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# NASA TECHNICAL
# MEMORANDUM

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## COMPUTERIZED DATA COLLECTION AND REDUCTION
## FROM AN X-RAY DIFFRACTOMETER

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**NASA**

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## INTRODUCTION

A series of computer programs has been written for use with a Philips X-ray Diffractometer and a Hewlett Packard 9825A Desk Top Computer. These programs permit the collection and storage on disk of the number of X-ray counts and the associated 2-theta angles across line profiles. Automatic background subtraction, integrated intensity, correction for the angular dependence of the Lorentz, polarization, and atomic scattering factors, peak location, K-alpha 2 removal, and calculation of Fourier coefficients are performed. This technical note is documentation for these programs and should provide a guide to their use. The programs are written in HPL which is a Hewlett Packard variation of BASIC. The programs are written for a computer configured with a disk drive, but they can be easily modified to run from the cassette tape drive that is integral to the 9825A Computer.

Copies of these programs are available on cassette from the author.

## HARDWARE

With the exception of the Angle Mode Programmer (AMP) and the Output Interface, the Philips Electronics equipment used is standard X-ray diffraction hardware.

The operation of the AMP and Output Interface is as follows: data initiation is started by pushing "run" on the AMP and the diffractometer advances to the first angle that has been programmed into the AMP. This angle is sent to the Output Interface. Control is turned over to the Scaler/Timer. After a preset length of time the Scaler/Timer stops data acquisition, sends the number of counts that it has collected and the length of time that it collected data to the Output Interface, and sends a signal to the AMP that it has completed data acquisition. The AMP causes the diffractometer to advance by the step size set on the Motor Controller and compares the new angle of the diffractometer with the scan stop angle that has been preprogrammed into the AMP. If the new angle of the diffractometer exceeds the scan stop angle, data acquisition is halted, and the measurement is completed. If the new angle does not exceed the scan stop angle, the data acquisition cycle is repeated.

During this cycle the Output Interface has received the number of counts collected during the preset time, the length of the preset time, and the angle of the diffractometer. This data is already digitized going into the interface. The Output Interface appropriately formats this string of data for the kind of output device that is used. The formatting controls should be set as follows:

Mode --- repeat

Parity --- odd

Format --- normal

Output --- TTY.

With this formatting a typical output appearing on the DEC writer is shown in Figure 1. Column A is the number of counts collected. Column B is 100 times the number of seconds in which the counts were collected. Column C is 100 times the diffractometer 2-theta angle. Column D has no significance here.

To interface the Hewlett Packard 9825A Computer to the Philips equipment a Newlett Packard 983036A Option 001 Serial Input/Output (I/O) Interface is required. Pin 1 is connected to instrument ground, and pin 3 is connected to the output signal of the Philips Output Interface. Since the Philips data output is BNC and the Serial I/O interface is a 25 pin connector, these connections must be made carefully to avoid bending or shorting pins. Certain switches internal to the I/O interface must be set for proper operation. The switches must be set to: "Current Loop," 2 stop bits, Odd Parity, and 8 bits/character. The device select code is 11 and can be set on the outside of the I/O interface.

The basic 9825A computer accepts Read Only Memory (ROM) chips that extend the software capabilities. The programs described in this report assume that the Advanced Programming, Advanced I/O, String Variable, and Disk Control ROMs are in place. The Hewlett Packard 9885M Flexible Disk Drive must also be connected to the computer. The 9825A has an integral cassette tape drive that can be used in place of the disk drive. During line by line documentation of the programs, some of the program modifications that are required to operate this cassette drive will be mentioned. Generally, disk operation is preferable because of more flexible addressing, greater capacity and speed, and a lower error rate.

## SOFTWARE

### "datrd"

This program is stored on track 0, file 1 of the cassette and reads pairs of X-ray counts and the diffractometer 2-theta angle, prints out this data, and stores the counts and angles on disk for future use. A listing of the program is in Figure 2. The following discussion of the program should help the user to understand how the program works and suggests possible modifications that may be useful for particular applications. The numbers refer to lines in the program.

1. The user is asked by the computer how many data points are to be collected. The number of points, of course, depends on how wide the line is and the step size between angles.

4. D is a dummy variable and is not used except as a storage for serially output data.

5. C is the vector containing the X-ray counts.

7. B is 100 times the number of seconds in which data is collected. If operation with variable time increments 's desired, the counts vector can be normalized by dividing by B to give counts per second instead of just counts.

8. A is the vector containing 100 times the 2-theta angle of the diffractometer.

10. The correct 2-theta angle is printed.

14. The names of the files under which the data are stored are listed. The first word after "files" is the name of the file under which the angles are stored, and the second word after "files" is the name of the file under which counts are stored. These names must be entered before the program is run and space must be reserved on the disk for them using an "open" command. Any previous information in these files will be lost.

## "Xfoure"

This program reads data off the disk, performs a background subtraction, computes the integrated intensity of the line, corrects the line for the angle dependence of the polarization factor and the atomic scattering factor, calculates the peak by a three point parabolic fit, subtