} from axial 2θ values -- the program uses $\sin\theta$ as weights.
11. Calculate θ, $\sin\theta$, 2θ and $\sin\theta/\lambda$ for all reflections along any line in reciprocal space from the d or d* of the first reflection along this line.
12. Calculate the total number of reflections which can occur in the tore of reflection for any radiation.

III. Source: Revised from an original program by R. Snyder for the IBM 1130.

IV. Procedure: The geometric equations pertinent to each of the cameras are summarized by R. Snyder in the Hewlett-Packard Journal V. 4[1], 1972 in an article describing a version of this program for a Hewlett-Packard programmable calculator.

V. Data required: The raw data obtained by measuring the various types of x-ray diffraction photographs.

VI. BTM execution: Assign SOCELDIM, FSNYDER to M:SI, call the compiler, loader and execute. All instructions will be provided by the program.

SOFORMF

I. Program language and type: FORTRAN IV - interactive; requires an input and output file.

II. Function: To produce atomic scattering factors for any element in a format compatible with the programs in this writeup.

III. Source: Original program by R. Snyder.

IV. Procedure: The atomic scattering factors for all elements and ions except hydrogen are taken from Cromer and Waber, Acta Cryst., 18, 104 (1965). The hydrogen form factor is from R. Stewart, private communication. All scattering factors are contained on the file F10FORMF as functions of sin θ/λ. After the user specifies his λ the program reads the form factors of interest from the file and performs a four-point Aitken interpolation to produce the needed scattering factors as a function of sin θ. The final values are printed and written as file 20.

V. Data required: The wavelength of the radiation of interest and the chemical symbols and oxidation states of the elements whose form factors are desired.

VI. BTM execution: Assign SOFORMF, FSNYDER to M:SI, compile and load. When the loader prompts F: reply as follows:

F:10 = F10FORMF, FSNYDER, IN
F:20 = ANYNAME, OUT

then execute. Program will supply all necessary instructions.

SOPLANE

I. Program language and type: FORTRAN IV - interactive; requires standard coordinate input file.

II. Function: Calculates the least square plane through a set of atomic coordinates.

III. Source: Original program for the IBM 7090 by Shirley Chu, revised for the IBM 1130 by R. Shiono, revised and made interactive for the XDS Σ 5 by R. Snyder.

IV. Procedure: The least squares plane through any set of atoms specified from the coordinate file is computed and the distances of each of these atoms from the plane are output. The program also calculates the distances from the plane to all the other atoms on the coordinate file not included in the least squares.

V. Data required: The only input data to this program comes from the standard coordinate file described in the introduction. The file need only be built down to the coordinate card terminator; the subsequent symmetry information is not read by SOPLANE.

VI. BTM execution: Assign SOPLANE, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = NAME OF COORDINATE FILE, IN

then execute. All instructions will be supplied by the program.

SODAC

I. Program language and type: FORTRAN IV -interactive, requires standard coordinate input file.

II. Function: Calculates interatomic distances, angles and conformation (dihedral) angles.

III. Source: Revised by R. Snyder from the original IBM 1130 program by E. L. McGandy.

IV. Procedure: Geometric relations in a general triclinic coordinate system are used.

V. Data required: This program requires, on logical unit number 10, the standard coordinate file described in the introduction. The file need only be built down to the coordinate card terminator. This program does not use or read the symmetry information.

VI. BTM execution: Assign SODAC, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: reply as follows

F:10 = Coordinate file name, IN

then execute. All instructions will be provided by the program.

SOANGLE

I. Program language and type: FORTRAN IV - interactive; requires standard coordinate input file.

II. Function: Calculates interatomic distances and angles with standard deviations from standard errors output by least squares.

III. Source: Original program by R. Snyder.

IV. Procedure: The normal geometric relations are used to compute interatomic distances and angles. The estimated standard deviations of the coordinates which are obtained by the full matrix least squares program (ORFLS) from the variance-covariance matrix are used to estimate the standard deviation in the distances and angles. These are the conventional standard deviations reported in the literature but beware; it has been well established in the last few years that these errors are too low by as much as a factor of two.

V. Data required: This program requires the full standard coordinate file including symmetry information on logical unit 10. The errors for each coordinate as printed by the full matrix least squares program will be requested at execution time.

To specify the atoms to be used for each bond angle and distance calculation three quantities must be specified for each atom:

1. The sequence number of the atom on the coordinate file,
2. The unit cell the atom should be translated to (e.g., 555, see below),
3. The sequence numbers from the coordinate file of the symmetry element to be applied to the atomic coordinates.

If two atom identifiers are input then only the distance between them is calculated. If three are input then the second atom is treated as the apex and both distances and the angle are calculated. If the symmetry code is left blank the identity operation is assumed (i.e., XYZ). If the cell code is left blank the 555 cell is assumed.

NOTATION for translational symmetry:

Three numbers with one digit for each are used to represent the translation in each axial direction. A digit 5 is for no translation, a 4 is a translation of minus one unit cell, and a 6 is for a translation of plus one unit cell.

e.g., 555: $(0)\bar{a} + (0)\bar{b} + (0)\bar{c}$ (i.e., the central unit cell)

654: $(6-5)\bar{a} + (5-5)\bar{b} + (4-5)\bar{c}$

or $(1)\bar{a} + (0)\bar{b} + (-1)\bar{c}$.

This translation symbol represents the translation required to generate the coordinate from the originally given coordinate values after the application of any symmetry operations. Since this translation symbol has no relation to the actual unit cell, the atoms 155501 and 255503 (i.e., atoms one and two untranslated but having symmetry operation 1 applied to atom one and three applied to atom two) may or may not be in the same cell. It depends on the initial XYZ coordinates supplied by the user.

VI: BTM execution: Assign SOANGLE, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply as follows:

F:10 = COORDINATE FILE NAME, IN

then execute. All instructions will be supplied by the program.

SOTETRA

I. Program language and type: FORTRAN IV - interactive, requires the standard coordinate file as input and an output file.

II. Function: To calculate the coordinates of two tetrahedral sites at a specified bond distance away from another site. Usually used to calculate hydrogen positions in structures where they are not observable.

III. Source: Revised by R. Snyder from original IBM 1130 program by G. L. Gartland and D. Schwarzenbach.

IV. Procedure: Based on a matrix transformation procedure described by G. L. Gartland, May, 1968, Crystallography Department, University of Pittsburgh (available from R. Snyder).

V. Data required: A. This program requires, on logical unit number 10, the standard coordinate file described in the introduction. Since the symmetry information is neither used nor read it need not be included on the file.

B. SOTETRA will write the generated coordinates in ORFLS format on logical unit 20 which therefore must be assinged to an output file.

C. The program will explain how it is to be used and request at execution time which coordinates are to be calculated.

VI. BTM execution: Assign file SOTETRA, FSNYDER to M:SI and call the compiler and loader. When the loader prompts F: enter the following:

F:10 = COORDINATE FILE NAME, IN
F:20 = OUTPUT FILE NAME, OUT

then execute. All instructions will be provided by the program.

SOEQUIV

I. Program language and type: FORTRAN IV - interactive; requires two standard coordinate files as input.

II. Function: To find any coordinates on unit 10 which are equivalent to any coordinates on unit 20. Generally used in analyzing Fourier, difference Fourier and E maps.

III. Source: Original program by R. Snyder.

IV. Procedure: This program enables one to tell whether or not two Fourier maps have common peaks by taking the coordinates output by the peak searching routine in the Fourier program and matching them within a user specified error window.

V. Data required: Two standard coordinate files are required, one on unit 10 and the other on unit 20. Each may contain up to 200 coordinates.

VI. BTM execution: Assign SOEQUIV, FSNYDER to M:SI, call the compiler and loader. When the loader prompts F: reply as follows

F:10 = Name of standard coordinate file 1, IN
F:20 = Name of standard coordinate file 2, IN

then execute. All instructions will be supplied by the program.

SOTRANSFORM

I. Program language and type: FORTRAN IV - interactive.

II. Function: To transform atom position coordinates from one space group to another.

III. Source: Original program by R. Snyder.

IV. Procedure: The position vector XYZ for any atom can be transformed from one space group to any other by multiplying by the proper transformation matrix. Instructions for building such a transformation matrix are given in the International Tables for Crystallography.

V. Data required: 3 x 3 transformation matrix and the XYZ values to be transformed.

VI. BTM execution: Assign SOTRANSFORM, FSNYDER to M:SI and call the compiler, loader and execute. All instructions will be provided by the program.

SOLINUS

I. Program language and type: FORTRAN IV - batch processing mode.

II. Function: To perform a linear least squares and plot the data and resulting straight line on the CALCOMP plotter and/or line printer.

III. Source: Original program by R. Snyder.

IV. Procedure: The least squares is performed by a generalized subroutine called LLS. The CALCOMP plot is performed by the general subroutine GENPLOT, and the line printer plot is performed by subroutine TTPLOT.

V: Data setup: This program may be set up from terminal by executing SULINUS (see section II. A 3 of this writeup). To set up by hand the following cards should be used:

Item 1: !JOB Users account information and priority (e.g. ECLASS, 7800 (NAME), 9).

Item 2: !ASSIGN M:SI (FILE, SOLINUS, FSNYDER)

Item 3: !FORTRAN BC, GO

Item 4: !ASSIGN M:PL (DEVICE, PLAØ6)

Item 5: !LOAD (GO) (UNSAT (:PLOTLIB))

Item 6: !RUN

Item 7: !DATA

Item 8: Plot control and title for printed output (I1, 19A4)
Col 1 NPLOT = 0 plot on both CALCOMP and line printer
= 1 line printer plot only
= 2 no plots -- least squares only
Col 2-27 Any title information

Item 9: Controls for treatment of data (6G13.6)

Col 1-13 AX	Col 14-26 BX	Col 27-39 TX
Col 40-52 AY	Col 53-65 BY	Col 66-78 TY

If TX or TY is 1.0 then each input X and/or Y value will be evaluated as X(I) = A * log (X(I)*BX) (Base 10 log)

If TX or TY is 0.0 then each X and/or Y value will be evaluated as Y(I) = AY * Y(I)**BY

e.g., to leave the Y values as read and take 1/X use the following values

AX = 1.0, BX = -1.0, TX = 0.0, AY = 1.0, BY = 1.0, TY = 0.0

Item 10: Data (2G13.6, I1)
Col 1-13 X value
Col 14-26 Y value
Col 27 ITEST = 0, read another data card
= 1 last data card of last data set
= 2 last data card, another data set to follow this calculation

Items 11 and 12 should be included if NPLOT (Col 1 of item 8) is zero or one.

Item 11: XSIZE and YSIZE (2F10.4) - may be zero if NPLOT = 1
Col 1-10 size of X axis in inches - any size allowed
Col 11-20 size of Y axis in inches - 10.0 maximum

Item 12: X axis and Y axis titles (2(7A4))
Col 1-28 title for X axis - place a semicolon after last character in title
Col 29-56 titles for Y axis - place a semicolon after last character in title

If ITEST (Col 27 of item 10) is 2 go back to item 8 and start over; otherwise, go to item 13

Item 13: !EOD

VI: BPM execution: If the above items are punched on cards, submit deck at computer center. If they are built on a file, assign this file to M:SI and call the BPM subsystem.

SOGENPLOT

I. Program language and type: FORTRAN IV - batch processing mode.

II. Function: To plot one or more plots containing one or more sets of data.

III. Source: Original program by P. Prideaux.

IV. Procedure: The input X values may be plotted as read or program can take log base 10 or reciprocal of them. The input Y values may be plotted as read or after logs have been taken. If the numbers to be plotted already exist on file they may be input under user format control from logical unit 20. Control cards are read from logical unit number 10.

V. Data setup: This program may be set up from terminal by executing SUGENPLOT (see Section IIA4 of this writeup). To set up by hand the following cards should be used:

Item 1: !JOB User's account information and priority (e.g., ECLASS, 7800 (NAME), 9)

Item 2: !ASSIGN M:SI (FILE, SOGENPLOT, FSNYDER)

Item 3: !FORTRAN BC,GO

Item 4: !ASSIGN M:PL,(DEVICE, PLAØ6)

Item 5: !ASSIGN F:1Ø,(DEVICE, CRAØ3)

Item 6: If user's data (X and Y values) are to be input along with these items, use the following

!ASSIGN F:2Ø,(DEVICE, CRAØ3)

If data already exist on a file, use the following

!ASSIGN F:2Ø,(FILE, Name of data file)

Item 7: !LOAD (GO) (UNSAT, (:PLOTLIB))

Item 8: !RUN

Item 9: !DATA

Item 10: Number of data sets for first plot and pen control (2I2)
Col 1-2 NS = number of data sets for first plot right adjusted -10 maximum
Col 4 IPEN = 2 pen down between the data points
IPEN = 3 pen up between data points

Item 11: Boundaries for data sets (20I3)
Col 1-3 position in X and Y arrays of first data pointin data set one -- usually 001
Col 4-6 position in X and Y array of last data point in data set one
Col 7-9 position in X and Y arrays of first data point in data set two

.
.
.

Col n-(n+3) position in X and Y arrays of last data point in last data set

Item 12: XLEN and YLEN (2G)
Col 1-80 X axis length and Y axis length with decimal separated by commas. XLEN max = 12.0. YLEN max = 9.0.

Item 13: Graph type (A4) LNLN or LNLG or LGLN or LGLG or RTLN or RTLG (LN = linear-leave data alone, LG = base 10 log, RT = reciprocal). First two letters refer to X axis, second two to Y.
Col 1-4 one of the above codes.

Item 14: X axis title (79A1)
Col 1-79 Title for X axis enclosed in apostrophes (e.g., 'XTITLE')

Item 14: Y axis titles
Col 1-79 title for Y axis enclosed in apostrophes.

Item 16: Format controling the input X and Y values (6A4)
Col 1-24 The part of a FORTRAN format statement enclosed in parentheses. Includes the parentheses, e.g., (F6.1, 3X, E9.3).
If the data are to be entered, enter here, use (2G).

Item 17: X and Y values according to the format specified in item 16. Only include data here if the ASSIGN statement in item 6 is F:20, (DEVICE, CRAØ3). If it is assigned to a file, then include your X and Y values on that file.

Item 18: If another plot is desired, go back to item 19 and repeat through 17.

Last item: !EOD

VI: BPM execution: If the above items are punched on cards, submit at the computer center. If they are built on a file, assign it to M:SI and call the BPM subsystem.

LMINDEX1

I. Program language and type: FORTRAN IV - batch processing mode.

II. Function: Index an X-ray powder diffraction pattern from 2θ values.

III. Source: Original program by J. B. Goebel and A. S. Wilson for IBM 7090, modified by J. Gawthrop for IBM 360; modified for XDS Σ 5 by R. Snyder.

IV. Procedure: The full description of this program is available from the Clearinghouse for Federal Scientific and Technical Information, NBS, U.S. Department of Commerce, Springfield, Va., "Index: a Computer Program for Indexing X-ray Diffraction Powder Patterns" BNWL-22. A brief description follows:

A. Cubic Case: The lattice constant $\bar{a}$ and reflections of any cubic crystal must satisfy the Bragg relation

$$\sin^2\theta = \frac{\lambda^2}{4\bar{a}^2}(h^2+k^2+\ell^2).$$ Thus the program attempts to find a solution to a set of equations of the form

$\sin^2\theta_i = \bar{a} n_i$. Using only the high sin θ half of the reflections, a trial $\bar{a}$ is found by finding a set of integers n_k which satisfy

$$\bar{a} = \sin^2\theta_k/n_k \quad \text{and cause} \quad \left|\frac{\sin^2\theta_i}{\bar{a}} - n_i\right| < E$$

where E is an absolute error. The program keeps cycling, reducing E in steps of .01 until any further reduction causes no solution. Thus this method always produces a solution. Its validity may be judged by the value for E. $E < .25$ would normally indicate a valid solution. $E > .25$ would indicate the system is not cubic. The user should also look for the appearance of forbidden integers like 7 and 15 which cannot be expressed in the form

$$h^2+k^2+\ell^2$$

and for differences in the observed vs. calculated $\sin^2\theta_i$ values greater than .005 all of which indicate that the system is not cubic.

B. Tetragonal and Hexagonal Case: The basic equation used is

$$\sin^2\theta = XS + YL$$

where

for Hexagonal $X = \lambda^2/3\bar{a}_o^2$, $Y = \lambda^2/4\,\bar{c}_o^2$, $S = h^2+hk+k^2$, $L = \ell^2$

for Tetragonal $X = \lambda^2/4\bar{a}_o^2$, $Y = \lambda^2/4\bar{c}_o^2$, $S = (h^2+k^2)$, $L = \ell^2$.

All possible values of $S < 1000$ and $L < 32^2$ are generated. Starting with the high order reflections values for S and L are chosen for two reflections and two equations of the type

$$\sin^2\theta_i = XS_i + YL_i \quad i = 1 \ldots N \text{ are solved}$$

simultaneously. The values of X and Y are used to try to index the rest of the reflections so that the calculated $\sin^2\theta$ agrees with the observed within $\pm$ E, the assigned error. Then E is reduced by $\frac{1}{2}$ and another indexing is attempted. When E has decreased to its smallest value the first five solutions within this E are found and printed.

Note: Usually the five solutions printed are multiples of the first, obtained by doubling the length of one axis or in the hexagonal case multiplying an axis by $\sqrt{3}$. It is reasonable to conclude that the correct indexing is the one that has the smallest lattice constants and gives the best agreement between the observed and calculated $\sin^2\theta$ values, since this agreement could be made vanishingly small by allowing the lattice constants to increase without limit. In addition, if the empirical formula weight and observed crystal density are supplied the program will output Z the number of formula units per unit cell, under the heading number. The size of Z and its deviation from integral values are also an aid to selecting the valid solution.

C. Orthorombic Case: The basic equation used is $\sin^2\theta = XH + YK + ZL$

where $H = h^2$, $K = k^2$, $L = \ell^2$, $X = \lambda^2/4\bar{a}_o^2$, $Y = \lambda^2/4\bar{b}_o^2$ and $Z = \lambda^2/4\bar{c}_o^2$

A set of tentative values for H_i, K_i, and L_i are selected for i = 1, 2 and 3 and simultaneous solutions to the above equations are used to produce X, Y and Z values starting with the lowest order reflections. When the error (initially set equal to the smallest difference between successive $\sin^2\theta$ values) has decreased to the smallest value within which an indexing can be achieved, the first twenty solutions are printed. The principal limitation is that only combinations of the Miller indices 0, 1 and 2 are used. If the data set does not contain three independent reflections involving only 0, 1 and 2 indices the solutions produced will be false.

V. Data set up: This program may be set up from terminal by executing

SUINDEX1 (see section II B4).

To set up by hand use the following instructions:

Item 1: !JOB Users account information and priority (e.g., ECLASS, 7800 (NAME), 9)

Item 2: !ASSIGN F:1, (FILE, F1INDEX1, FSNYDER)

Item 3: !RUN (LMN, LMINDEX1, FSNYDER)

Item 4: !DATA

Item 5: title information (18A4)

cols. 1-72 any alphameric information

Item 6: Control parameters (I5, 6F10.5, 4I1)

cols. 4-5 cut number, right adjusted. All reflections below this sequential number will be treated as unresolved and $K\bar{\alpha}$ will be used. $K\alpha_1$ will be used for all reflections above this number. On our Norelco diffractometer resolution occurs around 40-45°.

cols. 6-15 $K\alpha_1$ wavelength)
cols. 16-25 $K\alpha_2$ wavelength) } if λ is for Cu these may be left blank

cols. 26-35 Maximum error between observed and calculated $\sin^2\theta$ values. If left blank .0005 will be used.

cols. 36-45 skip

cols. 46-55 Molecular weight of empirical formula - optional

cols. 56-65 Observed density in g/cc - optional

col. 66 = 0 attempt cubic indexing = 1 skip
col. 67 = 0 attempt hexagonal indexing = 1 skip
col. 68 = 0 attempt tetragonal indexing = 1 skip
col. 69 = 0 attempt orthorombic indexing = 1 skip

Item 7: Two theta values in degrees, seven on a card (7F10.2)

cols. 1-10 $2\theta_1$ cols. 11-20 $2\theta_2$ ... cols. 61-70 $2\theta_7$

Use as many cards as necessary to input all data

Item 8: last card cols. 1-80 all blanks.

Item 9: If another data set is to be run go back to Item 5 and repeat through 8; after last data put !EOD

VI. BPM execution: If the above items are punched on cards submit deck at Computer Center. If they are built on a file, assign this file to M:SI and call the BPM subsystem.

LMCELREF

I. Program language and type: FORTRAN IV - batch processing mode .

II. Function: Refine lattice parameters and index diffraction data giving standard deviations from $\theta, 2\theta$ or d's .

III. Source: Original program by D. Appleman; revised for XDS Σ 5 by R. Snyder.

IV. Procedure: A least squares procedure is used, the standard deviation being obtained from the variance-covariance matrix. Indexing is accomplished simply by varying values for $hk\ell$ starting with zeros, calculating d's for each possible index and matching them within the calculated errors to the observed d's . If no reflections are supplied only the list of possible reflections will be produced.

V. Data set up: The following items may be either punched on cards or built on a file.

Item 1: !JOB Users account information and priority (e.g., ECLASS, 7800 (NAME), 9)

Item 2: !ASSIGN F:5, (DEVICE, CRAØ3)

Item 3: !ASSIGN F:6, (DEVICE, LPAØ2)

Item 4: !RUN (LMN, LMCELREF, FSNYDER)

Item 5: !DATA

Item 6:
- cols. 1 - 5 = the word TITLE
- col. 6 = blank
- cols. 7-72 any alphameric information
- cols. 73-80 not used

Item 7:
- cols. 1 - 5 = the word PARM
- col. 6 = blank
- cols. 7 - 15 crude value for $\overline{a}$
- cols. 16-24 crude value for $\overline{b}$
- cols. 25-33 crude value for $\overline{c}$
- cols. 34-36 the number of degrees in α (I3)
- cols. 37-41 the number of minutes in α (F5.3)
- cols. 42-44 the number of degrees in β (I3)
- cols. 45-49 the number of minutes in β (F5.3)
- cols. 50-52 the number of degrees in γ (I3)
- cols. 53-57 the number of minutes in γ (F5.3)
- col. 58 ITHT = 0 all following information will apply to 2θ values
  = 1 all following information will apply to θ values

cols. 9-61 THTMX (F3.0) the maximum value of 2θ (or θ if ITHT = 1) to be used in the first NCYC cycles of refinement. If a zero is supplied 40.0° 2θ will be assumed.

col. 62 NCYC (I1) the number of initial cycles using only the data with angle below THTMX. If left blank, 2 is assumed.

cols. 63-67 TOLMN (F5.4) the minimum tolerance allowed between the observed and calculated angles (θ or 2θ) - .04°-2θ is a reasonable value.

cols. 68-72 TOLMX (F5.4) the maximum tolerance -.2°-2θ is a reasonable error.

Note: If cols. 63-72 are left blank, reasonable values will be assumed by the program.

Item 8: cols. 1 - 6 = the word SYSEXT

cols. 7 - 11 one of the following eight names giving crystal system:

CUBIC, TETRA, ORTHO, MONOC, RHOMB, TRICL, HEXAG or HEXAR

where the final word (HEXAR) refers to a rhombohedral space group referred to a hexagonal axis.

cols. 12-14 THEMX (F3.0) the 2θ (or θ) value below which no reflections appear in the observed pattern.

cols. 15-20 PWL (F6.5) the wavelength of the X-radiation used. If a zero is input λ Cu Kα will be used.

The following 27 columns only apply if the space group is known. If it is the extinction condition as given by the International Tables for Crystallography will tell the user whether I = 2, 3, 4 or 6 should be entered in the appropriate column. If a column is left blank or a zero is entered that class of reflections will be calculated and included in the output. All formats are I1, ENTER the value for I in the following relations:

col.	21	h k ℓ	h+k = In	col.	22	h k ℓ	h+ℓ = In
col.	23	h k ℓ	k+ℓ = In	col.	24	h k ℓ	h+k, h+ℓ+k+ℓ = In
col.	25	h k ℓ	h+k+ℓ = In	col.	26	h k ℓ	-h+k+ℓ = In
col.	27	h h ℓ	h = In	col.	28	h h ℓ	ℓ = In
col.	29	h h ℓ	h+ℓ = In	col.	30	h h ℓ	2h+ℓ = In
col.	31	o k ℓ	k = In	col.	32	o k ℓ	ℓ = In
col.	33	o k ℓ	k+ℓ = In	col.	34	h o ℓ	h = In
col.	35	h o ℓ	ℓ = In	col.	36	h o ℓ	h+ℓ = In
col.	37	h k o	h = In	col.	38	h k o	k = In
col.	39	h k o	h+k = In	col.	40	h h o	h = In
col.	41	h h o	h = In	col.	42	o k o	k = In
col.	43	o o ℓ	ℓ = In	col.	44	h ℓ ℓ	h = In
col.	45	h ℓ ℓ	ℓ = In	col.	46	h ℓ ℓ	h+ℓ = In
col.	47	h ℓ ℓ	h+2ℓ = In				

Item 9: Data cards (A6, 3I5, F9.6, F8.6, 2F9.5) either θ , 2θ or d values may be entered.

col. 1 - 6	anything but the letters END in cols. 1-3
cols. 7 - 11	h if known
cols. 12-16	k if known
cols. 17-21	ℓ if known
cols. 22-30	d if θ or 2θ are not to be entered; otherwise leave blank
cols. 31-38	λ - this may be used to cause a different wavelength to be used in computing angles from this one d value. If blank or zero the value assigned to PWL will be used.
cols. 39-47	θ or 2θ depending on the value of ITHT.
cols. 48-56	the weight to be used for this reflection in the least squares procedure. If blank or zero is input sin (θ) will be used as a weighting factor. If unit weights are desired enter a 1.0.

Item 10: Data terminator

cols. 1-3 = the word END

Item 11: If a second data set is to be run this should be a TITLE card; go back and repeat items 6-10. After last END card of last data set enter:
cols. 1 - 6 FINISH

Item 12: !EOD

VI. BPM execution: If the above items are punched on cards submit at Computer Center. If they are built on a file assign to M:SI and call BPM subsystem.

I. Program language and type: FORTRAN IV - batch processing system .

II. Function: Calculate values of particle size, strain, faulting and true lattice constants by analyzing X-ray diffraction line profiles.

III: Source: Original program by C.N.J. Wagner (Department of Engineering and Applied Science, Yale Univ.) described in Technical Report No. 15 to Office of Naval Research. Peak smoothing routine added and adapted to XDS Σ 5 by R. Snyder.

IV. Procedure: This program analyzes the peak profiles, i.e., calculates peak position, Fourier coefficients, integral breadth and variance. From these quantities, one can deduce the values of particle size, strain, faulting and true lattice parameter.

The first step in the program consists of correcting the measured profile for polarization and geometric factors, and to convert the 2θ-scale to equal intervals in $\eta = \sin\theta$. The Rachinger method is applied to separate the $K\alpha$ doublet. The $K\alpha_1$ peak profile is used to determine the position of the peak maximum and the center of gravity, the integral breadth and the variance, and the lattice parameter corresponding to the individual reflection (h k ℓ) for cubic crystals.

The Fourier coefficients are calculated for different values of $L = na_3$ normal to the reflecting planes, say at 10 or 25A interval. The corresponding coefficients of the standard are used to correct for instrumental broadening by the Stokes method. The integral breadths are corrected with the parabolic relationship

$$b_{cor}/b_{uncor} = 1 - (b_{stand}/b_{uncor})^2 .$$

The corrected variance is given by $W_{cor} = W_{uncor} - W_{stand}$.

The Fourier coefficients are used to separate the particle size and strains by the Warren-Averbach method. The integral breadth particle size and strain are obtained from the parabolic relationship $b_{particle\ size}/b_{cor} = 1 - (b_{strain}/b_{cor})^2$.

The $K\alpha_1$ peak profile, the Fourier coefficients of the first and second order peak, and the particle size coefficients and the strain values are directly output on the line printer.

V. Data set up:

Item 1: !JOB Users account information and priority of zero(e.g., ECLASS, 7800 (NAME), 0) . A zero priority is required on this job so that the operation may raise the priority when time sharing is not running. This is due to the the need for more memory than is available to the batch partition during BPM/BTM operation.

Item 2: !MESSAGE RUN THIS JOB UNDER BTMX

Item 3: ! ASSIGN M:SI, (FILE,SOBROAD,FSNYDER)

Item 4: ! FORTRAN BC,GO,LS

Item 5: ! ASSIGN F:5,(DEVICE,CRAØ3)

Item 6: ! ASSIGN F:6,(DEVICE, LPAØ2)

Item 7: ! LOAD (GO)

Item 8: ! RUN

Item 9: ! DATA

Item 10: 2F10.6 format

cols. 1 - 10 wavelength of $K\alpha_1$ radiation
cols. 11-20 difference between $K\alpha_1$ and $K\alpha_2$ radiations ($\lambda K\alpha_2 - \lambda K\alpha_1$)

Item 11: Indicies of reflection to consider and title information (3I1,3A4)

col. 1 = h
col. 2 = k
col. 3 = ℓ
cols. 4 - 16 any title information

Item 12: I2,F10.5 format

cols. 1 - 2 NFC = number of Fourier coefficients to use (< 101)
cols. 3 - 12 VIK interval ΔL between Fourier coefficients
(NFC = 50 and VIK = 10 are reasonable values)

Item 13: col. 1 = NRAC = 0 No Rachinger correction = 1 use correction

Item 14: col. 1 = NACW = 1 annealed peak only is to be supplied
= 2 this peak is for annealed sample, cold worked data to follow
= 3 this peak is for cold worked sample, annealed data has already been read and GR(L) and GI(L) values calculated
= 4 this peak cold worked, read GR(L) and GI(L) values
= 5 this peak cold worked, read GBA(L) values

Item 15: col. 1 = NSTR = 0 no strain calculation
= 1 do strain calculation for this peak and following one
= 2 do strain calculation for this peak and preceding one

Item 16: cols. 1 - 10 ALPHA 2θ angle that monochromter is set at.

Item 17: cols. 1 - 10 TWCH (1) - $2\theta_1$ value for first data point of peak

Item 18: cols. 1 - 10 DTWCH = $\Delta 2\theta$ - interval between data points

Item 19: cols. 1 - 3 NDP = number of data points (≤ 400)

Item 20: Intensity values (10F7.3) 10 per card

cols. 1 - 7 first Intensity value
cols. 8 - 14 second value ...

Item 21: this and items 22 & 23 should only be included if NACW (Item 14) = 5

cols. 1 - 2 NPG = Number of Fourier coefficients (GBA(L)) to be read ($\leq$ 101)

cols. 3 - 12 VG = interval ΔL (in Å) between Fourier coefficients

Item 22: Fourier coefficients from previous run (GBA(L)) 10F7.3 (only included if NACW=5)

Item 23: cols. 1 - 10 BINTS - integral breadth standard from previous output

Item 24: GR(L) and GI(L) L = 1, NFC (10F7.3) only include this item if NACW=4

cols. 1 - 7 GR(1) from previous output
cols. 8 - 14 GI(1)
cols. 15-21 GR(2) ...

Item 25: Repeat items 11-20 for cold worked sample

Item 26: !EOD

VI. BPM execution: If the above items are punched on cards, submit at Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem.

NOTE: You will not get immediate execution as running of this program requires the shutting down of terminals.

SODELITE

I. Program language and type: FORTRAN IV - Batch processing mode .

II. Function: To carry out a Delaunay reduction on any general set of lattice parameters producing the standard Delaunay cell--possibly exposing hidden symmetry.

III. Source: Originally programmed at Brookhaven National Laboratory for the CDC 6600; revised for the IBM 1800 by A. Bednowitz and for the XDS Σ5 by R. Snyder.

IV. Procedure: Delaunay's method for the reduction of the most general primitive cell of any lattice to a standard form involving four vectors which make obtuse angles with one another is described in the International Tables for Crystallography and in various text books. The Delaunay reduced cell permits the recognition of the symmetry properties of the lattice.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g., ECLASS,7800 (NAME),9)

Item 2: !ASSIGN M:SI, (FILE,SODELITE,FSNYDER)

Item 3: !FORTRAN BC,GO

Item 4: !LOAD (GO)

Item 5: !RUN

Item 6: !DATA

Item 7: cols. 1 - 80 any title information (20A4)

Item 8: Cell parameters (7F10.4)

cols. 1 - 10	$\bar{a}$ or a*
cols. 11-20	$\bar{b}$ or b*
cols. 21-30	$\bar{c}$ or c*
cols. 31-40	cos (α) or cos (α*) or α or α*
cols. 41-50	cos (β) or cos (β*) or β or β*
cols. 51-60	cos (γ) or cos (γ*) or γ or γ*
cols. 61-70	Leeway factor for determining the equality of dot products ($\approx .1$)

Item 9: !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem. There will be an interactive version of this program at some time in the future.

I. Program language and type: FORTRAN IV - Batch Processing mode

II. Function: To analyze the principle directions of preferred orientation normal to the surface of a polycrystalline sample.

III. Source: Original program by W. Carr and R. Snyder.

IV. Procedure: The method is based on the comparison of observed intensities of an X-ray diffraction pattern to the intensities of a calculated pattern. A full description of the procedure will appear in the Proceedings of the Conference on Surfaces and Interfaces held in August 1973 at the NYS College of Ceramics.

Briefly the function

$$Q_{hk\ell} = \frac{\Sigma I_{h'k'\ell'} \cos \varphi_{hk\ell}}{\Sigma I_{h'k'\ell'}}$$

is evaluated for an observed and a calculated X-ray powder diffraction pattern for each of the 7 principal zones (100, 010, 001, 110, 101, 011, 111). When calculating Q's for the observed pattern $\Sigma I_{h'k'\ell'}$ is the sum of the intensities of all reflections in the observed pattern which match peaks in the calculated pattern. $\varphi_{hk\ell}$ is the angle each direction $[hk\ell]$ makes with the zone in question. For the calculated pattern the sum $(\Sigma I_{h'k'\ell'})$ is taken over all input I_{cal} values. Q values are evaluated for a large number of directions and ΔQ $(Q_{obs}-Q_{cal})$ are then plotted against φ for each of the 7 zones. Plots showing a negative slope are directions of preferred orientation.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g., ECLASS, 7800 (NAME),9)

Item 2: !ASSIGN M:PL, (DEVICE,PLAØ6)

Item 3: !RUN (LMN,LMPREF,FSNYDER)

Item 4: !DATA

Item 5: cols. 1-80 any title information: the first 16 columns should contain the chemical formula or name centered around col. 8. This column will be used to identify any plots.

Item 6: Cell parameters (6F10.4)

cols. 1-10 $\bar{a}$ in Å cols. 11-20 $\bar{b}$ cols. 21-30 $\bar{c}$
cols. 31-40 α in degrees cols. 41-50 β cols. 51-60 γ

Item 7: Control parameters (10I1)

col. 1 =0 calculated and observed pattern to be input
=1 observed pattern only will be input--only Q observed will be calculated

col. 2 =0 output a list of I_o^3/I_c and Lotgering f factors (cf. J. Inorg. Nucl. Chem 9, 113, 1959)
=1 skip this option

col. 3 =2 calculate the scaled differences in intensity (I_o-I_c) and plot for each of the 7 principal zones vs. the angle that each reflection makes with the zone.
=1 calculate the above and print results but skip plot
=0 skip this option

NOTE: This routine is not very useful and should normally be skipped.

col. 4 =0 calculate the observed (Q_o), calculated (Q_c) and difference (Q_o-Q_c) Q factors for the 7 principal zones and plot vs. the angle each makes with the zone
=1 skip plotting features
=2 skip routine

col. 5 =0 last data set
=1 another data set to follow item (repeat Items 5 -14)

col. 6 =1 plot Q observed vs. angle for the 7 principal zones
=0 no Q_o plots

col. 7 =1 plot Q calculated vs. angle for the 7 principal zones
=0 no Q_c plots

col. 8 =1 plot Delta Q (Q_o-Q_c) vs. angle for the 7 principal zones
=0 skip Δ Q plots

NOTE: Normally only ΔQ plots are of interest.

Item 8: Control parameters for listing and plots (4F10.4)

cols. 1-10 X=Maximum angle output for table listing for option 3 of Item 7 (180.0 gives all values)

cols. 11-20 X1 = Maximum angle to be plotted for option 3 of Item 7

cols. 21-30 X2 = Maximum angle to be output for table listing of option 4 of Item 7 (90.0 gives all values)

cols. 31-40 X3 = Maximum angle to be plotted for option 4 of Item 7

Item 9: Observed pattern parameters (I4,2F10.4)

cols. 1-4 MAXPKN = Maximum number of unmatched observed peaks to calculated peaks to be tolerated. If more than this number occur run will abort. A value of 200 will force calculation no matter how many peaks match.

cols. 5-14 SINT = the full scale setting of recorder in counts per second when observed pattern was recorded

cols. 15-24 BCKGRD-average background value from strip chart in chart units

cols. 25-34 FACTR-a multiplier which controls the size of any plots to be run. If 1.0 plots will be 10 x 10 inches; if .5 they will be 5 x 5 etc.

Item 10: cols. 1-10 Wavelength of X-radiation used

Item 11: Observed pattern

cols. 1-10 2θ
cols. 11-20 unscaled or scaled intensity

Item 12: Blank to terminate observed pattern.

Item 13: Calculated pattern (F17.2, 7XF7.3, T34, 3I3, T51I4)
(if one is to be entered)

This uses the format punched by POWDER (see section IV 9 of this write up).

cols. 1-17 $2\theta_c$ cols. 25-32 d_c cols. 34-36 h
cols. 37-39 k_c cols. 40-42 ℓ_c cols. 51-54 peak intensity

Item 14: Blank to terminate calculated pattern.

Item 15: !EOD

VI. BPM execution: If the above items are punched on cards, submit them at the Computer Center. If they are built on a file, assign it to M:SI and call the BPM subsystem.

SODATLST

I. Program language and type: FORTRAN IV - Batch processing mode.

II. Function: To produce a list of possible reflections for any crystal system and include spaces on which to record multiple film intensities.

III. Source: Original program by J. Ibers; revised at Brookhaven for the CDC 6600 by R. Rudman; for the IBM 1620 and XDS Σ 5 by R. Snyder.

IV. Procedure: All reflections within the range determined by TMAX and the cell constants and the limiting integers J1, K1, L1 are generated. To eliminate the listing of any systematically absent reflections a user supplied subroutine REJECT may be written. The call has the arguments (J, K, L, SL, NRJCT) where J, K, L refer to the h k ℓ indices that will not be printed if the subroutine returns a 1 for NRJCT. If a 0 is returned for NRJCT the reflection will be printed. SL is $\sin\theta/\lambda$ value. A sample subroutine follows:

```
      SUBROUTINE REJECT (J,K,L,SL,NRJCT)
C     EXAMPLE TO REJECT ALL REFLECTIONS OF TYPE OK(-L)
      IF(J)1,2,1
    2 IF(L)3,1,1
    3 NRJCT=1
      GO TO 4
    1 NRJCT=0
    4 RETURN
      END
```

The program as compiled will accept all reflections. If a new reject subroutine is to be added, copy SODATAV into your account, and add your subroutine in place of the dummy currently in source.

If desired the Wissenberg equi-inclination Lp factor together with $\sin\theta/\lambda$ values will be output for each reflection. The output includes spaces on which to record the intensities from five multiple films. There is an option to punch cards containing h, k, ℓ and reflection number to aid the key punching of the intensity data.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g. ECLASS, 7800(NAME), 9)

Item 2: !ASSIGN M:SI, (FILE, SODATLST, FSNYDER)

Item 3: !FORTRAN BC, GO

Item 4: !LOAD (GO)

Item 5: !RUN

Item 6: !DATA

Item 7: cols. 1 - 48 any title information (12A4)

Item 8: Cell constants (6F10.6)

cols. 1 - 10	$\overline{a}$
cols. 11-20	$\overline{b}$
cols. 21-30	$\overline{c}$
cols. 31-40	cos (α)
cols. 41-50	cos (β)
cols. 51-60	cos (γ)

Item 9: 2F10.5, 2I10

cols. 1 - 10	wavelength of radiation used
cols. 11 - 20	the maximum Bragg angle TMAX in degrees within which one wants the reflections listed.
col. 30	IPCH = 0 printed output only = 1 punched output only = 2 printed and punched output
col. 40	LP = 0 do not calculate Lp factors = 1 calculate Lp factors

Item 10: J1, K1, L1, M1, M2, M3 (6I1)

col. 1 = J1	= 0 h index will range from 0 to maximum = 1 h index will range from -max to +max
col. 2 = K1	= 0 or 1 for limits on k index
col. 3 = L1	= 0 or 1 for limits on ℓ index
col. 4 = M1	
col. 5 = M2	
col. 6 = M3	where M1, M2 and M3 refer to the slowest (1), next slowest (2) and fastest (3) varying indicies. Thus, if M1, M2, M3 = 1 2 3 then h value is slowest, k next slowest and ℓ fastest. The index associated with the axis along which the crystal is orientated should move slowest.

Item 11: !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem.

SOFILMFAC

I. Program language and type: FORTRAN IV - Batch processing mode.

II. Function: Generate a table of powers of film to film factors multiplied by relative Intensity Units to be used in scaling intensities to the first film in multiple film techniques involving up to 10 films.

III. Source: Original program by R. Snyder.

IV. Procedure: The film to film intensity reduction factors are used to create a table so that any relative intensity unit on any film may be referred to its intensity on the first film.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g., ECLASS,7800 (NAME),9)

Item 2: !ASSIGN M:SI, (FILE,SOFILMFAC,FSNYDER)

Item 3: !FORTRAN LS, GO

Item 4: !LOAD (GO)

Item 5: !RUN

Item 6: !DATA

Item 7: cols. 1 - 80 any title information (20A4)

Item 8: (I5,F5.0,I1)

cols. 1 - 5	highest relative intensity unit on your film strip
cols. 6 - 10	the interval desired between each intensity value (usually 1.0)
col. 11	= 0 another cycle of this program to follow = 1 end job after this run

Item 9: Film factors (5F10.4)

cols. 1 - 10	film factor between film 1 and film 2
cols. 11-20	film factor between film 2 and film 3
cols. 21-30	film factor between film 3 and film 4
cols. 31-40	film factor between film 4 and film 5
cols. 41-50	film factor between film 5 and film 6

Item 10: Last four film factors (4F10.4)

cols. 1 - 10	film factor between film 6 and film 7
cols. 11-20	film factor between film 7 and film 8
cols. 21-30	film factor between film 8 and film 9
cols. 31-40	film factor between film 9 and film 10

Item 11: If another job is to follow repeat items 7 to 10; otherwise put !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem.

SOSTRUFAC

I. Program language and type: FORTRAN IV - Batch, requires an output file .

II. Function: To compute structure factors from intensity data obtained by the equi-inclination Weissenberg technique. Options allow for the scaling of layers to a common scale, application of spot shape correction and calculation of weights based on a modified Cruckshank scheme.

III. Source: Revised from an original KINGSTRAN program by R. Snyder for the IBM 1620.

IV. Procedure: The spot shape correction(s) are after D. C. Phillips Acta. Cryst. 7, 746 (1954). The principal equation used is $F^2 = S\ Lp\ S_f I$ where

S = spot shape correction
Lp = Lorentz polarization correction
S_f = scale factor I = intensity

The weight for each reflection is computed from

$$W = \frac{4C_1^2 I^2}{1+C_2^2}$$

where C_1 = the percent error in reading intense reflections (10% gives a good distribution)

C_2 = the error in reading weak reflections in the relative intensity units of the scale used (3 is a usual value)

NOTE: The printed weights are multiplied by 1000 and divided by F^2. The weights written on file 1 or punched are as calculated from the above equation.

V. Data set up: the following items may be either punched on cards or built on a file.

Item 1: !JOB Users log on code and priority (e.g., ECLASS,7800(ANYNAME),9)

Item 2: !ASSIGN M:SI,(FILE,SOSTRUFAC,FSNYDER)

Item 3: !FORTRAN LS, GO

Item 4: !ASSIGN F:1, (FILE,ANYNAME),(OUT)

Item 5: !LOAD (GO)

Item 6: !RUN

Item 7: !DATA

Item 8: Cell constants (6F10.6)

cols. 1-10	$\bar{a}$
cols. 11-20	$\bar{b}$
cols. 21-30	$\bar{c}$
cols. 31-40	cos α
cols. 41-50	cos β
cols. 51-60	cos γ

Item 9: Control parameters (8I1)

col. 1	= 1 if $\bar{a}$ is oscillation axis = 0 if not
col. 2	= 1 if $\bar{b}$ is oscillation axis = 0 if not
col. 3	= 1 if $\bar{c}$ is oscillation axis = 0 if not
col. 4	= 0 if Lp corrections are to be applied = 1 if not
col. 5	= 0 if spot shape correction is to be made = 1 if not
col. 6	= 0 if weights are to be calculated = 1 if not
col. 7	= 0 output will be punched in addition to being written on logical Unit Number 1 = 1 no punched output
col. 8	= 0 all scale factors will be set to 1.0 = 1 factors will be applied

If scale factors are to be applied, then the next two items (10 & 11) should be treated as batch cards and should precede each layer of data for which the scale factor differs.

If col. 8 = 0 they need only be put in once.

Item 10: Batch card 1 Title (16A4)

cols. 1-64	any alphameric information

Item 11: Batch card 2

cols. 1-10	wavelength of radiation used in Å
cols. 11-20	C_1 the error in reading strong reflections in percent (usually 10.)
cols. 21-30	C_2 the error in reading weak reflections in relative intensity units (usually 2. or 3.) If col. 6 of Item 9 is 1 then C_1 and C_2 may be ignored.
cols. 31-40	the scale factor by which all reflections in this batch will be multiplied.

Item 12: Data (3I3, F10.0)

cols. 1-3	h
cols. 4-6	k
cols. 7-9	ℓ
cols. 10-19	intensity

Item 13: Terminator after last data card in batch or entire run (71XI1)

col. 72	= 1 means read two new batch cards and a new set of reflections = 2 means end of data call exit

Item 14: !EOD

VI. BPM execution: If the above items are punched on cards simply submit deck at Computer Center. If they are built on a file, assign the file to M:SI and call BPM subsystem to submit run to the batch job stream.

I. Program language and type: FORTRAN IV - Batch processing mode.

II. Function: Calculate and print a two dimensional Patterson projection.

III. Source: Revised from an original program by R. Snyder for the IBM 1620.

IV. Procedure: This program will produce the density map of a two dimensional Patterson projection along any one of the three principal crystallographic directions. The general triclinic Patterson function is evaluated, thus assuming that all intensity data will be input. If only unique data for othorombic or higher symmetry is available, then the space group specific equation (found in Vol. I of the International Tables) should be inserted in subroutine FUNCT.

V. Data required: The following items may be either punched on cards or built in a file.

Item 1: !JOB Users log on code and priority (e.g., ECLASS,7800(ANYNAME),9)

Item 2: !ASSIGN M:SI, (FILE,SOPATMAP,FSNYDER)

Item 3: !FORTRAN LS, GO

Item 4: !LOAD (GO)

Item 5: !RUN

Item 6: !DATA

Item 7: Cell constants (6F10.4)

cols. 1-10	$\bar{a}$
cols. 11-20	$\bar{b}$
cols. 21-30	$\bar{c}$
cols. 31-40	α
cols. 41-50	β
cols. 51-60	γ

Item 8: Limits on density map as fractional coordinates (6F10.2)

cols. 1-10	upper limit on X (U)
cols. 11-20	lower limit on X
cols. 21-30	upper limit on Y (V)
cols. 31-40	lower limit on Y
cols. 41-50	upper limit on Z (W)
cols. 51-60	lower limit on Z

NOTE: the limits for the projection axis must be 0.0

Item 9: Control parameters (3F5.0, I5)

cols. 1-5	the interval desired between each X (U) value (as a fractional coordinate)
cols. 6-10	the interval desired between each Y (V) value
cols. 11-15	the interval desired between each Z (W) value
cols. 19-20	= -1 all values will be printed on density map = 0 all negative values will be omitted = +N only values greater than N will be printed

Item 10: Data - as output from SOSTRUFAC (3I9, F9.2)

cols. 1-9	h
cols. 10-18	k
cols. 19-27	ℓ
cols. 28-36	F^2

Item 11: Data terminator (I1)

col. 1	= 1 means read 4 new set up cards (Items 7-10) and a new set of data = 2 means call exit

Item 12: !EOD

VI. BPM execution: If the above items are punched on cards simply submit at Computer Center. If they are built on a file, assign the file to M:SI and call the BPM subsystem to submit the run to the batch job stream.

I. Program language and type: FORTRAN IV - Batch Processing mode

II. Function: Perform a Wilson plot to get overall scale and temperature factors and use these to calculate normalized strucutre factors (E values)

III. Source: Original program for the IBM 1130 by R. Shiono; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: Starting with a set of observed reflection data, this program calculates the Wilson plot method of finding an overall scale factor and temperature factor by linear or second order equation fitting.

With the calculated scale and temperature factors or those supplied by the user, the program prepares normalized structure factors (E's), and if so specified, repeats the calculation, changing various factors, to bring the average E^2 for different combinations to 1.0 or nearer to it. The final set of E values will be written on Unit 106; if unassigned to a file they will be punched on cards with or without sorting on the magnitude of E .

V. Data set up:

Item 1: !JOB Users account information and priority
(e.g., ECLASS, 7800(NAME),9)

Item 2: !ASSIGN F:1, (FILE,NAME OF REFLECTION FILE),
(OUTIN) or (INOUT), (SAVE)

File 1 is the binary reflection file. If it has been created by a previous run of SOWILSON or SOFC or SOCRYLS or SOFOURIER or any data reduction program, you may input your data on it (specify INOUT); otherwise input your data as Item 16 below and it will be created by the program(specify OUTIN).

Item 3: !ASSIGN F:106, (FILE,ANYNAME)

The output normalized structure factors will be output on this file. If Item 3 is omitted the E's will be punched.

Item 4: !RUN (LMN,LMWILSON,FSNYDER)

Item 5: !DATA

Item 6: Title card (20A4)

cols. 1 - 80 any title information

Item 7: Control card 1 (6I2,3F6.2)

col. 2 KN1 = 0 reflection data on cards (Item 16) (SOFC or SOCRYLS input format
= 1 reflection data on cards (Item 16) (SOFOURIER input or SOFC or SOCRYLS output format)
= 2 reflection already on binary file input on Unit 1; must use for all repeat cycles of program

col. 4 KN2 = 0 isotropic B is used (linear first order regression)
= 1 second order temperature factors B_1 and B_2 are used

col. 6 KN3 = 0 normal operation
= 1 unitary structure factors $U_{h\,k\,\ell}$ will replace F_{obs} on File 1

col. 8 KN4 = 0 call Wilson plot to obtain B and K
= 1 no Wilson plot B and K supplied by user
= 2 K and B taken from previous cycle (no card needed)

col. 10 KN5 = 0 no punching of E's on cards or output to Unit 106
= 1 E values to be punched without sorting
= 2 punch (write 106) E values in descending order of magnitude

col. 12 KN6 = 0 normal; reads various weighting factors from cards (Items 10-12)
= 1 use factors stored or modified by the previous cycle

cols. 13-18 a damping factor (fraction of shift to be applied) for the shifts of multiplicity factors for each zone (i.e., h k ℓ, hko, ok ℓ, etc.)

cols. 19-24 a damping factor for the shifts of factors for the parity groups (e.e., EEE, EOE, etc.)

cols. 25-30 a damping factor for the shift of factors for the sin θ groups (i.e., 0-.1, .1-.2, etc.)

NOTE: If cols. 13-30 are left blank program will assign the value of 0.4 to each. If no shifts are to be applied, use 1.0

Item 8: Control card 2 (8F8.3)

If Wilson plot is going to be calculated (KN4 = 0) use a blank card here.
If KN4 = 1 supply the necessary factors here.
If KN4 = 2 skip this card entirely.

cols. 1 - 8 scale factor K for F_{obs} (if KN2=0)
cols. 9 - 16 isotropic temperature factor B (if KN2=0)
cols. 25 - 32 scale factor for second order B's (if KN2=1)

cols. 33 - 40 B_1 (if KN2=1)
cols. 41 - 48 B_2 (if KN2=1)

Item 9: Control card 3 (10F5.1)

The total number of each kind of atom present in the entire unit cell (not asymmetric unit). The order of the types of elements specified here should correspond to the order in which the atomic scattering factors are entered.

cols. 1 - 5 the number of atoms of element 1 in unit cell (with decimal)
cols. 6 - 10 the number of atoms of element 2 in unit cell up to a maximum of 10 elements
cols. 11- ...

Item 10: Control card 4 (7F5.1)

Relative weight of the reflections in each zone. If left blank, 1.0 is assumed for each. These classes are exclusive of each other (e.g., o o ℓ is not included in h o ℓ). If h o o is present, only when k is even you should use a factor of 2.0 .

cols. 1 - 5 h k ℓ class
cols. 6 - 10 h k o
cols. 11-15 o k ℓ
cols. 16-20 h o ℓ
cols. 21-25 h o o
cols. 26-30 o k o
cols. 31-35 o o ℓ

Item 11: Control card 5 (8F5.1)

Weighting factors for each class of reflections with h, k or ℓ, even (E) or odd (O). If all are to be equally weighted at 1.0 use a blank card.

cols. 1 - 5 EEE class
cols. 6 - 10 EEO
cols. 11-15 EOE
cols. 16-20 EOO
cols. 21-25 OEE
cols. 26-30 OEO
cols. 31-35 OOE
cols. 36-40 OOO

Item 12: Control card 6 (10F5.1)

Weighting factors for reflections with various ranges of $\sin\theta$. There are 10 groups of $\sin\theta$, 0.0 to 1.0 in steps of .1 . If all weights are to be 1.0 use a blank card.

cols. 1 - 5 $\sin\theta$ 0.0-0.1
cols. 6 - 10 $\sin\theta$ 0.1-0.2
cols. 11-15 $\sin\theta$ 0.2-0.3
cols. 16-20 $\sin\theta$ 0.3-0.4
cols. 21-25 $\sin\theta$ 0.4-0.5
cols. 26-30 $\sin\theta$ 0.5-0.6
cols. 31-35 $\sin\theta$ 0.6-0.7
cols. 36-40 $\sin\theta$ 0.7-0.8

cols. 41-45 $\sin\theta$ 0.8-0.9
cols. 46-50 $\sin\theta$ 0.9-1.0

Item 13: Cell constants (3F7.3, 4F7.4)

cols. 1 - 7 $\overline{a}$ (Å)
cols. 8 - 14 $\overline{b}$
cols. 15-21 $\overline{c}$
cols. 22-28 cos (α)
cols. 29-35 cos (β)
cols. 36-42 cos (γ)
cols. 43-49 λ wavelength of X-rays used

Item 14: Atomic scattering factors (8(7F10.4/))

X-ray scattering factors for $\sin\theta = 0.0$ to 1.0 in steps of .02 on eight cards for each element in ORFLS format. These can be produced by program SOFORMF (see IIC 2 of this write up). Be sure to include them in the same order as the elements were entered in Item 9.

Item 15: Blank card terminating atomic scattering factors

Item 16: Reflection data - only include if KN1=0 or 1 .
If KN1=0 then input is in the normal least squares format (3I9, 2F9.2, F9.0, I5, 2F6.3)

cols. 1 - 9 h
cols. 10 - 18 k
cols. 19 - 27 ℓ
cols. 28 - 36 F_{obs}
cols. 37 - 47 σ (F_{obs})
cols. 46 - 54 scale factor designation (not used)
col. 59 IO = 0 observed reflection; = 1 unobserved reflection
cols. 60 - 65 RA (not used)
cols. 66 - 71 RB (not used)

If KN1=1 then data is in the form produced by SOFC or SOCRYLS for SOFOURIER (3I4, 6F7.2, I3, F72)

cols. 1 - 4 h
cols. 5 - 8 k
cols. 9 - 12 ℓ
cols. 13-19 F_{obs}
cols. 20-26 F_{cal}
cols. 27-33 A_{obs}
cols. 34-40 A_{cal}
cols. 41-47 B_{obs}
cols. 48-54 B_{cal}
cols. 55-59 $\sin\theta$
col. 62 IO=0 observed; =1 unobserved
cols. 63-67 $\sigma(F_{obs})$

Item 17: Blank card to terminate reflection data

Item 18: Control card 7 (3I5,3F5.3)

This is only used for the Wilson plot. If a Wilson plot is not to be calculated then this card should NOT be included.

cols. 1-5	number of divisions in $\sin\theta$ range (≤ 30)
col. 10	=0 use all reflection data
	=1 omit reflection with $F_{obs} = 0$
	=2 for unobserved reflections (IO=1) use F_o=Fo x factor. This factor should be entered in cols. 26-30.
col. 15	=0 normal operation
	=1 use F_{cal} instead of Σf's
cols. 16-20	minimum value of $\sin\theta$ to be included in Wilson plot (blank=0.0)
cols. 21-25	maximum value of $\sin\theta$ (blank=1.0)
cols. 26-30	a factor to be used in handling unobserved reflections if col. 10 = 2 .

Item 19: OPTION 1: Automatic recycling to obtain better E statistics for the various zones - follow control card 7 (Item 18) with another title card (Item 6) and control card 1 (Item 7) with KN1=2, KN4=2 and KN6=1 . As many sets of title cards and control card 1 should follow as cycles desired. After last card place a !EOD.

OPTION 2: To recycle changing the various weighting factors by hand - follow control card 7 with:

(1) Title card (Item 6)
(2) Control card 1 (Item 7) (with KN1=2 and KN6=0)
(3) Control card 2 (Item 8) (only included if KN4=0 or 1)
(4) Control cards 3 to 6 (Items 9 to 12)
(5) Control 7 (Item 18) (only include if KN4=0 or 1)
(6) As many cycles with either option 1 or 2 as desired may follow ending with !EOD

OPTION 3: If this is the first run you may want to stop after the initial calculation. If this is the case put !EOD after Item 18.

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem. There will be an interactive version of this program at some time in the future.

I. Program language and type: FORTRAN IV - Batch Processing mode

II. Function: To perform Fourier, Patterson, difference Fourier or F_{cal} synthesis.

III. Source: Original program for the IBM 1130 by R. Shiono; revised for the XDS Σ5 by R. Snyder.

IV. Procedure: This program reads F_{obs} in the normal ORFLS input format to perform an F^2 Patterson. To perform either a Fourier, difference Fourier or F_{cal} synthesis the required phases must be calculated by SOFC, SOCRYLS or ORFLS and the file or cards created by these programs should be input.

Electron Density Expression used in the program: The general Fourier series expression for electron density is:

$$\rho\,(XYZ) = \frac{1}{V} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} F\,(hk\ell)\, \exp\,\{-2\pi(hX+kY+\ell Z)\}$$

The program uses the simplified forms of the above expression for each space group, which are listed in the International Tables for X-ray Crystallography, Vol. I, (page 374-525) for standard axial settings. The expressions listed should be further expanded to make all trigonometric functions into the product form of

$\begin{matrix}\cos\\ \sin\end{matrix} 2\pi hX$, $\begin{matrix}\cos\\ \sin\end{matrix} 2\pi kY$, $\begin{matrix}\cos\\ \sin\end{matrix} 2\pi \ell Z$. The phase angle α should be combined with F (hkℓ) to become A(hkℓ) and B(hkℓ). The resulting expression for general case would be

$$\begin{aligned}\rho\,(XYZ) = \frac{1}{V} F(000) + \frac{M}{V} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} \sum_{-\infty}^{\infty} \Big[A(hk\ell) \Big\{ &\Big(\pm \begin{matrix}\cos\\ \sin\end{matrix} 2\pi hX \begin{matrix}\cos\\ \sin\end{matrix} 2\pi kY \begin{matrix}\cos\\ \sin\end{matrix} 2\pi \ell Z\Big)\\ &+\Big(\pm \begin{matrix}\cos\\ \sin\end{matrix} 2\pi hX \begin{matrix}\cos\\ \sin\end{matrix} 2\pi kY \begin{matrix}\cos\\ \sin\end{matrix} 2\pi \ell Z\Big)\\ &+(\ \ldots\ldots\ldots\ \ )\\ &+(\ \text{up to 4 terms}\ \ )\Big\}\\ + B(hk\ell) \Big\{ &\Big(\pm \begin{matrix}\cos\\ \sin\end{matrix} 2\pi hX \begin{matrix}\cos\\ \sin\end{matrix} 2\pi kY \begin{matrix}\cos\\ \sin\end{matrix} 2\pi \ell Z\Big)\\ &+(\ \ldots\ldots\ldots\ \ )\\ &+(\ \text{up to 4 terms}\ \ )\Big\}\Big]\end{aligned}$$

The expression inside the square brackets [ ] is for a type of indices (even, odd) and there may be up to four different expressions to be added together for the electron density. In the above expressions, the Miller indices h, k, ℓ may be positive as well as negative depending on the crystal class. Therefore, for example, in monoclinic class, (hkℓ) and $(\bar{h}k\ell)$ reflexions are represented by the same expression.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g., ECLASS, 7800 (NAME),9)

Item 2: !ASSIGN M:SI, (FILE,SOFOURIER,FSNYDER)

Item 3: !FORTRAN BC, GO

Item 4: !ASSIGN F:1, (FILE,NAME OF DATA FILE FROM LEAST SQUARES), (IN)

If data is to be input from cards, F:1 should be assigned to a file of anyname and be specified as OUTIN rather than IN. After execution this file will contain data information and may be used for future input to Fourier or Least Squares programs.

Item 5: !ASSIGN F:2, (FILE, ANYNAME),(OUTIN) - The point by point electron density summation is written on this file and may be saved for a peak finding program yet to come.

Item 6: !LOAD (GO)

Item 7: !RUN

Item 8: !DATA

Item 9: Control card 1 (5I4,6F5.3,2I4)

col. 4 This specifies which of the values of the input reflexion data are to be used as amplitudes.

digit		
1	Fourier summation	(A_{obs} and B_{obs} are used)
2	F_{cal} Fourier	(A_{cal} and B_{cal} are used)
3	Difference Fourier	(A_{obs}-A_{cal}, B_{obs}-B_{cal} are used)
4	Patterson Function	(F_{obs}^2's are used)

col. 8 Direction of summation. The summation is done section by section in the direction of increasing h_3 axis.

h_1 The direction appears horizontally in the output.

h_2 The direction appears vertically in the output.

h_3 The direction of consecutive sections.

digit	h_1	h_2	h_3
1	h	k	ℓ
2	h	ℓ	k
3	k	h	ℓ
4	k	ℓ	h
5	ℓ	h	k
6	ℓ	k	h

cols. 9 - 12 The highest absolute value of h_2 index. The value is required only when the reflexion data are on disk. The field may be left blank otherwise and the program will find the value when it reads in the data. If a larger value than the actual value is used, it will slow down the calculation.

cols. 16, 20 These two columns specify the tests on indices, if any, to choose a trigonometric combination. If there is only one test, use column 16. For two tests, the first test in column 16 and the second in column 20 (see items 12-15).

digit	indices to be tested
0	no test
1	h
2	k
3	ℓ
4	h+k
5	h+ℓ
6	k+ℓ
7	h+k+ℓ

zone	
cols. 21-25	okℓ
cols. 26-30	hoℓ
cols. 31-35	hko
cols. 36-40	hoo
cols. 41-45	oko
cols. 46-50	ooℓ

Multiplicity factors for different zones. If a zone has equal weight as hkℓ, 1.0 should be used. For half weight, punch 0.5. This arises from the fact that only independent reflexions are used.

col. 54
- 0 card input for reflexion
- 1 reflexion data already on disk (File 1)

col. 58
- 0 reflexion cards in the standard format (A) (see item 16)
- 1 reflexion cards in the alternate format (B)

Item 10: Control card 2 (9F4.2)

This card specifies the starting and ending point of three axial directions with the increments in fractions of a cell.

Minimum increment = .001 .

cols. 1-4 starting value for x
cols. 5-8 ending value for x
cols. 9-12 increment for x

cols. 13-16 starting value for y
cols. 17-20 ending value for y
cols. 21-24 increment for y

cols. 25-28 starting value for z
cols. 29-32 ending value for z
cols. 33-36 increment for z

If only one section is calculated, specify the ending value equal to the starting value with an arbitrary non-zero increment.

NOTE: (No. of grid points in h_1 direction) x (Max. h_2 index + 1) ≤ 1581

No. of grid points in h_1 direction ≤ 150

If any of these limits are exceeded, the program will halt with a message.

EXAMPLE: To calculate x = 0.00 → 0.50 in steps of 0.02
y = 0.00 → 1.00 in steps of 0.04
z = 0.00 → 0.25 in steps of 0.05

the card would contain

.00 .50 .02 .00 1.0 .04 .00 .25 .05

Item 11: Control card 3 (F7.5, F7.2, E10.3, 2I2)

cols. 1-7 scale factor to be applied to the input coefficients; if blank, 1.0 will be assumed

cols. 8-14 a constant to be added to the final sum, for example, F(000)/V.

cols. 15-24 highest density to scale the output to within ± 999.

Normally, you may leave this field blank, then the program will use the highest value actually calculated.

If any value is punched here, the program uses the higher value of the two.

col. 26 =0 input data in format as produced by SOFC or SOCRYLS
=1 input in ORFLS format

col. 28 =0 data in logical unit 1 written by SOFC or SOCRYLS
=1 data from cards

Items 12-15:

Control cards No. 4, 5, 6, 7 (32I2)

These cards specify the signs and the trigonometric functions of triple products for the electron density expression.

If there is no test of indices, that is, all reflexions use the same set of expressions, then Control card No. 4 is used to specify the products and Control cards No. 5, 6 and 7 are blank.

If there is one test of indices, then Control card No. 4 is for the expressions for the even reflexions, and Control card No. 5 is for the odd. Control cards Nos. 6 and 7 are blank.

When there are two tests of indices, then all four cards are used to specify.

	no test	one test	two tests	
			1st test	2nd test
Card No. 4	for all reflexions	even	even	even
5	(blank)	odd	even	odd
6	(blank)	(blank)	odd	even
7	(blank)	(blank)	odd	odd

Within each card, cols. 1-32 are used for A part and cols. 33-64 are for B part of the expression.

The electron density is expressed by one or more of the triple products

$$\begin{matrix}+\\-\end{matrix}\begin{matrix}\cos\\\sin\end{matrix} 2\pi hX \begin{matrix}\cos\\\sin\end{matrix} 2\pi kY \begin{matrix}\cos\\\sin\end{matrix} 2\pi \ell Z$$

and four integers are used to specify each of the products.

The following digits are used

digit	symbol
1	+
2	-
1	cos
2	sin

Eight columns (four digits) each are used to specify a product and up to four products each for A or B part of the expression on each card.

cols. 2, 10, 18, 26	sign of product	
4, 12, 20, 28	cos or sin $2\pi hX$	for A
6, 14, 22, 30	cos or sin $2\pi kY$	
8, 16, 24, 32	cos or sin $2\pi \ell Z$	
34, 42, 50, 58	sign	
36, 44, 52, 60	cos or sin $2\pi hX$	for B
38, 46, 54, 62	cos or sin $2\pi kY$	
40, 48, 56, 64	cos or sin $2\pi \ell Z$	

If there is only one term for example, then cols. 1-8 are used to specify A (hkℓ) part and cols. 34-40 are used for B (hkℓ) part. Any unused field should be left blank.

For Patterson function, an appropriate expression for it should be specified (International Tables, Vol. I, p. 526).

Examples:

i) Space group $P\bar{1}$, no test of indices

$$\zeta(XYZ) = \frac{2}{V} \sum\sum\sum F(hk\ell) \cos 2\pi(hX+kY+\ell Z)$$

(Intn'l. Tables, Vol. I, p. 374)

The trigonometric part without the constant term is expanded into

$$\begin{aligned} &+ \cos 2\pi hX \cos 2\pi kY \cos 2\pi \ell Z \\ &- \cos 2\pi hX \sin 2\pi kY \sin 2\pi \ell Z \\ &- \sin 2\pi hX \cos 2\pi kY \sin 2\pi \ell Z \\ &- \sin 2\pi hX \sin 2\pi kY \cos 2\pi \ell Z \end{aligned}$$

Accordingly, Control card No. 4, cols. 1-32 are

1 1 1 1 2 1 2 2 2 2 1 2 2 2 2 1

cols. 33-64 are blank

Cards No. 5, 6 and 7 are all blanks (these cards must be present)

ii) Space group $P2_1/c$, one test (Intn'l. Tables, Vol. I, P. 383)

The expanded expression for A (hkℓ) parts are

$k+\ell = 2n$ + cos2πhX cos2πkY cos2πℓZ - sin2πhX cos2πkY sin2πℓZ

$k+\ell = 2n+1$ - sin2πhX sin2πkY sin2πℓZ - cos2πhX sin2πkY sin2πℓZ

Control card No. 4 cols. 1-16 1 1 1 1 2 2 1 2
No. 5 cols. 1-16 2 2 2 1 2 1 2 2
No. 6&7 blank

iii) Space group $P2_1$ (2nd setting) one test (Intn'l. Tables Vol. I, p. 375)

$k = 2n$ + A (cos2π hX cos2πkY cos2π ℓZ - sin2πhX cos2πkY sin2πℓZ)
+ B (cos2π hX sin2πkY cos2π ℓZ - sin2πhX sin2πkY sin2πℓZ)

$k = 2n+1$ - A (sin2π hX sin2πkY cos2π ℓZ + cos2πhX sin2πkY sin2πℓZ)
+ B (sin2π hX cos2πkY cos2π ℓZ + cos2πhX cos2πkY sin2πℓZ)

For this specification, the signs in front of A or B should be transferred into the products in the brackets since each terms are added algebraically.

Control card No. 4 cols. 1-16 1 1 1 1 2 2 1 2
cols. 33-48 1 1 2 1 2 2 2 2

Control card No. 5 cols. 1-16 2 2 2 1 2 1 2 2
cols. 33-48 1 2 1 1 1 1 1 2

Control cards Nos. 6 & 7 all blank

iv) Space group $P2_12_12_1$, two tests (Intn'l Tables, Vol. I, p. 386)

h+k = 2n	+ cos2πhX cos2πkY cos2π ℓZ	for A (hkℓ)
k+ℓ = 2n	- sin2π hX sin 2πkY sin2π ℓ Z	for B (hkℓ)
h+k = 2n	- cos2πhX sin2πkY sin2π ℓ Z	for A (hkℓ)
k+ℓ = 2n+1	+ sin2π hX cos2πkY cos2π ℓ Z	for B (hkℓ)
h+k = 2n+1	- sin2πhX cos2πkY sin2π ℓ Z	for A (hkℓ)
k+ℓ = 2n	+ cos2πkY sin2πk Y cos2πℓ Z	for B (hkℓ)
h+k = 2n+1	- sin2πhX sin2πkY cos2πℓZ	for A (hkℓ)
k+ℓ = 2n+1	+ cos2πhX cos2πkY sin2πℓZ	for B (hkℓ)

Control card No. 4 cols. 1-8 1 1 1 1 cols. 33-40 2 2 2 2
No. 5 cols. 1-8 2 1 2 2, cols. 33-40 1 2 1 1
No. 6 cols. 1-8 2 2 1 2, cols. 33-40 1 1 2 1
No. 7 cols. 1-8 2 2 2 1, cols. 33-40 1 1 1 2

Item 16: Reflexion data if not on file

A. Data as punched by SOFC or SOCRYLS or SOWILSON (3I4, 6F7.2, F5.3, I3)

cols. 1-4 h cols. 5-8 k cols. 9-12 ℓ cols. 13-19 F_{obs}

cols. 20-26 F_{cal} cols. 27-33 A_{obs} cols. 34-40 A_{cal}

cols. 41-47 B_{obs} cols. 48-54 B_{cal} cols. 55-59 $\sin\theta$

col. 62 IO=0 observed reflexion; =1 unobserved

cols. 63-69 $\sigma(F_{obs})$

B. Data in standard ORFLS input format as produced by all data reduction programs.

cols. 1-9 h cols. 10-18 k cols. 19-27 ℓ cols. 28-36 F_{obs}

cols. 37-54 $\sigma(F_{obs})$ cols. 53-54 scale factor designation (not used)

col. 59 IO=0 observed reflection; =1 unobserved

Item 17: Blank card to terminate data

Item 18: !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign this file to M:SI and call the BPM subsystem. An interactive version of this program will be available at some time in the future.

I. Program language and type: FORTRAN IV - Batch Processing mode

II. Function: To calculate structure factors, for up to 100 atoms, to test a structure model or for Fourier input.

III. Source: Original program by R. Shiono for the IBM 1130; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: This program is essentially similar to SOCRYLS. The input for both of these programs and for ORFLS are similar.

V. Data set up:

Item 1: !JOB Users account information and priority (e.g., ECLASS, 7800 (NAME),9)

Item 2: !ASSIGN F:1, (FILE,NAME OF REFLECTION DATA FILE IF AVAILABLE)(INOUT)

If a reflection file has not already been created this program will create one on unit 1. Assign it to file of any name with paramater OUTIN.

Item 3: !RUN (LMN,LMFC,FSNYDER)

Item 4: !DATA

Item 5: Cell parameter (3F7.3,4F7.4)

cols. 1-7	$\overline{a}$ (Å)
cols. 8-14	$\overline{b}$
cols. 15-21	$\overline{c}$
cols. 22-28	cos (α)
cols. 29-35	cos (β)
cols. 36-42	cos γ
cols. 43-49	λ

Item 6: Control card 1 (3I5)

col. 5	=0 reflection data in ORFLS format for data reduction program
	=1 reflection data as output by SOFC, SOCRYLS, or SOWILSON
col. 10	=0 data from cards to be input here
	=1 data on logical unit number 1

If col. 5 and col. 10 are 1 the input file already contains f values; thus, the next item to include is Control card 2 (Item 11).

col. 15 =0 just write output on unit 1
=1 write on unit 1 and punch calculated structure factors in SOFOURIER input format

Item 7: Atomic scattering factors (8(7F10.4/)) only included if data is from cards. X-ray scattering factors for $\sin\theta$ =0.0 to 1.0 in steps of .02 on eight cards for each element in ORFLS format. These should be prepared by using program SOFORMF (see II C2 of this write up).

Item 8: Blank card to terminate reading of f's .

Item 9: Reflection data if input from cards only.

If col. 5 Item 6=0 data in standard ORFLS input format.

cols. 1-9 h cols. 10-18 k cols. 19-27 ℓ cols. 28-36 F_{obs}

cols. 37-45 σ (F_{obs}) may be blank col. 59 IO=0 observed reflection; =1 unobserved

If col. 5 Item 6=1 data was punched by SOFC, SOCRYLS or SOWILSON

cols.1-4 h cols. 5-8 k cols. 9-12 ℓ cols. 13-19 F_{obs}

col. 62 IO=0 observed reflection; =1 unobserved cols. 63-69 $\sigma(F_{obs})$

Item 10: Blank card to terminate reading of reflections

Item 11: Control card 2 (7I5)

col. 5 0 centrosymmetric
1 non-centrosymmetric
cols. 6-10 number of symmetry cards (≤ 24)
cols. 13-15 number of atoms (coordinate cards) used (≤ 100)
col. 20 0 isotropic, anisotropic temperature factors or mixture of both.
1 (no effect in this program)

col. 25 0 normal structure factor calculation mode.
1 partial structure factor calculation. The A_c, B_c's on the input are added to the newly calculated values. For this mode, the input data must be the output of a previous calculation. Contributions of atoms may be added to or subtracted from the already calculated values.

col. 30 0 normal mode
1 punch A_c and B_c parts based on the E values, rather than the actual A_{cal} and B_{cal}. (for E card input only)

col. 35 0 final F_{obs}' are automatically scaled to F_{cal}'s
1 suppress the rescaling and keep F_{obs} unchanged

Item 12: Symmetry cards (F11.6, 2I2, F11.6, 2I2, F11.6, 2I2)

This is the common format for all programs described in this write up.

If centrosymmetric, only those not related by the center of symmetry are required. Those symmetry related by pure translation may be handled by increasing the occupancy factors for the atomic parameter cards. The identity relation, x, y, z must be present.

Symmetry	Digit to be punched
0	blank
x	1
-x	-1
y	2
-y	-2
z	3
-z	-3

cols. 1-11	translation for a direction
cols. 12, 13	symmetry for a axis direction
cols. 14, 15	
cols. 16-26	translation for b
cols. 27-28	symmetry for b direction
cols. 29-30	
cols. 31-41	translation for c direction
cols. 42, 43	symmetry for c direction
44, 45	

Where there is only one symmetry symbol to punch, either one of two fields may be used.

Item 13: Scale factor card (F9.6)

An overall scale factor to be multiplied by the F_{obs} values. If you are inputing a disk file from a previous run, the F_{obs} is already scaled; use 1.0 .

Item 14: Atomic parameter cards (2 cards per atom)

The format is common to all the programs described in this write up.

Up to 100 atoms may be used in one run. If more than 100 are necessary, the calculation may be split into two or more runs and each contribution may be added by use of the partial structure factor calculation mode. This partial mode enables you to speed up the calculation when it is necessary to change only a part of the structure and the remainder is unchanged.

a) Positional parameter card (A4, A2, 3X5F9.6, 14X I2)

cols. 1-6	any six Hollerith characters (or blank) for identification
cols. 10-18	atomic scattering factor identifier (1.0~10.0). This corresponds to the order of atomic scattering factor tables being read in.

cols. 19-27 multiplier or occupancy factor a_i, usually 1.0 . This may be used for adjusting F_{cal}'s in a non-primitive cell.

cols. 28-36 x (fractional coordinate)
cols. 37-45 y
cols. 46-54 z
col. 70 If a 1 is punched here, this atom contribution will be subtracted from A_c and B_c This may be used to replace an atom with the partial mode calculation.

b) Thermal parameter card (6F9.6)

cols. 1-9 isotropic temperature factor B or β_{11}
cols. 10-18 β_{22} (this field must be zero (blank)for an isotropic temperature factor)
cols. 19-27 β_{33}
cols. 28-36 β_{12}
cols. 37-45 β_{13}
cols. 46-54 β_{23}

The program identifies an isotropic temperature factor by testing β_{22} field.

The above two cards (a) and (b) are always paired in that order. The expression for the anisotropic temperature factor is

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

Item 15: !EOD

VI. BPM execution: If the above items are punched on cards, submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem. An interactive version of this program will be available at a future time.

SOCRYLS

I. Program language and type: FORTRAN IV - Batch Processing mode

II. Function: Carry out a block-diagonal least squares structure refinement on up to 50 atoms.

III. Source: Original program for the IBM 1130 by R. Shiono; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: This program calculates structure factors for a given set of reflections with atomic coordinates and symmetry relations. It also refines the atomic parameters by the method of least-squares using the block-diagonal approximation. The algorithm for the procedure is explained, for example, by J. S. Rollett in "Computing Methods in Crystallography," (Editor, J. S. Rollett, 1965) page 67.

The blocks used are 2 x 2 for scale factor and over-all temperature factor, 3 x 3 for positional parameters and 2 x 2 or 7 x 7 for occupancy factor and isotropic or anisotropic temperature factors.

In order to handle atoms in special positions, subroutine entries are provided for the user to write his own subroutines. In this way, any necessary constraint to the parameters may be introduced.

Card formats used in the program are common with all other related programs and only minimum amount of hand punching is required.

For the purpose of calculating structure factors only without any refinement, a separate program SOFC is available which enables twice as many atoms to be used in one pass.

V. Data set up:

Item 1: !JOB Users Account information and priority (e.g., ECLASS, 7800 (NAME),9)

Item 2: !ASSIGN F:1, (FILE, NAME OF REFLECTION DATA FILE), (INOUT)

If data are from cards assign F:1 to any file and specify OUTIN.
At end of this run file will contain data information.

Item 3: !RUN (LMN,LMCRYLS)

Item 4: !DATA

Item 5: Cell parameters (3F7.3, 4F7.4)

cols. 1-7 $\bar{a}$ (Å) cols. 8-14 $\bar{b}$ cols. 15-21 $\bar{c}$ cols. 22-28 $\cos(\alpha)$

cols. 29-35 $\cos(\beta)$ cols. 36-42 $\cos(\gamma)$ cols. 43-49 λ

Item 6: Control card 1 (3I1, 2X, 3I5, 6F8.4)

col. 1	=0 reflection data on disk file 1 ; Control card 2 (Item 11) follows this item
	=1 reflection data from cards
col. 2	=0 reflection data in ORFLS input format from data reduction programs
	=1 reflection data produced by SOFC, SOCRYLS
col. 3	=0 write results on disk file 1
	=1 write on disk file 1 and punch results
col. 10	=0 weights taken as $1/\sigma^2$ from σ's supplied with reflection data
	=1 Hughes' weighting scheme; requires F_{min} in cols. 21-28
	=2 Cruickshank's weighting scheme, A, B and C are required
	=3 $W = 1/(\sin\theta/\lambda)$
	=4 constant weight of 1.0
cols. 21-28	A for Cruickshank's scheme or F_{min} for Hughes' scheme
cols. 29-36	B for Cruickshank's scheme
cols. 37-44	C for Cruickshank's scheme
cols. 45-52	D } any information which may be desired in a user
cols. 53-60	E } supplied subroutine--not used by normal program
cols. 61-68	F }

NOTE: On weighting schemes used in Program:

In the calculation, the weight of each reflection ω is taken as $\omega = 1/(\sigma)^2$. If $\sigma = 0$, then the program sets $\omega = 0$. What you punch on the reflection data cards or calculate in execution time according to some scheme and written on the intermediate tape are σ's and not ω. The program will derive ω from σ each time needed.

Some of the commonly used weighting schemes are built in the program and may be specified on Control Card No. 1. F_{obs} values used here are those on the input data cards and they are not affected by the scale factors you provide in the calculation.

i) Hughes' scheme

E. W. Hughes (1941) J. Amer. Chem. Soc. 63, 1737

$$\omega = 1/|F_o|^2 \quad \text{if} \quad F_o \geq 4F_{min}$$

$$\omega = 1/|4F_{min}|^2 \quad \text{if} \quad F_o < 4F_{min}$$

$$\omega = 0 \quad \text{if} \quad F_o = 0 .$$

ii) Cruickshank's scheme

"Computing Methods and the Phase Problem in X-ray Crystal Analysis," Edit. Pepinsky et al (1961) p. 45

$$\omega = 1/(A + BF_o + CF_o^2) .$$

You may alter the weights by using the subroutines MODIFY and RSETW if so desired.

If the disk file input is used, you may use RSETW only, since the first part of the program is completely bypassed.

Item 7: Atomic scattering factors ((8(7F10.4)) (only included if data is from cards)

X-ray scattering factors for $\sin\theta = 0.0$ to 1.0 in steps of .02 on eight cards for each element in ORFLS format. These should be prepared by executing program SOFORMF (see II C 2 of this write up).

Item 8: Blank card to terminate reading of f's .

Item 9: Reflection data if input from cards only.
If col. 2 of Item 6 = 0 data in standard ORFLS input format

col. 1-9 h cols. 10-18 k cols. 19-27 ℓ cols. 28-36 F_{obs}

cols. 37-45 $\sigma(F_{obs})$ may be blank if col. 10 Item 6 is non zero.

col. 59 IO = 0 observed reflection, = 1 unobserved.

If col. 2 of Item 6 = 1 data prepared by SOFC or SOCRYLS

col. 1-4 h cols. 5-8 k cols. 9-12 ℓ cols. 13-19 F_{obs}

col. 62 IO = 0 observed reflection, = 1 unobserved

cols. 63-69 $\sigma(F_{obs})$ may be blank if col. 10 Item 6 is non zero.

Item 10: Blank card to terminate reading of reflection data.

Item 11: Control card 2 (4I5)

col. 5
- 0 (blank) centro-symmetric
- 1 non-centrosymmetric

cols. 9-10 number of symmetry cards (≤ 24) - If centrosymmetric, only those not related by a center are required. For a face or body-centered lattice, only those not related by pure translations are necessary. However, you have to adjust the multiplier (occupancy) on parameter cards to obtain the $F_{cal's}$ on absolute scale.

col. 15
- 0 (blank) normal, isotropic, anisotropic temperature factors may be intermixed.
- 1 All isotropic temperature factors will be converted to anisotropic mode before refinement. Parameter selection cars should be made for anisotropic temperature factors. Those that are already anisotropic remain unchanged.

Item 12: Control card 3 (4I5)

col. 5 number of refinement cycles
0 (zero) for structure factor calculation only

cols. 9-10 number of atoms used (≤ 50)
If more than 50 are needed, use the partial mode calculation.

col. 15	0 (blank)	new calculation
	1	partial calculation Previously calculated A_{cal} and B_{cal} on the input are added to the current calculation. This required A_c and B_c on the input.

Item 13: Control card 4 (4F9.6)

Unlike the full matrix refinement, the block-diagonal approximation refinement will generally give the parameter shifts too large and necessitate the use of damping factors. This card specifies the damping factors for the following shifts. Generally a value of 0.5 ~ 0.75 will be adequate.

cols. 1-9	factor for the overall scale factor shift If this is zero, the scale factor will be held constant.
cols. 10-18	factor for the overall temperature factor shift If this field is zero, no overall temperature factor shift is applied.
cols. 19-27	factor for positional parameter shifts. If this field is left blank (zero), the program assumes the value of 0.75.
cols. 28-36	factor for the thermal parameters and the occupancy (multiplier) factor shifts If this field is left blank, the program assumes the value of 0.75.

If no refinement is made, just use a blank card.

Item 14: Symmetry cards (F11.6, 2I2, F11.6, 2I2, F11.6, 2I2)

This is the standard format used in all programs in this write up. For a centrosymmetric structure, those symmetry relations related by a center are not required. The identity relation x. y. z is always necessary.

symmetry	digit to be punched
0	blank
x	1
-x	-1
y	2
-y	-2
z	3
-z	-3

cols. 1-11 translation for $\bar{a}$ direction	$\overbrace{12,13}$	$\overbrace{14,15}$ symmetry for $\bar{a}$ direction	16-26 translation for $\bar{b}$ direction	$\overbrace{27,28}$	$\overbrace{29,30}$ symmetry for $\bar{b}$ direction
cols. 31-41 translation for $\bar{c}$ direction	$\overbrace{42,43}$	$\overbrace{44,45}$ symmetry for $\bar{c}$ direction			

When there is only one symmetry symbol to punch, either one of two fields may be used.

Item 15: Scale factor card (F9.6)

The scale factor will multiply the F_{obs} values.
If data is from disk the F_{obs} have already been scaled and the factor should be close to 1 .

Item 16: Atomic parameter cards

The format is common to all other programs in this write up.

a) Postional Parameter Card (A4, A2, 3X5F9.6, 14X I2)

cols. 1-6	any 6 Hollerith characters (or blank) for indentification.
cols. 10-18	atomic scattering factor identifier (1.0 ~ 10.0) This corresponds to the order of atomic f tables being read in item 7.
cols. 19-27	multiplier or occupancy a_i , usually 1.0 .
cols. 28-36	x (fractional coordinate)
cols. 37-45	y
cols. 46-54	z
col. 70	If a 1 is punched here, this atom contribution will be subtracted from A_c and B_c . This may be used to replace an atom in the partial mode calculation.

b) Thermal Parameter Cards (6F9.6)

cols. 1-9	isotropic temperature factor B or β_{11}
cols. 10-18	β_{22}
cols. 19-27	β_{33}
cols. 28-36	β_{12}
cols. 37-45	β_{13}
cols. 46-54	β_{23}

The program identifies an isotropic temperature factor by testing β_{22} field being zero.

The above two cards are always paired for each atom.

Item 17: Parameter selection cards (8011)

These cards specify which of the parameters are to be refined or varied. Ten columns each are allocated for each atom, thereby eight atoms may be specified by a card. Continue to next card for more atoms. The order of atoms here should correspond to the order of atomic parameter cards read.

Punch 1 for refinement and leave blank for fixed parameter.

cols.	1	2	3	4	5	6	7	8	9	10
	x_i	y_i	z_i	a_i	$B(\beta_{11})$	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}

Each column has a fixed designation to a parameter, i.e., columns 1, 11, 21, 31, etc. always refer to x. Use as many cards as necessary.

Item 18: !EOD

NOTE: After each refinement cycle the new parameters are punched on cards.

VI. BPM execution: If the above items are punched on cards submit them at the Computing Center. If built on a file assign it to M:SI and call the BPM subsystem. Be careful about the number of cycles asked for and your priority--this program can run into a number of hours of execution time.

SODIST

I. Program language and type: FORTRAN IV - Batch Processing mode - requires standard coordinate file.

II. Function: To calculate all distances and angles, between user set limits, for any set of atomic coordinates and symmetries.

III. Source: Original program by S. Chu for the IBM 7090; revised for the IBM 1130 by R. Shiono; revised for the XCS Σ 5 by R. Snyder.

IV. Procedure: Given a set of atomic coordinates with the unit cell dimensions and the symmetry relations, this program calculates all possible distances of less than a specified maximum value between two atomic positions. The program generates the coordinates of symmetry related positions and also those with the translation of one unit cell length in one or more of the three axial directions to scan for the total of 27 sets of translations.

In order not to miss a distance shorter than the given maximum, the program first translates all those original coordinates beyond ± 1/2 of the unit cell by adding or subtracting one to or from the coordinates. All coordinates are translated back to the original after the calculation for the output.

The distances are calculated from the atomic position i (original) to the atomic positions 1 through N and their symmetry related positions with or without twenty-seven different sets of translations applied.

Because of the way in which the program generates the coordinates, sometimes not all the distances calculated in the part from an atom i to an atom j, will be duplicated in the part from the atom j to the atom i, or vice versa. Therefore, for the complete set of distances around an atom, not only the particular part of the output, but also the rest of the distance output should be examined.

The angles are calculated by forming two sides with all possible combinations of the lines around an atom, which have been formed in calculating distances in the first part.

The maximum distance to be used as a side to form an angle may be specified independently as less than the maximum used for distance calculation. This will reduce the number of angles calculated.

V. Data set up: This program requires the full standard coordinate file described in the introduction of this write up on logical unit 10. All symmetry relations must be supplied including those related by centers of symmetry and non primitive Bravais lattices. If only the distances among the coordinates supplied are desired then only the identity operation X, Y, Z need be entered.

Item 1: !JOB Users account information and priority (e.g., ECLASS,7800(NAME),9)

Item 2: !ASSIGN F:10, (FILE,NAME OF COORDINATE FILE),(IN)

Item 3: !ASSIGN F:1, (FILE,JUNK),(OUTIN),(REL)
This is a scratch file required by calculations.

Item 4: !RUN (LMN,LMDIST,FSNYDER)

Item 5: !DATA

Item 6: Control card (4I1,3F6.2)

col. 1	IAGL =0	distance calculation only
	=1	distance and angles
	=2	calculate angles and suppress output of distances
col. 2	ITRN =0	all 27 translations applied
	=1	no translations applied--the program uses the original coordinates with only the symmetry relations applied.
col. 3	ISOR =0	calculated distances will be printed in groups of same ending atoms
	=1	for each starting atom distances will be sorted in increasing magnitude
col. 4	NCARD =0	only position parameters appear on coordinate file
	=1	thermal parameters are interspersed with coordinates on file 10
cols. 5-10	DMAX =	the maximum distance to be calculated
cols. 11-16	DMIN =	the minimum distance to be included (may be zero)
cols. 17-22	DANG =	the maximum distance to be used in angle calculation (to reduce the very large numbers of angles generated) If left blank, DMAX will be used.

Item 7: !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file, assign it to M:SI and call the BPM subsystem.

SOTRANS

I. Program language and type: FORTRAN IV - Batch Processing mode - requires the standard coordinate file.

II. Function: To calculate the symmetry generated positions of a set of coordinates in the central cell and all 27 adjacent cells and output them in angstroms--to be used in building structure models.

III. Source: Original program for the XDS Σ 5 by R. Snyder.

IV. Procedure: Each atomic position is symmetry transformed within a central unit cell and then translationally transformed into all 27 adjacent cells. The coordinates are converted to Angstroms and output. The results are a convenient reference for use in building models of crystal structures based on a 1 inch/Å scale.

V. Data set up: This program requires the standard coordinate file described in the introduction to be input on unit 10. The full symmetry set is required.

Item 1: !JOB Users account information and priority (e.g., ECLASS,7800(NAME),9)

Item 2: !ASSIGN M:SI, (FILE,SOTRANS,FSNYDER)

Item 3: !FORTRAN LS, GO

Item 4: !ASSIGN F:10, (FILE,NAME OF STANDARD COORDINATE FILE)

Item 5: !ASSIGN F:1, (FILE, JUNK),(OUTIN),(REL)
This is a scratch file required by the program.

Item 6: !LOAD (GO)

Item 7: !RUN

Item 8: !DATA

Item 9: Control card (2I1)

col. 1	=0	coordinates only on file 10
	=1	temperature parameters interspersed with coordinates
col. 2	=0	calculate for all 27 adjacent cells
	=1	calculate positions only in the 555 cell

Item 10: !EOD

VI. BPM execution: If the above items are punched on cards submit at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem. There will be an interaction version of this program at some future date.

SODIFGEN

I. Program language and type: FORTRAN IV – Batch processing mode.

II. Function: To generate diffractometer settings for the collection of single crystal diffraction data.

III. Source: Original program for the IBM 1130 by E. L. McGandy and N. C. Seeman; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: The full description of this program is available as published by the Crystallography Department, University of Pittsburgh, Pa. 15213, under the title "DIFN4: an IBM 1130 Fortran Program to Generate Diffractometer Setting Cards," January 1969 by E. L. McGandy and N. C. Seeman. This description is quite useful and also may be obtained from R. Snyder. The program can perform a large number of functions, many of which do not apply to the generation of settings for our GE single crystal orienter in θ-2θ scan mode. Thus the data set up given here ignores many unrelated items and uses fixed input items for a number of parameters.

V. Data set up:

Item 1: !JOB Users account information and priority
(e.g., ECLASS,7800(NAME),9)

Item 2: !ASSIGN M:SI, (FILE,SODIFGEN)

Item 3: !FORTRAN BC,GO

Item 4: !ASSIGN F:10, (FILE,JUNK),(OUTIN),(REL)

This is a scratch file used by program.

Item 5: !LOAD (GO)

Item 6: !RUN

Item 7: !DATA

Item 8: Title card cols. 1-72 any alphameric information

Item 9: Control card all parameters in I format (2(1X,3I1),18I4)

col. 2	= most rapid varying index 1=h, 2=k, 3=ℓ
col. 3	= second most rapid varying index 1=h, 2=k, 3=ℓ
col. 4	= slowest moving index 1=h, 2=k, 3=ℓ
col. 6	= most rapid varying angle 1=d, 2=χ, 3=λ d*
col. 7	= second most rapid varying angle 1=d, 2=χ, 3=λ d*
col. 8	= slowest moving angle 1=φ, 2=χ, 3=λ d*
col. 12	= 0 read the h k ℓ's whose angles are desired from cards
	= 1 generate all h k ℓ's
col. 16	= 0 ignore limits on φ, χ, and λ d*
	= 1 observe limits

cols. 27-28	number of extinction routines to use = 0 use all h k ℓ's generated = 1 $P2_1$, = 2 $P2_1/c$, = 3 $P2_1\,2_1\,2_1$, = 4 Fd3 the user may supply his own extinctions by modifying subroutine XTINC
col. 44	= number of reference reflections to be used (0 to 20)
col. 48	= number of reflections to be printed between references
col. 52	= 2
cols. 55-56	= 75
cols. 58-60	= 100
cols. 63-64	= 75
col. 68	= 0
cols. 70-72	= sequence number of first reflection to be generated (usually 1)
col. 76	= 1
col. 80	= 0 end program when through = 1 go back to Item 8 and read a new set of control cards

Item 10: Cols. 1-10 λ - wavelength of radiation desired (.71068 or 1.5418)

Item 11: Known reflection information--at least <u>three</u> non co-planer reflections, one to a card, must be specified to allow calculation of the orientation matrix. (3F5.0, 3F10.5)

col. 5 h col. 10 k col. 15 ℓ
cols. 16-25 d setting cols. 26-35 χ cols. 36-45 2θ

Item 12: Terminate reading known reflection cards.

col. 2 = 1

Item 13: B-Matrix card (9F8.7) 9 elements; order: B_{11}, B_{21}, B_{31}, B_{12}, B_{22}, B_{32}, B_{13}, B_{23}, B_{33}

This matrix specifies upper limit, lower limit, and stepping interval of h, k, and ℓ scanning.

	col.	low limit	col.	high limit	col.	step
h	1-8	B_{11}	25-32	B_{12}	49-56	B_{13}
k	9-16	B_{21}	33-40	B_{22}	57-64	B_{23}
ℓ	17-24	B_{31}	41-48	B_{32}	65-72	B_{33}

Example: To scan h from -7 to +7, k from -12 to -4 in steps of 2, and to hold ℓ constant at +2 use this card:

-7	-12	2	7	-4	2	1	2	1
h	k	ℓ	h	k	ℓ	h	k	ℓ
low limit			high limit			step		

Notice that even though ℓ is not to change, a non-zero step must be used.

A blank card is satisfactory if hkℓ are not used as limits for generating reflections.

Also, if one wishes to segment the calculation and the scan sequence (columns 2, 3, 4 on control card) is 231, the run could be divided into two groups on h with two cards:

-7	-12	2	0	-4	2	1	2	1
0	-12	2	7	-4	2	1	2	1

Also note that for generating concentric spherical shells, limits of all three indices hkℓ must pass through zero, even for the outer shells.

Item 14: C-Matrix card (9F8.7)

Nine elements; order: C_{11}, C_{21}, C_{31}, C_{12}, C_{22}, C_{32}, C_{13}, C_{23}, C_{33}.

This matrix specifies upper limit, lower limit, and stepping interval of Φ, χ and d* scanning ranges.

	col.	low limit	col.	high limit	col.	step
Φ	1-8	C_{11}	25-32	C_{12}	49-56	C_{13}
χ	9-16	C_{21}	33-40	C_{22}	57-64	C_{23}
λd*	17-24	C_{31}	41-48	C_{32}	65-72	C_{33}

Example: To scan Φ from 90° to 270° in two quadrant-steps, χ from 90° to 180° in one step, and λ d* from 0.50 to 0.80 in 0.15 steps, use this card:

89	89	0.50	271	181	0.80	91	92	0.15
Φ	χ	λ d*	Φ	χ	λ d*	Φ	χ	λ d*
low limit			high limit			step		

Notice that slightly larger angular ranges have been used to insure inclusion of axial reflections. Be sure that step values add to the low limit to give exactly the high limit.

As in the B-matrix card, never use zero step values.

Item 15: Reference reflections (1X,3I3)

cols. 2-4 h cols. 5-7 k cols. 8-10 ℓ

Item 16: Reflection cards (1X,3I3)

Same as reference reflections. The contents of columns 1 and 11-80 are irrelevant.

Item 17: !EOD

VI. BPM execution: If the above items are punched on cards submit them at the Computer Center. If they are built on a file assign it to M:SI and call the BPM subsystem. There are plans to have an interactive version of this program available at some future date.

CELREF

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: Refine lattice parameters and index diffraction data giving standard deviations from $\theta, 2\theta$ or d values.

III. Source: Original program by D. Appelman; revised for the XDS $\Sigma 5$ by R. Snyder.

IV. Procedure: This program is also available to be run under the Batch Processing mode and is described in section III B2 of this write up under the name LMCELREF.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:5,(DEVICE,CRAØ3)

Item 3: !ASSIGN F:6, (DEVICE,LPAØ2)

Item 4: !RUN (LMN,CELREF,FSNYDER)

Item 5: !DATA

Item 6 - Item 12 are described in section III B2 and apply here.

VI. XRAY execution: The card deck must be submitted at the Computer Center with instructions that it is to be run on the XRAY system at night.

DATAP

I. Program language and type: FORTRAN IV - large XRAY system only

II. Function: General Data reduction program--takes raw diffractometer intensity and background measurements, applies Lp and Gaussian absorption corrections and sets quantities for applying the Zachariasen extinction correction.

III. Source: Original program for the CDC 6600 by P. Coppens, revised by W. C. Hamilton. Revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: Diffractometer intensity information for either Xrays or neutrons are input and Lp corrections applied. The optional absorption correction is by numerical Gaussian integration (Acta Cryst. 18, 1035 (1965)). The necessary quantities for making extinction corrections in the Zachariasen approximation are calculated (Acta Cryst. A26, 71 (1970) and 23, 558 (1967)).

For a full description of program and input parameters execute the following cards on the BPM system:

Item 1: !JOB Users account information and priority
(e.g., ECLASS,7800(NAME),9)

Item 2: !PCL

Item 3: COPY SODATAP ON LP

Item 4: END

Item 5: !EOD

The instructions will be listed on the line printer.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:2,(FILE,ANY NAME),(OUT)
This file will contain the structure factors in ORFLS format - BCD

Item 3: !ASSIGN F:4,(FILE,ANY NAME),(OUT)
This file if requested will contain the binary input information for the least squares program.

Item 4: !RUN (LMN,DATAP,FSYNDER)

Item 5: !DATA

Item 6: Title card (1X79H)
cols. 2-80 any title information

Item 7: Cell constants (7F9.6)

cols. 1-9 $\bar{a}$ or a* cols. 10-18 $\bar{b}$ or b* cols. 19-27 $\bar{c}$ or c*

cols. 28-36 α, α*, cos(α) or cos(α*) cols. 37-45 β, β*, cos(β) or cos(β*)

cols. 46-54 γ, γ*, cos(γ) or cos (γ*) cols. 55-63 λ

Item 8: Reflection cards for calculation of orientation matrix

A. Blank card

B. Angle zero settings (4F9.4)

cols. 1-9 φ zero ccls. 10-18 ω zero cols. 19-27 2θ zero

cols. 28-36 χ zero

C. Three cards specifying the diffractometer settings of three non-coplaner reflections (3(3F9.0,4F9.4/))

cols. 1-9 h cols. 10-18 k cols. 19-27 ℓ

cols. 28-36 observed φ cols. 37-45 observed ω

cols. 46-54 observed 2θ cols. 55-63 observed χ

D. repeat C for reflection 2

E. repeat C for reflection 3

Item 9: Control integers (16I5) ICN(I), I=1,16

col. 5
=0 no absorption corrections
=1 absorption corrections applied--crystal boundary planes described by h, k, ℓ indices and D in cm

col. 10
=0 skip extinction features
=1 calculate extinction parameters necessary for least squares extinction refinement (not allowed in XRAY version of ORFLS)

col. 15
=0 do not call scale subroutine
=1 scale data relative to standards collected during data collection

col. 20
=0 normal operation
=1 calculate distance between given pairs of vertices (see Item 11); vertex cards must follow crystal plane card

col. 25
=0 for Xray data
=1 neutron data

col. 30
=0 no punched output or BCD tape 2
=1 punch cards in ORFLS input format
=2 write tape 2 in ORFLS input format

col. 35 =-1 no output on binary tape 4
= 0 new binary tape 4 will be written
= 1 update an old tape 4--adds new reflections to end

col. 40 = 0 input from cards --format controlled by subroutine IMP

col. 45 = 0 normal operation
= N to check setting angle calculation; if non zero, this card should be followed by N cards in 3F3.0, F9.3 format containing h, k, ℓ and true ω (corrected for the ω zero setting)

col. 50 = 0 always

cols. 51-80 contain ICN(I), I=11, 16 which are not used by program but may be used for any purpose in the user supplied subroutines

Item 10: Supply only if col. 5, Item 9=1

A. Specification of Gaussian Grid for absorption or extinction corrections.

The number of Grid points in the directions $\bar{a}$, $\bar{b}$ and $\bar{c}$ must be such that their product is less than 5000. The number of points in any direction ($\bar{a}$, $\bar{b}$ or $\bar{c}$) must be an even number between 2 and 32. (4I5)

cols. 1-5 number of Grid points along $\bar{a}$
cols. 6-10 number of Grid points along $\bar{b}$
cols. 11-25 number of Grid points along $\bar{c}$
cols. 26-30 number of boundary planes NB

B. (4F10.6) one card for each of the NB boundary planes.

Boundary planes are given in terms of the Miller indices of the faces of the crystal and the perpendicular distances in cm to these planes from an arbitrary origin within the crystal.

Item 11: Supply only if col. 20, Item 9=1

Calculation of distance between theoretical intersection of vertices. The Vertex numbers must be known. Since the program prints these numbers, this option can only be run on a second or later pass. It is intended only as a check.

Item 12: Reflection batch card (I5, 7F10.5)

cols. 1-5 IQ = scale factor number. IQ will be punched on output cards if NSCALE is set to 1 in IMPD.

cols. 16-25 C(1) - the program will calculate σ^2 (I-B) (observed variance) as (I+B) + C(1)^2 · (I-B)^2 + C(2)^2 · (I corrected-I)^2

cols. 26-35 C(2) - the three terms represent the statistical error, a proportional error and the uncertainty in the absorption correction.

cols. 36-45 μ - absorption coefficient in reciprocal cm. Program SOMUONRO (see section II B 11) will calculate μ/ρ for your compound.

cols. 46-55 scale factor by which F^2 is to be multiplied (usually 1.0)

cols. 56-65 ω_o value which is subtracted from ω value on card

cols. 66-75 φ_o value which is subtracted from φ on card to get true φ

cols. 76-80 2θ for the monochrometer--if 0.0 normal Lp factor will be used

Item 13: Reflection data if read from cards

Format is handled in the user supplied subroutine IMPD.

Item 14: !EOD

Subroutine IMPD -- this user supplied subroutine has the following form:

```
SUBROUTINE IMPD(FH,FK,FL,S,B,SCB,OM,PHI,SLO,SLB,
1OBSFI,BACFK,IDENT,NSCALE,ICN,NBACK)
DIMENSION ICN(16)
```

A call is made to this subroutine to read each reflection in turn until IDENT is returned as a termination code.

FH, FK, FL Miller indices (real)
S = peak intensity B = total intensity of all backgrounds
SCB = scale factor -- usually 1.0
OM = observed ω PHI = observed φ
SLO = peak scan length time in sec. SLB = total background counting time (sec.)
OBSFI = identical to S BACFK = identical to B
NSCALE - a scale factor number transferred to output
ICN - the 16 control parameters read in Item 9
NBACK - number of backgrounds observed; number of terms contributing to B
IDENT = Data termination signal
= 1 read a new batch card (Item 12) and call IMPD again
= 2 run is terminated
= 3 start a complete new run (go back to Item 6 and supply new set of control cards)
> 3 read another data card (call IMPD again)

NOTE: for a standard reflection set FH=FH+100000.

VI. XRAY execution: Punch the above items and submit deck to Computer Center with instructions that it is to be run on the XRAY system at night.

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: To take data from DATAP sort and average equivalent reflections and produce a unique data set for least squares input.

III. Source: Original program (SORT 1) for the IBM 1130 by R. Snyder; revised for the IBM 360 (SORT 3) and for the XDS Σ 5 (SORT 5) by R. Snyder.

IV. Procedure: SORT 5 is a general program to sort crystallographic reflection data on hkℓ, khℓ or ℓkh and/or interscale up to 10 batches of data, determining inter-set R values and/or average all equivalent reflections. This program performs the final three steps in the processing of raw intensity data to produce a set of independent structure factors suitable for use in various Fourier and least squares programs.

The program accepts the output from any of the data processing programs presently in use here. A futher feature is that the output sequential disk file (Unit 2) from DATAP is compatible with input file number 10 of SORT 5, thus eliminating the necessity of punching the structure factor data before scaling and averaging. The final unique data set is also output onto file 20.

The sorting procedure used is the rapid shell sort algorithim. As the reflections are read they are written on a random scratch file (Unit 1) in partitions depending on the value of the slowest moving index. Each of these partitions may contain up to 640 reflections.

Partition 1 contains reflections with slowest moving index (SMI) ≥ -10

⋮

Partition 11 contains reflections with SMI = 0

⋮

Partition 21 contains reflections with SMI ≥ 10

Due to this arrangement the slowest moving index should be chosen so as to not put more than 640 reflections on any one file. For the case when the SMI has no negative values a special option may be called which will more efficiently use the 21 partitions of the random data file by averaging the data as follows:

Partition 1 contains reflections with SMI = 0

Partition 21 contains reflections with SMI ≥ 21

If more than 5000 data are to be processed this option should be used and the data sort should be specified making that index which ranges closest to 21 the SMI.

If averaging of equivalent reflections is desired for Laue groups other than monoclinic or orthorhombic (2/m or mmm), a Laue group specific subroutine SPACE, must be provided. This subroutine must convert the indices of all reflections to an independent segment of the sphere of reflection. An example of this subroutine for Laue group 2/m (which is already contained in the program) which converts all indices to +h +k ± ℓ is :

```
      SUBROUTINE SPACE (J,K,L,IREJ)
      IREJ = 0
      IF(J)20, 200, 100
10    IF(L)100, 200, 200
20    IF(L)200, 100, 100
100   J = IABS(J)
      K = IABS(K)
      L = IABS(L)
      RETURN
200   J = IABS(J)
      K = IABS(K)
      L = IABS(L)
      RETURN
      END
```

NOTE: If IREJ is set to other than zero then the reflection rejected and excluded from all processing.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:10,(FILE,NAME OF DATAP FILE 2),(IN)
This is only included if data is to be input from tape.

Item 3: !ASSIGN F:20,(FILE,ANY NAME),(OUT)
This is the BCD data output file in ORFLS format

Item 4: !ASSIGN F:1,(FILE,JUNK),(RANDOM),(OUTIN),(REL),(RSTORE,544)

Item 5: !ASSIGN F:2,(FILE,JUNK1),(RANDOM),(OUTIN),(REL),(RSTORE,176)
These (1 and 2) are scratch files released at the end of job.

Item 6: !RUN (LMN,SORT5,FSNYDER)

Item 7: !DATA

Item 8: Control card (9I1)

cols. 1, 2 and 3 specify the order of sorting reflections h=1, k=2, ℓ=3
cols. 1, 2, 3 = 231 means sort data so that h moves slowest, ℓ next slowest and k fastest
col. 1 = fastest moving index
col. 2 = next fastest moving index
col. 3 = slowest moving index (SMI)

col. 4	= 0 Read one batch of data and do not scale.
	= 1 Read up to 10 batches of data, determine inter-set R values and scale all sets to first batch read.
col. 5	= 0 Do not average equivalent reflections.
	= 1 Average equivalent reflections for Laue group 2/m.
	= 2 Average equivalent reflections for Laue group mmm.
	= 3 Average equivalent reflections for any other Laue group.
	User must supply subroutine SPACE (see above).
col. 6	= 1 Punch the final data set.
	= 0 Do not punch--data is still written on file 20.
col. 7	= 0 Input data from cards.
	= 1 Data from tape 2 produced by DATAP.
col. 8	= 0 Slowest moving index (SMI) can be negative.
	= 1 SMI is only positive.
col. 9	= 0 normal operation
	= 1 Only determine R values between batches and call exit.

Item 9: First batch of reflection data (normal ORFLS format 3I9, 2F9.2, 13XI1)

cols. 1-9 h cols. 10-18 k cols. 19-27 ℓ cols. 28-36 F_{obs} (or I_{obs})

cols. 37-45 σ (F_{obs}) col. 59 IUN = 0 observed reflection, = 1 unobserved

Item 10: End of batch indicator

cols. 7-9 =998 means end of current batch; read another data set next
=999 means end of last data set; begin processing

Item 11: If Item 10 = 998 then Items 9 and 10 should be repeated for as many data sets as are to be entered.

When Item 10 = 999 then place the following at end of data
!EOD

VI. XRAY execution: The above data deck should be submitted to the Computer Center with instructions that it is to be run on the special XRAY system at night.

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: General three dimensional crystallographic Fourier analysis program.

III. Source: Original program by A. Zalkin; revised in numerous stages at Brookhaven National Laboratory, particularly by J. Ibers; extensively revised by R. Shiono for the IBM 7090 and 360; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: The program first expands the given independent reflections to fill one half of the reciprocal space, according to the symmetry relations. Then the Fourier summation is done in P1 or $P\bar{1}$ space group with the expanded data. The resulting electron densities are then written on a tape as the output. Since the summation is done with one half of the limiting sphere, a factor of two (or 2/volume) should be multiplied to obtain the absolute density. This may be done by the subroutine ALTER.

The F(000)/V term may be added by providing a value on a control card. This is added as a constant to all the grid points and is not affected by the subroutines ALTER and REJECT. Therefore, if used, this must be in the same scale as the general reflections after any modification.

A grid interval of 1/1000th of a cell or larger may be used.

The results of Fourier summation are printed in orthogonal mesh with the axial directions and the grid point coordinates properly indicated. Depending on the way each section is calculated, the print-out has the following fixed directions:

Sections perpendicular to	Axis in output print horizontal	vertical
a*	z	y
b*	x	z
c*	x	y

The electron density values may be printed in numeric code with three-digit integer with a sign or in alphabetic one-letter representation with a specified grade of not more than 20. The program keeps record of the highest calculated electron density and scales the results appropriately before printing. The scale may be chosen in such a way so that the highest peak will be printed as 999 (or -999) or as the true value multiplied by a factor of $10^{\pm n}$ in three-digit number.

Negative values may be suppressed in printing and they will appear as a 0 (zero) or . (decimal point).

The number of grid points which may be printed on a single page before continuing to the second one are:

i) Numeric
- 26 points horizontally
- 51 points vertically with single space
- or 26 points vertically with double space
- or 17 points vertically with triple space.

ii) Alphabetic
- 101 points horizontally with no blank space
- 51 points horizontally with one blank space
- 35 points horizontally with two blank spaces
- 26 points horizontally with three blank spaces
- same as numeric case vertically.

Headings for the coordinate in the horizontal direction are printed for the first 26 grids only, and therefore they will not match properly to the grids in an alphabetic mode except the one with three blank spaces.

Fourier Peak program searches the summation result and records all grid points whose densities are higher than the neighboring points, in order of the magnitude of calculated density. Since peaks on the first and the last section as well as on the edge of each section can not be counted as peaks, an extra section or an extra row of grids may have to be calculated in order to include these peaks. The coordinates of all peaks may be punched in ORFLS format.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:4,(FILE,NAME OF TAPE 10 or 4 from ORFLS),(IN)
Include this item only if data is from binary least squares tape (the usual case).

Item 3: !ASSIGN F:9,(FILE,ANY NAME),(OUTIN),(SAVE)
This tape contains the actual Fourier summation as printed for future reference (e.g., peak finding or minimum function). If saving is not desired replace SAVE with REL.

Item 4: !ASSIGN F:3,(FILE,JUNK1),(OUTIN),(REL)

Item 5: !RUN (LMN,FOURIER,FSNYDER)

Item 6: !DATA

Item 7: Title card (72H)

cols. 1-72 Any alphanumeric information.

Item 8: Control card No. 1 (8I1, 3I4, F10.4)

col. 1
- 0 bypass Fourier print-out
- 1 call Fourier print-out or punch-out (FRPRNT)
- 2 call Fourier print and also repeat the entire program with a new set of control cards

col. 2
- 0 print out in numeric
- 1 print out in alphabetic
- 2 punch out in numeric, a printed page at a time
- 3 punch out in alphabetic, a printed page at a time
- 4 punch out in numeric horizontally across up to last value using as many cards per line as necessary
- 5 punch out in alphabetic as above

NOTE: Options 4 and 5 are used for punching the Fourier in a format that can be read by other programs (e.g., minimum function, etc.).

col. 3
- 0 print or punch all values
- 1 print or punch positive values only and suppress negative values

col. 4
- 0 use RMAX from the calculation or from your specified value, whichever the greater. The normalization factor will be c = 999/RMAX. This is recommended for an alphabetic print mode.
- 1 let the program choose a factor $c = 1 \times 10^n$ to print the true value, except the decimal point position, in three digits or less. $c \geq c' = 1 \times 10^n$. Using this mode for an alphabetic print may result in a complete loss of details.
- 2 same as 0, except that the output values are in one digit with a sign

col. 5
- 1 single space vertically between lines
- 2 double spaces vertically between lines
- 3 triple spaces vertically between lines

col. 6
- 0 bypass Fourier peak search
- 1 call Fourier peak search (FRPEAK)

col. 7
- 0 search up to 1000 peaks
- n search up to n x 100 peaks

col. 8
- 0 no space between letters horizontally in alphabetic print out.
- 1 one blank
- 2 two blanks
- 3 three blanks

cols. 11-12 ND the number of grades to be used in the alphabetic print out (punch) for positive or negative values. Usually

$$1 \geq ND \geq 20$$

but if the negative values are suppressed, this may be as big as 40.

col. 16
- 0 for regular Fourier calculation (call RIP and SIG)
- 1 to bypass the Fourier summation part (RIP and SIG) and to call only the print and/or the peak search parts. Fourier results must be on tape 9 when this is specified.

cols. 18-20 LMTD upper limit of density for alphabetic print out if a value less than 999 is desired. Any density greater than this (absolute value) will be printed as the highest grade.

cols. 21-30 RMAX the maximum electron density. Usually this field may be left blank. This may be used to changed the normalizing factor in FRPRNT if the value punched here is greater than the RMAX calculated.

Item 9: Control card No. 2 (7I3, 5F10.3)

cols. 1-3 NEQUIV half the multiplicity of the Laue group, as given in the following table. Used by the program in expanding the input data to full set.

Laue Group	NEQUIV	Laue Group	NEQUIV
$\bar{1}$	1	$\bar{3}$	3
2/m	2	$\bar{3}$m	6
mmm	4	6/m	6
4/m	4	6/mmm	12
4/mmm	8	m3	12
		m3m	24

cols. 4-6 NREF number of sets of equivalent reflections (as expanded by RIP) to be listed. This serves as a convenient check, but uses lots of paper. This is ordinarily zero.

col. 9 NTAPIN 0 for the reflection data on cards
1 for the data on tape from the LS program (NDATAP- binary)

col. 12 NSP 0 Fourier (Fo synthesis)
1 Difference Fourier
2 Patterson (program squares F_{obs})
3 F_{cal} Fourier
4 F_{cal} Patterson (program squares F_{cal})
5 Partial difference Fourier

col. 15 NREJ 0 subroutine REJECT is not used
1 to enter subroutine REJECT

col. 18 NALT 0 subroutine ALTER is not used
1 to enter subroutine ALTER

cols. 19-21 NXT extra integer field usually not used. This may be used for ALTER or REJECT subroutines.

cols. 22-31 FOOO F(000)/V for electron density map
$F(000)^2/V$ for Patterson map. This value must be on the same scale as the rest of reflection data.

cols. 32-41 42-51 52-61 62-71	EXT(I)	I=1, 4	Extra floating point numbers field for use by REJECT or ALTER subroutines. When not used, these may be left blank.

Item 10: Control card No. 3 (9F5.3, 5X, I3)

cols. 1-5	XMIN	ρ (x, y, z) is computed for points such that XMIN ≥ x ≥ XMAX, YMIN ≥ y ≥ YMAX, ZMIN ≥ z ≥ ZMAX where the limits are stated as fractions of the cell edges.
6-10	XMAX	
11-15	YMIN	
16-20	YMAX	
21-25	ZMIN	Allowable ranges for the limits of x, y and z are -1 ≥ limit ≥ + 1, and the length of the ranges must be equal to or less than one unit cell. The increments (DX, DY, DZ) must be multiples of 0.001. If a specified range (MAX-MIN) is one unit cell, the program always readusts the range and calculates from -0.5 to +0.5 regardless of your specification.
26-30	ZMAX	
31-35	DX	
36-40	DY	
41-45	DZ	

cols. 51-53	NORIEN	100	sections perpendicular to a* axis or projection along a axis.
		010	sections perpendicular to b* axis or projection along b axis.
		001	sections perpendicular to c* axis or projection along c axis.

Example: sections perpendicular to b* axis.

x: -.01 0.51 with 1/100th
y: 0.0 0.50 with 1/40th
z: 0.0 0.98 with 1/50th

cols. 1-5	6-10	11-15	16-20	21-25	26-30	31-35	36-40	41-45
-.01	0.52	0.	0.5	0.	.98	.01	.025	.02

cols. 51-53
010

For a projection, the increment along the projection axis should be specified as a non-zero number with MIN=MAX=0 .

Item 11: Symmetry relations in least squares format (3(F11.6, 2I2))

NEQUIV of these cards: do not include positions related by a center of symmetry or pure translations, such as a face or body-centered relation. These cards are used to set up the transformation matrices for expanding the input reflection data. Caution: Besure to use the symmetry of the Patterson function for Pattersons.

Symmetry codes: 1 = X , -1 = -X , 2 = Y , -Z = -Y , 3 = Z , -3 = -Z

cols. 1-11	translational part of X
cols. 12-13	symmetry code for X direction -- use either space
cols. 14-15	if only one code is required
cols. 16-26	translational part of Y
cols. 27-28	symmetry code for Y
cols. 29-30	" " " " " "
cols. 31-41	translational part of Z
cols. 42-43	symmetry code for Z
cols. 44-45	" " " " " "

Item 12: Reflection Data Cards (3I4, 6F7.2, F5.3, I3)

These cards are used only when NTAPIN=0 (col. 9 of item 9).

cols. 1-4	h
cols. 5-8	k
cols. 9-12	ℓ
cols. 13-19	F_{obs}
cols. 20-26	F_{cal}
cols. 27-33	A_{obs}
cols. 34-40	A_{cal}
cols. 41-47	B_{obs}
cols. 48-54	B_{cal}
cols. 55-59	$\sin\theta$
cols. 60-62	ID

For normal Fourier summations, h, k, ℓ and A_{obs}, B_{obs} terms are used by the program. Any unecessary field may be left blank.

In order to calculate a Patterson synthesis with the data cards in ORFLS format, Part I of the least-squares program should be used to create an input tape.

Item 13: Reflection Data Termination Card (I4)

Use only if data is from cards.

cols. 2-4 =999

Item 14: Control card No. 4 (F10.5,2I5)

Use only if FRPEAK (Fourier Peak search) is called.

cols. 1-10	RMIN the smallest density value to be considered a peak. Zero is usually suitable.
col. 15	=0 normal operation
	=1 punch coordinates of peaks in least squares format
col. 20	=0 search and print all peaks--include those maxima occurring on borders of summation as peaks.
	=1 exclude peaks on boundaries.

Item 15: !EOD

VI. XRAY execution: Submit the above items punched on cards to the Computer Center with instructions that it is to be run on the special XRAY system at night.

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: General crystallographic least squares refinement program.

III. Source: Original program by W. Busing, K. Martin and H. Levy of Oak Ridge. Extensively revised by W. C. Hamilton and others at BNL and by R. Shiono at the University of Pittsburgh. Extensively revised for the IBM 360 and XDS Σ5 by R. Snyder.

IV. Procedure: The general method is well described in the literature. The specific approaches of this program are described in the original write up available from theFederal Documents Clearinghouse as "ORFLS, A FORTRAN Crystallographic Least Squares Program" by W. R. Busing, et al, ORNL-TM-305 and in Technical Report No. 48, Dept. of Crystallography, University of Pittsburgh by R. Shiono.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:10,(FILE,NAME OF TAPE 10 or 4 from previous ORFLS run),(INOUT)
If data is not to be input from a previous ORFLS run, assign this to any file and specify (OUTIN).

Item 3: !ASSIGN F:4,(FILE,ANY NAME),(OUTIN)
At end of run this file contains the latest F_{cal} information and should be input as tape 10 for a subsequent run.

Item 4: !ASSIGN F:9,(FILE,NAME OF BCD OUTPUT FILE from SORT5 or DATAP or ANY NAME),(IN)
This card is only required if data is to be input from a data reduction program output tape or output tape for program ANGLE is to be written. If so, it must be specified as (OUT).

Item 5: !RUN (LMN,ORFLS,FSNYDER)

Item 6: !DATA

Item 7: Title card - cols. 1-72 any title information.

Item 8: Control card No. 1 (5I5, 6F8.4)

col. 5 JB
- 0 Input reflection data from cards.
- 1 Input reflection data on tape (tape 9). An output tape of the data reduction programs.
- 2 Input reflection on cards, run only part I to produce an intermediate output tape (10) for use in Patterson synthesis.
- 3 Input reflection data on tape from a previous least squares calculation. The tape should be mounted on 10.

All information on the tape are used without change and the program bypasses Part I. Control card 2, item 12 follows this card.

col. 10 JA 0 Refine on F_{obs}

1 Refine on $(F_{obs})^2$. This causes $(F_{obs})^2$ to be written on tape 10. Do not use this mode if F_{obs}'s are already squared.

col. 15 JW 0 Standard error σ's are punched on the data cards and/or they will be assigned by the subroutine MODIFY.

1 Hughes' weighting scheme. When this is specified, F_{min} (not $4F_{min}$) value should be punched as A in cols. 26-33.

2 Cruickshank's weighting scheme. A, B, C values below should be supplied.

3 $\omega = 1/(\sin\theta/\lambda)$

4 Constant weight, $\omega = 1.0$

col. 20 JC 0 Subroutine MODIFY is not used.

1 Enter subroutine MODIFY.

col. 25 JD 0 Normal

1 set $\omega = 0.0$ for unobserved reflections with ID = 1

cols. 26-33 A F_{min}, value for Hughes' or A for Cruickshank's scheme. This may be used for any other purpose in your MODIFY subroutine.

cols. 34-41 B For Cruickshank's B or blank.

cols. 42-49 C For Cruickshank's C or blank.

cols. 50-57 D For use in MODIFY subroutine.

cols. 58-65 E For use in MODIFY subroutine.

cols. 66-73 F For use in MODIFY subroutine.

Weight ω is taken as $\omega = 1/(\sigma)^2$. If $\sigma = 0$, then the program sets $\omega = 0$. What you punch on the reflection data cards or calculate according to some scheme and write on the tape is σ, and not ω. F_{obs} values used here are those on the input cards, or on the tape 9 and they are not affected by the scale factors you provide.

i) Hughes' scheme:

(E. W. Hughes (1941) J. Amer. Chem. Soc. 63, 1737)

$$\omega = 1/\left|Fo\right|^2 \quad \text{if } Fo \geq 4F_{min}$$

$$\omega = 1/\left|4F_{min}\right|^2 \quad \text{if } Fo < 4F_{min}$$

$$\omega = 0 \quad \text{if } Fo = 0$$

ii) Cruickshank's scheme:
("Computing Methods and the Phase Problem in X-ray Crystal Analysis", Edit. Pepinsky et al (1961) p. 45)

$$\omega = 1/(A + BFo + CFo^2)$$

When a 3 is punched in column 5, the rest of the fields in this card are irrelevant, and the following items (9), (10) and (11) are not used.

Item 9: Cell constant card (3F7.3, 4F7.4)

Skip Items 9 - 11 if data is from tape 10.

cols. 1-7 $\bar{a}$ cols. 8-14 $\bar{b}$ cols. 15-21 $\bar{c}$

cols. 22-28 $\cos\alpha$ cols. 29-35 $\cos\beta$ cols. 36-42 $\cos\gamma$

cols. 43-49 λ (wave length used)

$\bar{a}$, $\bar{b}$, $\bar{c}$ and λ in Å units

Item 10: Atomic scattering factor cards (7F10.4)

This is the table of f vs. $\sin\theta$, 8 cards per atomic kind. (51 entries of f). Atomic f's are punched in increasing order of corresponding $\sin\theta$ value, from 0.00 to 1.00 with an increment of 0.02. Program SOFORMF (see section II C2 of this write up) will produce these cards in the proper format. The order of sets for each atomic kind determines the number to be used on the parameter cards. Up to 10 sets. A blank card terminates the atomic f cards.

Item 11: Reflection data cards (3I9, 2F9.2, F9.0, I5, 2F6.3) - if data from cards only.

If data from tapes 9 or 10, skip this item.

cols. 1-9 h index
cols. 10-18 k index
cols. 19-27 ℓ index
cols. 28-36 F_{obs}
cols. 37-45 σ if used, or blank
cols. 53-54 Scale factor designation. 1~20. If blank, 1.0 is assumed.
col. 59 < 0 observed reflection
1 unobserved reflection

cols. 60-65 RA Extra fields for any desired values if needed.
cols. 66-71 RB The values will be transferred to the input and the output tape of the refinement part and available in the calculation. Blank if not used.

A blank card terminates the reflection data.

Item 12: Control card No. 2 (I6I5)

col. 5 NC The number of cycles to be run. If NC = 0, a set of structure factors will be calculated, but no refinement will be made.

cols. 8-10 NA The number of atoms in the asymmetric unit, which are specified by the parameter cards. (item 16)

cols. 14-15 NQ The number of scale factors used, and appearing in the parameter list.

col. 20 ITF 0 for isotropic temperature factors and anisotropic temperature factors, or mixed.
1 for conversion of isotropic temperature factors on the parameter cards to anisotropic mode before refining. If some of the atoms have already anisotropic temperature factors, this will not affect them.

cols. 23-25 NV The number of parameters to be varied and refined. If NC = 0 (SF only), then NV is irrelevant.

cols. 29-30 NAS The number of anomalous scattering atoms in the parameter cards to apply the correction. The parameter cards for those atoms must be grouped and placed in front of other atoms.

col. 35 NPT 0 normal calculation
1 Partial mode calculation. A_c, B_c are taken from the input tape and added to the current calculated values. This assumes that an output tape of previous calculation is mounted on 10 as input.

Any atom with anomalous dispersion correction should be in the new part and may not be in the input tape.

col. 40 NPRN 0 Print structure factors for every cycle.
1 Print only the final structure factors and suppress the print out of other cycles.

col. 45 NR 0 Normal calculation with no parameter selection change.
1 First run of repeat calculations with change in parameter selection cards. This makes the program go back and read a new set of control cards.
2 Second and more run of the above cycle. The program will go back and read more controls.
3 Final run of the recycling. The program terminates at the end of this specification.

col. 50 NRW 0 normal

1 Copy back the final output results on tape 4 to tape 10. For this tape 10 must have the protector ring in. This copying takes place only when the final calculation has been successfully run.

col. 55 ISTP 0 Program will be terminated, if a non-positive definite temperature factor results.

1 Program will proceed in the above case, by resetting the temperature factor to 0.0001 (for isotropic) or the original value (for anisotropic).

Item 13: Control card No. 3 (6I5)

col. 5 NF The number of different x-ray form factors. NF = 0 for neutron diffraction.

col. 10 ICENT 1 for centrosymmetric
2 for non-centrosymmetric

col. 14-15 NS The number of symmetry cards. For centrosymmetric structure, NS is equal to one-half the number of equivalent positions. The original x, y, z should be included. 1 ~ 24.

col. 20 IFSQ 1 to refine on (scale x F)
2 to refine on (scale x $F)^2$

cols. 24-25 IXFE 0 for no extra tape for ORFFE
-1 write the parameters and errors based on diagonal elements on file 9. This is the input tape for program ANGLE.
1 for extra tape for ORFFE. This may not be specified if the input tape 9 is used.
2 punch the same on cards for ORFFE

Item 14: Symmetry cards (F11.6, 2I2, F11.6, 2I2, F11.6, 2I2)

For a centrosymmetric structure, those positions related by the center of symmetry are not required. The basic x, y, z position must be included. For a centered-lattice, those symmetries related by pure translations are not required, but the atom multiplier should be increased.

Symmetry	Digit
0	blank
x	1
-x	-1
y	2
-y	-2
z	3
-z	-3

cols. 1-11 translational part of x

cols. 12-13
14-15 symmetry for x direction

cols. 16-26 translational part of y

cols. 27-28 29-30	symmetry for y direction
cols. 31-41	translational part of z
cols. 42-43 44-45	symmetry for z direction

Item 15: Scale factor cards (8F9.6)

cols. 1-9	first scale factor S_1
cols. 10-18	second scale factor S_2 etc.

If there are more than eight scale factors, continue to additional cards. All scale factors in this program apply to the F_{obs} values, rather than to the F_{cal} values. When an output tape of a previous calculation is used as the input, F_{obs} values were already scaled, so that the scale factors used here should be 1.0.

Item 16: Atomic parameter cards

a) First card (A6, 3X, 5F9.6, 2F6.2)

cols. 1-6	Any 6 Hollerith characters identifying atom i.
cols. 10-18	X-ray scattering factor identifier, to specify which atomic f to use. (1.0 ~ 10.0), for neutron problem, this is the neutron scattering factor itself.
cols. 19-27	A multiplier, a_i, this number is usually 1.0, except for a special position or disordered atom, or for a centered-lattice.
cols. 28-36	x_i, fractional coordinate
cols. 37-45	y_i
cols. 46-54	z_i
cols. 55-60 cols. 61-66	$\Delta f'$ $\Delta f''$ } if anomalous dispersion correction is applied, the values are taken as constant for sin θ value.

b) Second card (6F9.6)

cols. 1-9	T_i, the isotropic temperature factor, or β_{11}.
cols. 10-18	β_{22}, (if the field for β_{22} is zero, the program assumes isotropic temperature factor)
cols. 19-27	β_{33}
cols. 28-36	β_{12}
cols. 37-45	β_{13}
cols. 46-54	β_{23}

If anomalous dispersion correction is applied for some atoms, the parameter cards for those atoms should be placed first.

Item 17: Parameter selection cards (72I1)

These cards specify the NV parameters to be varied, each column of the cards for each parameter, in the order:

NQ scale factors

scattering factor multiplier	or	scattering factor multiplier
x_i		x_i
y_i		y_i
z_i		z_i
B_i		β_{11}
		β_{22}
		β_{33}
Punch 0 for holding constant		β_{12}
1 for refinement		β_{13}
		β_{23}

The set of six or eleven columns repeat for all atoms used. Continue from column 72 of one card to column 1 of next card. At present the total number of parameters to be used including those not to be varied is 811. This card is not used if the number of cycles is zero (SF only).

The number of parameters to be specified for each atom is either 6 or 11 depending on whether the temperature factor of an atom is isotropic or anisotropic. When using mixed mode of temperature factors, that is, some atoms have isotropic and others have anisotropic temperature factors, care must be taken to count and fill up the columns properly for 6 or 11. There should be no gap between atoms, and the order of atoms here are identical to the order in which the atomic parameter cards are read.

Item 18: !EOD

V. XRAY execution: Submit the above items punched on cards at the computer center with instructions that it be run on the special XRAY system at night.

ANGLE

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: To calculate interatomic bond lengths and angles with standard deviations from an input tape prepared by ORFLS.

III. Source: Original program for the IBM 7090 by R. Snyder; revised for the IBM 360 and XDS Σ 5 by R. Snyder.

IV. Procedure: There is an interactive version of this program available on our time sharing system (SOANGLE), but it does not use the ORFLS tape.

ANGLE is a general program to calculate angles and distances from fractional coordinates. The standard deviations are derived from the standard errors of the coordinates as shown in the parameter list printed after a cycle of least squares refinement. These errors may be obtained by punching from this list or they may be directly written on tape 9 by ORFLS. It should be noted that these errors are taken from the diagonal elements of the variance-covariance matrix and thus do not take covariance (cross terms) into account.

The specification of symmetry operations is similiar to that used in ORFEE. Translational symmetry is in reference to the 555 cell so that a translation of +1 in the x direction would be specified as 655. The symmetry element to be applied to a coordinate is the sequential number of the symmetry element as read by this program.

The present program is dimensioned for 200 coordinates and 99 symmetry cards. An unlimited number of specification cards may be used.

V. Data set up:

Item 1: !JOB FXRAY,75(USERS NAME),5

Item 2: !ASSIGN F:9,(FILE,Name of file 9 ORFLS output),(IN)

Item 3: !RUN (LMN,ANGLE,FSNYDER)

Item 4: !DATA

Item 5: Control card (3I5)

col. 5 = ITAP
- =0 data from tape 9 prepared by ORFLS
- =1 input all data from cards

cols. 9-10 =ISYMT =
- the number of symmetry elements to be input from tape 9
- =0 symmetry elements on tape ignored
- =-1 all symmetry elements used in least sqaures will be input
- =N the first N symmetry elements used in ORFLS will be input

col. 15 =ISYMC = the number of symmetry elements to be input from cards

Case 1, ISYMT=ISYMC=0: program will use one identity symmetry element. The symmetry specification number on the specification card (item 10) may be left blank. If ITAP=0 then item 10 follows this card.

Case 2, FSYMT=N ISYMC=M: N symmetry elements will be read from tape and M elements will be read from cards. (N+M elements will be used)

Remember: the symmetry elements used by ORFLS are not a complete set; those due to a center of symmetry or lattice translations are not included.

Item 6: Cell constants - only include if ITAP=1 (3F7.3,3F4.4)

cols. 1-7 $\bar{a}$(Å) cols. 8-14 $\bar{b}$(Å) cols. 15-21 $\bar{c}$(Å)

cols. 22-27 $\cos\alpha$ cols. 28-35 $\cos\beta$ cols. 36-42 $\cos\gamma$

Item 7: ISYM symmetry cards in standard format (3 (F11.6, 2F2.0))

only include if ITAP=1 or if ITAP=0 and ISYMC > 0

cols. 1-11	Translation for x
col. 13	Symmetry for x
col. 15	Second symmetry for x (if needed)
cols. 16-26	Translation for y
col. 28	Symmetry for y
col. 30	Second symmetry for y (if needed)
cols. 31-41	Translation for z
col. 43	Symmetry for z
col. 46	Second symmetry for z (if needed)

where +x = +1, -x= -1, etc.

Item 8: Coordinates and least squares errors (A6, 1XA1, 5X2F13.7)

only include if ITAP=1

cols. 1-6	Atom Name
col. 8	letter x, y or z
cols. 14-27	coordinate x, y or z
cols. 28-41	standard error

Coordinate for any atom must be input in the order x, y, z.

Item 9: Terminate coordinate cards - only include if ITAP=1

cols. 14-27 999.0

Item 10: Specification cards (3 (I4, 1X3I1, I2), I5)

These cards specify the atoms to be used in the bond length and angle calculation. If the angle between three atoms is desired the center

atom must be input as J. If only distance is desired, leave K blank.

cols. 1-3	I the sequence number of atom desired
cols. 4-6	cell desired (e.g., 555)
cols. 7-8	symmetry element number to be applied
cols. 11-13	J another atom sequence number
cols. 14-16	cell
cols. 17-18	symmetry element number
cols. 21-23	K a third atom sequence number (if blank only distance I-J will be computed)
cols. 24-26	cell
cols. 27-28	symmetry element number
col. 35	=0 normal =1 Bonds I-J and J-K are chemically equivalent

Item 11: Blank card to terminate run.

Item 12: !EOD

VI. XRAY execution: Submit the above items punched on cards at the computer center with instructions that job be run on the large XRAY system at night. NOTE: the usual case is when data is input from ORFLS file 9; for this case item 10 usually follows item 5.

WEIGHT

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: To analyze the weighting scheme used in the least squares procedure from a tape prepared by ORFLS.

III. Source: Original program written for the CDC 6600 by R. Snyder; revised for the IBM 7090, 360 and XDS Σ 5 by R. Snyder.

IV. Procedure: WEIGHT is a general program for analyzing a least squares weighting scheme. It produces an idealized scheme based on the hypothesis that the average value of (FO-FC)/σ should equal 1.0 for all ranges of FO or $\sin\theta/\lambda$.

The program operates by reading FO, FC, SIGMA(FO), and SIN θ from tape 10 as written by ORFLS. $|FO-FC|/\sigma$ values are calculated and averaged over intervals of FO and $\sin\theta/\lambda$.

A WEIGHT subroutine, suitable for use in the least squares program, which will assign new σ's, causing the average $|FO-FC|/\sigma$ for each interval to equal 1.0, may be punched. In addition, the program will produce the following four plots on the CALCOMP plotter:

1. all $|FO-FC|/\sigma$ values vs. FO
2. all $|FO-FC|/\sigma$ values vs. $\sin\theta/\lambda$
3. the averaged $|FO-FC|/\sigma$ values vs. the intervals of FO
4. the averaged $|FO-FC|/\sigma$ values vs. the intervals of $\sin\theta/\lambda$

At present the program is dimensioned for 4500 observed reflections, all unobserved reflections being ignored. To increase this number it is only necessary to change each "4500" which appears in the DIMENSION statements of the main program and subroutines; no coding need be changed. Allowance is made for the use of up to 50 intervals of FO and $\sin\theta/\lambda$ but in general, 5 would be a reasonable number.

TAPE: The input tape from ORFLS must be mounted on logical drive number 10.

V. Data set up:

Item 1: !JOB FXRAY,75(USERSNAME),5

Item 2: !ASSIGN F:10,(FILE,Name of file 10 from least squares),(IN)

Item 3: !RUN (LMN,WEIGHT,FSNYDER)

Item 4: !DATA

Item 5: Control card (10I1, 2I5)

col. 1 =0 Punch weighting factors based on FO analysis.
=1 Do not punch.

col. 2 =0 Punch weighting factors based on $\sin\theta/\lambda$ analysis.
=1 Do not punch.

col. 3	=0 Plot all $\lvert FO-FC \rvert / \sigma$ vs. FO values. =1 Bypass plot.
col. 4	=0 Plot all $\lvert FO-FC \rvert / \sigma$ vs. $\sin\theta/\lambda$ values. =1 Bypass plot.
col. 5	=0 Plot averaged $\lvert FO-FC \rvert / \sigma$ vs. FO values. =1 Bypass plot.
col. 6	=0 Plot averaged $\lvert FO-FC \rvert / \sigma$ vs. $\sin\theta/\lambda$ values. =1 Bypass plot.
col. 7	=0 Input tape 10 from ORFLS
col. 8	=0 Do not list sorted FO list. =1 List FO's sorted on magnitude.
cols. 11-15	The number of FO values to be included in each interval. If blank, or zero, all data will be equally divided into 15 intervals.
cols. 15-20	The number of $\sin\theta/\lambda$ intervals to be used. These intervals will be set so as to include approximately equal numbers of reflections. If zero, or blank, 15 is assumed.

Item 6: !EOD

VI. XRAY execution: Submit the above items punched on cards at the computer center with instructions that it be run on the large XRAY system at night.

ORTEP

I. Program language and type: FORTRAN IV with two modified plotting subroutines written in assembly language (SYMBOL) - large XRAY system.

II. Function: To plot on the CALCOMP plotter a three dimensional (two stereo related) picture of any molecule or crystal structure.

III. Source: Original program by C. K. Johnson of Oak Ridge National Laboratory; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: The procedures used are described in the original publication, "ORTEP: A FORTRAN Thermal-Ellipsoid Plot Program for Crystal Structure Illustrations" by Carroll K. Johnson, Oak Ridge National Laboratory (1965), ORNL-3794. Available from the Federal Documents Clearinghouse. This program is very general and for proper use one must obtain the above publication. Copies are available for borrowing from R. Snyder. Instead of attempting to describe all the functions of this program here, the data set up section will describe how to draw the outlines of any unit cell and fill it with all the atoms occurring in it for any crystal structure in stereo. This should serve to make the full instructions more understandable.

V. Data set up:

Item 1: !JOB FXRAY,75(Users Name),5

Item 2: !ASSIGN F:5,(DEVICE,SI)

Item 3: !ASSIGN F:6,(DEVICE,LO)

Item 4: !ASSIGN F:7,(DEVICE,PO)

Item 5: !ASSIGN F:8,(FILE,JUNK),(OUTIN),(REL)

Item 6: !ASSIGN M:PL,(DEVICE,PLAØ6)

Item 7: !RUN (LMN,ORTEP,FSNYDER)

Item 8: !DATA

Item 9: cols. 1-72 any title information (18A4)

Item 10: Cell parameters (6F9.6)

cols. 1-9 $\bar{a}$ or a* cols. 10-18 $\bar{b}$ or b* cols. 19-27 $\bar{c}$ or c*

cols. 28-36 α, α^*, $\cos(\alpha)$ or $\cos(\alpha^*)$

cols. 37-45 β, β^*, $\cos(\beta)$ or $\cos(\beta^*)$

cols. 46-54 γ, γ^*, $\cos(\gamma)$ or $\cos(\gamma^*)$

reciprocal cell parameters defined by $\bar{a}$ $a^* = 1$

Item 11: Symmetry cards (I1, F14.10, 3F3.0, 2(F15.10, 3F3.0))

col. 1 =0 another symmetry card to follow,
=1 on last card only

cols. 2-15 T_1 translation for X

cols. 16-18 S_{11} cols. 19-21 S_{12} cols. 22-24 S_{13} = symmetries for X

cols. 25-39 T_2 translation for Y

cols. 40-42 S_{21} cols. 43-45 S_{22} cols. 46-48 S_{23} = symmetries for Y

cols. 49-63 T_3 translation for Z

cols. 64-66 S_{31} cols. 67-69 S_{32} cols. 70-72 S_{33} = symmetries for Z

where the transformed coordinates X_1 Y_1 Z_1 relate to the above as follows:

$$X_1 = T_1 + S_{11}X + S_{12}Y + S_{13}Z$$
$$Y_1 = T_2 + S_{21}X + S_{22}Y + S_{23}Z$$
$$Z_1 = T_3 + S_{31}X + S_{32}Y + S_{33}Z$$

Item 12: Atom position cards (A4, A2, 3X5F9.6, F9.0) standard ORFLS format and temperature parameters (I1, F8.6, 5F9.6, F9.0) one card of each type per atom. The first two atoms are false plot points.

Place Atom #1 at XYZ = 000 with B=0. Place Atom #2 at .5.5.5 with B=0. (no labels for either one)

A. Positional parameter card:

cols. 1-6 any alphameric atom identifier
cols. 28-36 X fractional coordinate
cols. 37-45 Y
cols. 46-54 Z
cols. 55-63 = 0 or blank

B. Temperature factor card:

col. 1 =0 another positional and temperature factor card to follow
=1 last atom position card

cols. 2-9 β_{11} or B-isotropic temperature parameter--if so, leave rest of card blank

cols. 10-18 β_{22} cols. 19-27 β_{33} cols. 28-36 β_{12}

cols. 37-45 β_{13} cols. 46-54 β_{23} cols. 55-63 blank

Item 13: From here on, most instructions come as pairs of cards--the first, the actual instructions with necessary parameters; the second, an explanation of the instructions which will appear on the output.

A. col. 3 = 3 cols. 7-9 201

B. cols. 1-80 = "Initialize the CALCOMP plot package."

Item 14: A. col. 3 = 3 cols. 7-9 = 301 cols. 10-18 11.0

cols. 19-27 11.0 cols. 28-36 12.0 cols. 37-45 0.5

B. cols. 1-80 = 11 by 11 inch plot with 5 inch margin and 12 inch stereo view distance

Item 15: A. col. 3 = 3 cols. 7-9 = 404 cols. 13-18 =255501

cols. 22-27 =255501

cols. 28-36 =3.0 the sequence number of the first <u>real</u> atom card supplied

cols. 37-45 =N the sequence number of the last atom card supplied (i.e., the total number of <u>real</u> atoms + 2) enter with decimal

cols. 46-54 =0.5
cols. 55-63 =0.5
cols. 64-72 =0.5

B. cols. 1-72 ='Fill the unit cell with atoms."

Item 16: Only include this instruction if species to be plotted is a molecule with shorter inter molecular distances than intra molecular distances. This instruction will add all atoms which fall within D_{max} of atoms in the unit cell to the list of those to be plotted.
(i.e., it will complete any molecules protruding out of the unit cell)

Be VERY careful in your choice of D_{max} if it exceeds an intra molecular distance, the program will go into an endless loop of adding atoms until the storage space for the atoms list is exceeded.

A. col. 3 = 3 cols. 7-9 = 406 cols. 13-18 =344401

cols. 19-27 (right adjusted) - N666M where N = the sequence number of last atom card supplied (minus sign required) and M = the total number of symmetry cards supplied (if < 10 enter digit preceded with a zero)

cols. 28-36 = 3.0
cols. 37-45 = N with decimal
cols. 46-54 D_{max} with decimal (1.75 is good value for an organic molecule)

B. cols. 1-72 ='Finish out all incomplete molecules."

Item 17: A. cols. 3 = 3 cols. 7-9 = 401 cols. 13-18 =155501

cols. 21-27 = -166601

B. cols. 1-72 = "Put corners of unit cell into atoms list."

Item 18: This instruction should be manipulated in later runs to obtain a clear view of the crystal structure. For the first run try a 20^{o} rotation around the crystallographic plotter X and Y axis.

A. col. 3 = 3 cols. 7-9 = 502

cols. 10-18 1.0 = X, 2.= Y, 3.= Z, -1.= [111] direction (120^{o}rotation), -2.= [111] direction (240^{o}rotation).

cols. 19-27 = 20.0 (number of degrees of right handed rotation)
cols. 28-36 = 2.0 (for Y axis rotation)
cols. 37-45 = 20.0

B. cols. 1-72 ="20 degree rotation around X and Y axis"

Item 19: A. col. 3 = 3 cols. 7-9 = 503 cols. 10-18 = 2.0 cols. 19-27 3.0

B. cols. 1-72 ="stereo rotation of 3 degrees about Y axis for left eye"

Item 20: A. col. 3 = 3 cols. 7-9 = 604

B. cols. 1-72 =auto scale and position to 9 x 9. 50% probability ellipsoids

Item 21: A. col. 3 = 3 cols. 6-9 = 1101

B. cols. 1-72 ="Begin saved sequence."

Item 22: A. col. 3 = 3 cols. 7-9 = 712

cols. 46-54 = .2 (height of atom label in inches)

cols. 55-63 = .6 (perpendicular offset of label in inches)

cols. 67-72 = .6 (parallel offset of label in inches)

If no labels on atoms are desired then leave cols. 46-72 blank.

B. cols. 1-72 "Plot thermal elipses for atoms and label."

Item 23: These three cards may be skipped if bonds are not desired between atoms.

A. col. 3 = 3 cols. 7-9 = 802

B. col. 3 = 3 col. 12 = 3 cols. 13-15 = N (total number of atom cards +2)
col. 18 = 3 cols. 19-21 = N col. 24 = 3

cols. 25-30 = D_{min} (do not draw bonds between atoms closer than D_{min} in Å)

cols. 31-36 = D_{max} (do not draw bonds between atoms farther apart than D_{max} in Å)

cols. 37-42 = .04

C. cols. 1-72 "Draw .04 Å stick bonds."

Item 24: A. col. 3 = 2 cols. 7-9 = 811

B. col. 3 = 1 col. 24 = 2

C. col. 3 = 1 cols. 13-18 =155501 cols. 22-27 = 165501
cols. 31-36 = 155501 cols. 40-45 = 156501
cols. 49-54 = 155501 cols. 58-63 = 155601

D. col. 3 = 1 cols. 13-18 = 165601 cols. 22-27 = 155601
cols. 31-36 = 165501 cols. 40-45 = 166501
cols. 49-54 = 165501 cols. 58-63 = 165601

E. col. 3 = 1 cols. 13-18 = 165601 cols. 22-27 = 166601
cols. 31-36 = 166501 cols. 40-45 = 156501
cols. 49-54 = 166501 cols. 58-63 = 166601

F. col. 3 = 3 cols. 13-18 = 156601 cols. 22-27 = 156601
cols. 31-36 = 156601 cols. 40-45 = 166601
cols. 49-54 = 156601 cols. 58-63 = 155601

G. cols. 1-72 "Draw in outline of unit cell."

Item 25: A. col. 3 = 3 cols. 6-9 = 1102

B. cols. 1-72 = "end saved sequence"

Item 26: A. col. 3 = 3 cols. 7-9 = 202 cols. 10-18 9.0

B. cols. 1-72 = "advance plotter 9 inches along X for right eye view"

Item 27: A. col. 3 = 3 cols. 7-9 = 503 cols. 10-18 = 2.0
cols. 19-27 = -3.0

B. cols. 1-72 = "stereo rotation for right eye"

Item 28: A. col. 3 = 3 cols. 6-9 = 1103

B. cols. 1-72 ="execute saved sequence"

Item 29: A. col. 3 = 3 cols. 7-9 = 902

B. col. 39 = A

Item 30: A. col. 3 = 3 cols. 7-9 = 902

B. col. 39 = B

Item 31: A. col. 3 = 3 cols. 7-9 = 902

B. col. 39 = C

Item 32: A. col. 3 = 3 cols. 7-9 = 202 cols. 10-18 = 10.

B. cols. 1-72 "Advance plotter 10 inches."

Item 33: A. col. 3 = 3 cols. 7-9 = 202

B. cols. 1-72 "Terminate plot."

Item 34: !EOD

VI. XRAY execution: The above items punched on cards should be submitted at the Computer Center with instructions to be run on the large XRAY system at night.

POWDER

I. Program language and type: FORTRAN IV - large XRAY system.

II. Function: Calculate an "ideal" X-ray powder diffraction pattern from crystal structure parameters.

III. Source: Original program by D. K. Smith for the IBM 360; revised for the XDS Σ 5 by R. Snyder.

IV. Procedure: The procedures are well described in the literature including such textbooks as "Elements of X-ray Diffraction" by Cullity.

V. Data set up: For routine applications of this program an interactive program SUPOWDER (see section IIB2 of this write up) is available which can be used to set up an input deck to execute POWDER. The full data set up follows for more nonroutine applications.

Item 1: !JOB FXRAY,75(Users Name),5

Item 2: !ASSIGN F:1(FILE,F1POWDER,FSNYDER),(IN)

Item 3: !ASSIGN F:2,(FILE,F2POWDER,FSNYDER),(IN)

Item 4: !ASSIGN F:3,(FILE,F3POWDER,FSNYDER),(IN)

Item 5: !ASSIGN F:4,(FILE,F4POWDER,FSNYDER),(IN)

Item 6: !ASSIGN F:5,(FILE,F5POWDER,FSNYDER),(IN)

Item 7: !ASSIGN F:6,(FILE,F6POWDER,FSNYDER),(IN)

The above files contain the space group symmetry, absorption factors, etc.

Item 8: !ASSIGN F:9,(FILE,JUNK),(OUTIN),(REL)

Item 9: !RUN (LMN,POWDER,FSYNDER)

Item 10: !DATA

Item 11: cols. 1-72 any title information. Follow the last character with a $. This title will also be used on the plot.

Item 12: Control card 1 (A2,I4,11I3,21X,2F10.5)

cols. 1-2 IWL = letters MO,CU,NI,CO,FE,CR or AG. If any other radiation is desired it may be supplied later, but absorption factors are only available for the above elements and anomalous dispersion factors are only available for Cu,Mo,Fe,Cr or Ag.

cols. 3-6 NSG = number code of space group as listed in the International Tables of X-ray Crystallography, Vol. I. (1969). If two orientations are given the first is entered as +NSG, the second as -NSG.

cols. 7-9 NA = the number of atoms in the assymetric unit--number of atom cards to be read.

cols. 10-12 NPLOT = 1

cols. 13-15 NLAMDA = 0 - d spacings based on $K_{\alpha 1}$ or electron wavelength

= 1 - d spacings based on $K_{\overline{\alpha}}$

= -1 - d spacings based on neutron wavelength input in cols. 61-70

cols. 16-18 NABS =0 read cylindrical absorption curve from files 1-6

=1 read curve from cards after last atom card. Format is (8F10.5) for Å^{-1} values from $\theta = 0^{o}$ to 90^{o} in 5^{o} intervals

cols. 19-21 NAS = number of anomalous scatterers in assymetric unit

cols. 28-30 ITRANS =0 use symmetry information as supplied on files 1 - 6

=1 to 5 transform axis and symmetry according to following code:

	axis setting	internal form NTRAN(3)
ITRANS = 0	abc	123
1	cab	321
2	bca	231
3	$a\overline{c}b$	$1\overline{3}2$
4	$ba\overline{c}$	$2\overline{1}3$
5	$\overline{c}ba$	$\overline{3}21$

Use of this code as directed in the book of Vol. I. of the International Tables allows the user to transform the standard space group into any non standard setting.

cols. 61-70 XLAMDA = $K_{\alpha 1}$, electron wavelength or neutron wavelength. Not needed if specified by IWL.

cols. 71-80 WLZ = $K_{\alpha 2}$ if needed

Item 13: Form factor specifications NNF(I) (20I3)

cols. 1-3 NNF (1) code number for first f-curve

cols. 4-6 NNF(2) code number for second f-curve

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cols. 58-60 NNF(20) code number for twentieth f-curve

NNF(I) =Identification number for f-curve on the master file tape. Code numbers follow.

Code numbers must be listed in ascending numerical order.
A zero NNF(I) results in termination of the reading of f-tables.

Code Numbers	Scattering Factor Type and Format
301-700	Cromer polynomial format 9 values to fit the equation $f = \sum_{i=1}^{4} \left(a_i e^{-\left(\frac{\sin^2\theta}{\lambda^2}\right) b_i} \right) + c$ in the order $a_1, b_1, \ldots, b_4, c$ Cromer (1972) and Cromer and Mann (1968).
701-750	The program will read NNF(I)-700 additional f-curves in Cromer polynomial format immediately after the Atom Cards.
751-850	Single value anomalous dispersion format - f' and f'' values for Mo, Cu, Cr, Ag, Fe Cromer and Liberman (1971).
851-900	The program will read NNF(I)-850 additional anomalous dispersion parameters as single value f' and f'' immediately after the Atom Cards.

The codes follow:

Code	Element	Source	Code	Element	Source	Code	Element	Source
301	H -1	HF	321	SI	HF	341	CR	HF
302	HE	HF	322	SI+4	HF	342	CR+2	HF
303	LI	HF	323	P	HF	343	CR+3	HF
304	LI+1	HF	324	S	HF	344	MN	HF
305	BE	HF	325	CL	HF	345	MN+2	HF
306	BE+2	HF	326	CL -1	HF	346	MN+3	HF
307	B	HF	327	AR	HF	347	MN+4	HF
308	C	HF	328	K	HF	348	FE	HF
309	N	HF	329	K +1	HF	349	FE+2	HF
310	O	HF	330	CA	HF	350	FE+3	HF
311	O -2	HF	331	CA+2	HF	351	CO	HF
312	F	HF	332	SC	HF	352	CO+2	HF
313	F -1	HF	333	SC+3	HF	353	CO+3	HF
314	NE	HF	334	TI	HF	354	NI	HF
315	NA	HF	335	TI+3	HF	355	NI+2	HF
316	NA+1	HF	336	TI+4	HF	356	NI+3	HF
317	MG	HF	337	V	HF	357	CU	HF
318	MG+2	HF	338	V +2	HF	358	CU+1	HF
319	AL	HF	339	V +3	HF	359	CU+2	HF
320	AL+3	HF	340	V +5	HF	360	ZN	HF

Code	Element	Source	Code	Element	Source	Code	Element	Source
361	Z N+2	HF	409	I	HF	457	AU	HF
362	GA	HF	410	I -1	HF	458	HG	HF
363	GA+3	HF	411	XE	HF	459	TL	HF
364	GE	HF	412	CS	HF	460	PB	HF
365	AS	HF	413	CS+1	HF	461	BI	HF
366	SE	HF	414	BA	HF	462	PO	HF
367	BR	HF	415	BA+2	HF	463	AT	HF
368	BR -1	HF	416	LA	HF	464	RN	HF
369	KR	HF	417	LA+3	HF	465	FR	HF
370	RB	HF	418	CE	HF	466	RA	HF
371	RB+1	HF	419	CE+3	HF	467	AC	HF
372	SR	HF	420	CE+4	HF	468	TH	HF
373	SR+2	HF	421	PR	HF	469	PA	HF
374	Y	HF	422	PR+3	HF	470	U	HF
375	Y +3	HF	423	PR+4	HF	471	NP	HF
376	ZR	HF	424	ND	HF	472	PU	HF
377	ZR+4	HF	425	ND+3	HF	473	AM	HF
378	NB	HF	426	PM	HF	474	CM	HF
379	NB+3	HF	427	PM+3	HF	475	BK	HF
380	NB+5	HF	428	SM	HF	476	CF	HF
381	MO	HF	429	SM+3	HF	477	ES	HF
382	MO+3	HF	430	EU	HF	478	FM	HF
383	MO+5	HF	431	EU+2	HF	479	MD	HF
384	MO+6	HF	432	EU+3	HF	480	NO	HF
385	TC	HF	433	GD	HF	481	LW	HF
386	RU	HF	434	GD+3	HF	482	H	SDS
387	RU+3	HF	435	TB	HF	483	H	HF
388	RU+4	HF	436	TB+3	HF	484	H -1	HF
389	RH	HF	437	DY	HF	485	HE	RHF
390	RH+3	HF	438	DY+3	HF	486	LI	RHF
391	RH+4	HF	439	HO	HF	487	LI+1	RHF
392	PD	HF	440	HO+3	HF	488	BE	RHF
393	PD+2	HF	441	ER	HF	489	BE+2	RHF
394	PD+4	HF	442	E R+3	HF	490	B	RHF
395	AG	HF	443	TM	HF	491	C	RHF
396	AG +1	HF	444	TM+3	HF	492	CVAL	HF
397	AG +2	HF	445	YB	HF	493	N	RHF
398	CD	HF	446	YB+2	HF	494	O	RHF
399	CD +2	HF	447	YB+3	HF	495	O -1	HF
400	I N	HF	448	LU	HF	496	F	RHF
401	I N+3	HF	449	LU+3	HF	497	F -1	HF
402	SN	HF	450	HF	HF	498	NE	RHF
403	SN+2	HF	451	TA	HF	499	NA	RHF
404	S N+4	HF	452	W	HF	500	NA+1	RHF
405	SB	HF	453	RE	HF	501	MG	RHF
406	SB+3	HF	454	OS	HF	502	MG+2	RHF
407	SB+5	HF	455	I R	HF	503	A L	RHF
408	TE	HF	456	PT	HF	504	A L+3	HF

Code	Element	Source	Code	Element	Source	Code	Element	Source
505	SI	RHF	553	SE	RHF	601	BA	RHF
506	SI V	HF	554	BR	RHF	602	BA+2	*DS
507	SI+4	HF	555	BR -1	RHF	603	LA	*RHF
508	P	RHF	556	KR	RHF	604	LA+3	*DS
509	S	RHF	557	RB	RHF	605	CE	*RHF
510	CL	RHF	558	RB+1	RHF	606	CE+3	*DS
511	CL-1	RHF	559	SR	RHF	607	CE+4	*DS
512	AR	RHF	560	SR+2	RHF	608	PR	*RHF
513	K	RHF	561	Y	*RHF	609	PR+3	*DS
514	K +1	RHF	562	Y +3	*DS	610	PR+4	*DS
515	CA	RHF	563	ZR	*RHF	611	ND	*RHF
516	CA+2	RHF	564	ZR+4	*DS	612	ND+3	*DS
517	SC	RHF	565	NB	*RHF	613	PM	*RHF
518	SC+3	HF	566	NB+3	*DS	614	PM+3	*DS
519	TI	RHF	567	NB+5	*DS	615	SM	*RHF
520	TI+2	HF	568	MO	RHF	616	SM+3	*DS
521	TI+3	HF	569	MO+3	*DS	617	EU	RHF
522	TI+4	HF	570	MO+5	*DS	618	EU+2	*DS
523	V	RHF	571	MO+6	*DS	619	EU+3	*DS
524	V +2	RHF	572	TC	*RHF	620	GD	*RHF
525	V +3	HF	573	RU	*RHF	621	GD+3	*DS
526	V +5	HF	574	RU+3	*DS	622	TB	*RHF
527	CR	RHF	575	RU+4	*DS	623	TB+3	*DS
528	CR+2	HF	576	RH	*RHF	624	DY	*RHF
529	CR+3	HF	577	RH+3	*DS	625	DY+3	*DS
530	MN	RHF	578	RH+4	*DS	626	HO	*RHF
531	MN+2	RHF	579	PD	*RHF	627	HO+3	*DS
532	MN+3	HF	580	PD+2	*DS	628	ER	*RHF
533	MN+4	HF	581	PD+4	*DS	629	ER+3	*DS
534	FE	RHF	582	AG	RHF	630	TM	*RHF
535	FE+2	RHF	583	AG+1	*DS	631	TM+3	*DS
536	FE+3	RHF	584	AG+2	*DS	632	YB	*RHF
537	CO	RHF	585	CD	RHF	633	YB+2	*DS
538	CO+2	RHF	586	CD+2	*DS	634	YB+3	*DS
539	CO+3	HF	587	IN	RHF	635	LU	*RHF
540	NI	RHF	588	IN+3	*DS	636	LU+3	*DS
541	NI+2	RHF	589	SN	RHF	637	HF	*RHF
542	NI+3	HF	590	SN+2	RHF	638	HF+4	*DS
543	CU	RHF	591	SN+4	RHF	639	TA	*RHF
544	CU+1	RHF	592	SB	RHF	640	TA+5	*DS
545	CU+2	HF	593	SB+3	*DS	641	W	*RHF
546	ZN	RHF	594	SB+5	*DS	642	W +6	*DS
547	ZN+2	RHF	595	TE	RHF	643	RE	*RHF
548	GA	RHF	596	I	RHF	644	OS	*RHF
549	GA+3	HF	597	I -1	RHF	645	OS+4	*DS
550	GE	RHF	598	XE	RHF	646	IR	*RHF
551	GE+4	HF	599	CS	RHF	647	IR+3	*DS
552	AS	RHF	600	CS+1	RHF	648	IR+4	*DS

Code	Element	Source	Code	Element	Source
649	PT	*RHF	697		BLNK
650	PT+2	*DS	698		BLNK
651	PT+4	*DS	699		BLNK
652	AU	RHF	700		BLNK
653	AU+1	*DS			
654	AU+3	*DS			
655	HG	RHF			
656	HG+1	*DS			
657	HG+2	*DS			
658	TL	*RHF			
659	TL+1	*DS			
660	TL+3	*DS			
661	PB	RHF			
662	PB+2	*DS			
663	PB+4	*DS			
664	BI	RHF			
665	BI+3	*DS			
666	BI+5	*DS			
667	PO	*RHF			
668	AT	*RHF			
669	RN	RHF			
670	FR	*RHF			
671	RA	*RHF			
672	RA+2	*DS			
673	AC	*RHF			
674	AC+3	*DS			
675	TH	*RHF			
676	TH+4	*DS			
677	PA	*RHF			
678	U	RHF			
679	U +3	*DS			
680	U +4	*DS			
681	U +6	*DS			
682	NP	*RHF			
683	NP+3	*DS			
684	NP+4	*DS			
685	NP+6	*DS			
686	PU	*RHF			
687	PU+3	*DS			
688	PU+4	*DS			
689	PU+6	*DS			
690	AM	*RHF			
691	CM	*RHF			
692	BK	*RHF			
693	CF	*RHF			
694		BLNK			
695		BLNK			
696		BLNK			

FORM FACTOR CODE - ANOMALOUS DISPERSION

751	LI
752	BE
753	B
754	C
755	N
756	O
757	F
758	NE
759	NA
760	MG
761	AL
762	SI
763	P
764	S
765	CL
766	AR
767	K
768	CA
769	SC
770	TI
771	V
772	CR
773	MN
774	FE
775	CO
776	NI
777	CU
778	ZN
779	GA
780	GE
781	AS
782	SE
783	BR
784	KR
785	RB
786	SR
787	Y
788	ZR
789	NB
790	MO
791	TC
792	RU
793	RH
794	PD
795	AG
796	CD
797	IN
798	SN
799	SB
800	TF
801	I
802	XE
803	CS
804	BA
805	LA
806	CE
807	PR
808	ND
809	PM
810	SM
811	EU
812	GD
813	TB
814	DY
815	HO
816	ER
817	TM
818	YB
819	LU
820	HF
821	TA
822	W
823	RE
824	OS
825	IR
826	PT
827	AU
828	HG
829	TL
830	PB
831	BI
832	PO
833	AT
834	RN
835	FR
836	RA
837	AC
838	TH
839	PA
840	U
841	NP
842	PU
843	AM
844	CM
845	BK
846	CF
847	
848	
849	
850	

Item 14: Cell parameters (6F10.5)

cols. 1-10 $\bar{a}$ in Å cols. 11-20 $\bar{b}$ cols. 21-30 $\bar{c}$

cols. 31-40 α in degrees cols. 41-50 β cols. 51-60 γ

Item 15: Control card 2 (6X, 4F6.2, F6.4, 4X, 13I2)

cols. 7-12 XMU the linear absorption coefficient (μ) in cm^{-1}. If XMU = 0.0 this program will look for a density value in cols. 19-24 and a mass absorption coefficient and Molecular Weight on files 1-6 to calculate μ.

cols. 13-18 XMAX the value the highest reflection should be scaled to (usually 100.0).

cols. 19-24 DENS the crystal density. Only needed if XMU= 0.0. If DENS and XMU= 0.0 the absorption options will be skipped.

cols. 25-30 TTHMAX maximum limit of 2θ to be calculated. If 0.0 THHMAX defaults to175.0°.

cols. 31-36 SC(4) multiplicity scale factor. Only the general symmetry positions are stored on files 1-6. Thus if atoms sit on special positions of lower multiplicity in order to get the correct absolute intensities and crystal density and μ, you must reduce the contribution of the atoms to the structure factor. This may be done by reducing the multiplicity of input atoms on the atom parameter cards or by reducing the overall multiplicity here. e.g., If the general multiplicity for a space group is 96 but the maximum multiplicity for any atom in your structure is 24 then SC(4) may be set to .25 and on the atom parameter cards set atoms with a multiplicity of 24 to 1.0 and those with 12 to .5 etc.

cols. 41-66 I1 to I13 extinction codes. These can be used to modify the reflection extinctions which occur on the master files 1-6. If a value is < 0 the value on the master file (for this run only) will be reset to 0. If a value is entered as zero (or blank) leave the condition on the master file alone. If a position value is entered this condition will be added to the condition (or override the specification) on the master files.

Lattice type code

col. 42 I1=1 A-centered ($k+\ell=2n$)
=2 B-centered ($h+\ell=2n$)
=3 C-centered ($h+k=2n$)
=4 F-centered ($h+k=2n$, $h+\ell=2n$, $k+\ell=2n$)
=5 I-centered ($h+k+\ell=2n$)
=6 R-observe ($-h+k+\ell=3n$)
=7 R-reverse ($h-k+\ell=3n$)
=8 Hexagonal ($h-k+\ell=3n$)
=9 or 0 Primitive (no conditions)

h k 0 reflections

col. 44 I 2=0 no conditions
=1 a-glide (h=2n)
=2 b-glide (k=2n)
=3 n-glide (h+k=2n)
=4 d-glide (h+k=4n, h=2n, k=2n)

h 0 ℓ reflections

col. 46 I 3=0 no conditions
=1 a-glide (h=2n)
=2 c-glide (ℓ =2n)
=3 n-glide (h+ℓ =2n)
=4 d-glide (h+ℓ =4n, h=2n, ℓ =2n)

0 k ℓ reflections

col. 48 I 4=0 no conditions
=1 b-glide (k=2n)
=2 c-glide (ℓ =2n)
=3 n-glide (k+ℓ =2n)
=4 d-glide (k+ℓ =4n, k=2n, ℓ =2n)

h h ℓ reflections

col. 50 I 5=0 no conditions
=1 c(n)-glide (ℓ =2n)
=2 d-glide (2h+ℓ =4n)

$\bar{h}$ h ℓ reflections

col. 52 I 6=0 no conditions
=1 c(n)-glide (ℓ =2n)
=2 d-glide (2h+ℓ =4n)

h k h reflections

col. 54 I 7=0 no conditions
=1 b(n)-glide (k=2n)
=2 d-glide (2h+k=4n)

h k $\bar{h}$ reflections

col. 56 I 8=0 no conditions
=1 b(n)-glide (k=2n)
=2 d-glide (2h+k=4n)

h k k reflections

col. 58 I 9=0 no conditions
=1 a(n)-glide (h=2n)
=2 d-glide (2k+h=4n)

h k $\bar{k}$ reflections

col. 60 I 10=0 no conditions
=1 a(n)-glide (h=2n)
=2 d-glide (2k+h=4n)

h 0 0 reflections

col. 62 I 11=0 no conditions
=1 2_1 or 4_2 screw (h=2n)
=2 4_1 or 4_3 screw (h=4n)

0 k 0 reflections

col. 64 I 12=0 no conditions
=1 2_1 or 4_2 screw (k=2n)
=2 4_1 or 4_3 screw (k=4n)

0 0 ℓ reflections

col. 66 I 13=0 no conditions
=1 2_1, 4_2 or 6_3 screw (ℓ=2n)
=2 3_1, 3_2, 6_2 or 6_4 screw (ℓ=3n)
=3 4_1, or 4_3 screw (ℓ=4n)
=4 6_1 or 6_5 screw (ℓ=6n)

Item 16: Atom position cards (2A4, 2F6.1, 4F10.6, 18X, I2)

cols. 1-8 (Atom(N,I), N=1,2) atom label

cols. 9-14 SF(I) f-table identification number (sequence number on Form Factor Card) or thermal neutron scattering cross-section used when NLAMDA is < 0. (NOTE: this is a floating point number).

cols. 15-20 AI(I) multiplier. Used to distribute atoms over sites of partial occupancy (i.e., special positions). This number need not be absolute because the data are scaled to SC(4), but they must be relative to the multiplier of all the other atoms. AI(I) = AI(1)/SC(4)

cols. 21-30 XYZ(1,I) the x coordinate of atom I

cols. 31-40 XYZ(2,I) the y coordinate of atom I

cols. 41-50 XYZ(3,I) the z coordinate of atom I

cols. 51-60 BETA(1,I) the isotropic temperature factor of the atom. If this number is zero, the atom card must be followed immediately by an anisotropic temperature factor card (6F10.5)(BETA(K,I), K=1,6) for β_{ij}'s (uses ORFLS version with β_{12} containing factor of 2, etc.) Isotropic and anisotropic temperature factors may be mixed.

cols. 79-80 ISFA(I) I-format :

ISFA(I) anomalous form factor identification number (sequence number on Form Factor Card, including Cromer polynomial code numbers in the sequence).

Item 17: Optional cards placed after atom (and temperature factor) cards (called only if NNF code requests external form factor).

Card A Name Card (2A4)

cols. 1-8 any identifier

Card B Scattering Factor Data Cards

Cromer polynomial format, 2 cards, (8F10.5)

FX(9,I) 9 values to fit the equation

$$FI = \sum_{i=1}^{4} \left(a_i e^{-(\sin^2\theta/\lambda^2)b_i} \right) + C$$

in the order a_1, b_1, $a_2 \ldots$, b_4, c

URHO (NWL,I) mass absorption coefficient for the radiation used

WEIGHT (I) atomic weight

Anomalous dispersion - single value format, 1 card (8F10.5)

FX(NAS,I) f' - a single value valid for all $\sin\theta/\lambda$ for the radiation used

FX(NAS+1,I) f'' - a single value valid for all $\sin\theta/\lambda$ for the radiation used

Item 18: Absorption card (8F10.5) (usually omitted)

optional - included if NABS $\neq 0$

the cylindrical absorption curve for μR for A^{-1} values from $\theta = 0^o$ to $\theta = 90^o$ in 5^o intervals

cols. 1-10 A(1) A^{-1} for $\theta=0^o$

cols. 11-20 A(2) A^{-1} for $\theta=5^o$

cols. 21-30 A(3) A^{-1} for $\theta=10^o$

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cols. 21-30 (3rd card) A(19) A^{-1} for $\theta=90^o$

Item 19: Control card 3 (3F6.2,7I2,3X,5F5.4,F6.2,I2)

cols. 1-6 W in $^o2\theta$ cols. 7-12 TTHETA in $^o2\theta$

W is the half-width of a diffraction profile at the 2θ value specified by TTHETA. If W=0, W defaults to 0.075 at TTHETA = 40.0

cols. 13-18 SCMAX F-format

This number contains both the peak maximum for the plot routine and a code to control the ^{o}/in. horizontal scale. Best explained by example: 100.2 means a vertical scale of 100 at a horizontal scale of 2^{o}/in. This is the value assumed by the program in SCMAX = 0. Peaks over 100 will be truncated at 100. Other options of the decimal part are .1=4 in., .2=2^{o}/in., .3=1^{o}/in. and .4=0.5^{o}/in.

col. 20 blank
col. 22 =6
col. 24 =0 Cauchy curve will be used (usual case)
=1 Gaussian curve will be used
col. 26 =0
col. 28 =0
col. 30 =NPR the number of copies of the summary output desired. If greater than 2 a third copy will be punched--this is used as input to SOPREF.

cols. 31-32 NCC=0 plot pattern on CALCOMP plotter
=1 skip plot
cols. 36-40 SCA
cols. 41-45 SCB F-format
cols. 46-50 SCC Parameters for abridged listing
cols. 51-55 SCD
cols. 56-60 SCE

SCA - SCE are parameters used for abridging the summary. Reflections whose d are equal or greater than SCB will be listed if the integrated intensity is equal or greater than SCA. Reflections whose d lies below SCB and is equal or greater than SCD will be listed if the integrated intensity is equal or greater than SCC. Reflections whose d lies below SCD will be listed if the integrated intensity is equal or greater than SCE. In addition all reflections whose d lies below SCD will be listed if the integrated intensity is equal or greater than SCE. In addition all reflections whose peak intensity equals 0 (resulting from NLIST criterion) will be deleted. This summary should be suitable for listing in a publication

cols. 61-66 SCMAX2

If SCMAX 2 is non zero a second plot will be made using SCMAX2 as the scale factor and code control for horizontal scale. Number is used in the same way as SCMAX.

Item 20: Sentinal card (A2)

cols. 1-2 $* go back to Item 12 and rerun for a second data set
≠$* program will terminate

VI. XRAY execution: Submit the above items punched on cards at the Computer Center with instructions that it be run on the large XRAY system at night.

I. Program language and type: FORTRAN IV - large XRAY system

II. Function: to search the JCPDS diffraction file and match it against an unknown X-ray powder diffraction pattern.

III. Source: Original program by Vand and Johnson. The twelfth revised version of this program for the IBM 360 was extensively rewritten for the XDS Σ 5 by R. Snyder.

IV. Procedure: The input for this version of the search program has been kept compatible with that for version XII of the Johnson program. A description of the original program is available from the JCPDS, 1845 Walnut St., Philadelphia, Pa. 19103.

V. Data set up: For normal application of this program there is an interactive program which will set up and punch an input deck (see SUSEARCH section II B3). The full description follows:

Item 1: !JOB FXRAY,75(User's name),5

Item 2: !ASSIGN F:16,(FILE,ASTMFILE,FSNYDER),(IN)

Item 3: !ASSIGN F:5, (DEVICE,SI)

Item 4: !ASSIGN F:6, (DEVICE,LO)

Item 5: !ASSIGN F:77, (DEVICE,NO)

Item 6: !RUN (LMN,LMSEARCH,FSNYDER)

Item 7: !DATA

Item 8: col. 1-76 any title information

Item 9: Control card

The parameter card. The program will supply a reasonable set of parameters, default parameters, if a value of zero is given.

col. 1 (A) IFL, the subfile of the PDF to be searched.
blank = all subfiles
A = alloy
O = organic
I = inorganic
D = dual (i.e., both inorganic and organic)
M = mineral
Default = blank

col. 3 (I) RESOL, resolution condition.
0 = normal
1 = Guinier
Default = 0

cols. 5-8 (I) MM, the number of lines in unknown pattern
Default - computer will count number of peaks

cols. 9-12 (I) IW, the error window
Default = 2

cols. 13-16 (I) KUTØFF, the minimum acceptable value of log. int. match in range considered above backround
Default = 2

cols. 17-20 (I) NUMBER, the minimum acceptable number of line matches in range considered above background
Default = 3

col. 22 (I) KEYRD, input spacing data is
0 = d values
1 = degrees 2θ
Default = 0

col. 23 (I) KEYRAD, or Radiation type (only used if KEYRD = 1) CuKα , 2 = MoKα, 3 = CrKα . If molybdenum $K\alpha_1$ radiation, an error window of 3 should be used.

cols. 25-28 (I) IPERCT, the min. acceptable percent of line matches in range considered above background
Default = 33

cols. 29-32 (I) ICYCLE, the number of cycles
Default = 0

cols. 33-36 (I) IWCY, the increase of IW per cycle
Default = +1

cols. 37-40 (I) KUTOCY, the increase of KUTØFF per cycle
Default = +5

cols. 41-44 (I) NUMCY, the increase of NUMBER per cycle
Default = +1

cols. 45-48 (I) IPERCY, the increase of IPERCT per cycle
Default = +10

cols. 49-52 (I) JBKGR, the background intensity (0-100 scale)
Default = +1 or half lowest given intensity

cols. 53-60 (F) DHI, the upper limit of the d-spacing range which could be observed by the instrumentation used
Default = error window above largest measured d

cols. 61-68 (F) DLO, the lower limit of the d-spacing range observed
Default = error window below smallest measured d

cols. 69-73 (A) OPTION SOLID - Solid Solution,
MINOR - Minor Phase,
MAJOR - Major Component
Default = Major

Item 10: The positive element and preconceived possibilities card. Chemical elements on this card and the following card must be right justified, two columns per element, that is, single letter elements must be punched with a blank then the letter, e.g., a list of sodium, hydrogen, lithium, iron, nickel, oxygen and platinum would be punched NA HLIFENI OPT.

With this data starting in

col. 1 and none beyond col. 50, RE (Rare Earth) punched in column 49 and 50 will cause all the rare earth elements from La to Lu, inclusive, to be used as positive elements in addition to any other punched in column 1 - 48.

The letters TU (transuranium) punched in column 49 and column 50 of the position element card will cause all the elements from Ac to Fm to be included automatically in the positive element list.

A Q in column 1 calls for the periodic table

Preconceived possibilities: The PDF card numbers of patterns which are to be printed out in the order given even if not found to be a match by the search program. Each must consist of six digits with no spaces. (A maximum of five patterns, 1-24, 6-432, 11-4 and 16-432; the card would contain 010024060432110004160432 starting in column 51). In other words, the six numbers are divided into a two digit field for the card set and a four digit field for the card in that set. The minimum contents for this card is 000000.

Item 11: The negative element card. These mustbe punched right justified, two columns per element as in item 10 with none beyond column 80.

A Q punched in col. 1 will cause all elements (thru Fermium) not specifically designated as positive elements to be used as negative elements.

If Q is used, the undetermined elements start in column 51 with the same type of rules as specified for item 10. A total of 15 elements may be specified as undetermined.

Item 12: Positive functional groups. Those functional groups which are known to be present in the unknown (from spot or other Chemical tests or X-ray fluorescence).

Item 13: Negative functional groups. Those functional groups which are known to be absent in the unknown (from spot or other chemical tests)

NOTE: The input for both these cards is as follows:

Punch chemical group exactly as the group appears in ***output*** under formulae--notice the spaces--this is extremely important. Eight groups can be external starting in col. 1, 11, 21, etc. (i.e., ⌀h2⌀O..⌀S⌀O4..⌀O⌀H)

Item 14: These cards contain the pairs of d-spacings and intensities measured on the unknown pattern. These need not be in order.

Punch the d-spacing, then its intensity (scale 1-100). The d-spacing must contain a decimal point and the intensity must be given and must not contain a decimal point.

These cards are of the format (8.(F7.3,I3)). Then one blank card.

Items 8-14 may be repeated as many times as unknown diffraction patterns are available.

Item 15: !EOD

Interpretation of Program Output

The six sections of the program are labeled INPUT, OUTPUT, TOPONES, REPORT, MATCHD and SUBSTI.

a. INPUT. This is a summary and description of the input parameters and data and should be carefully checked for correctness.

b. OUTPUT. The output section gives various numerical measures of the degree of fit of the unknown to the PDF patterns, disregarding chemical information; hence, isostructural compounds will appear.

c. TOPONES. Four groups of 50 patterns each are possible as follows: chemically correct, chemically incorrect, chemically unknown no chemistry given, and disregarding chemistry.

d. REPORT. The entire powder pattern, for those standards retrieved, which are chemically correct, is printed out.

e. MATCHD. The matching of the d values (with the error window) of the standard is done under this section of the program output.

f. SUBSTI. The process of the subtraction of the scaled standard reference patterns with the unknown is done in this section of the program output.

VI. XRAY execution:

Submit the above items punched on cards at the Computer Center with instructions that it be run on the large XRAY system at night.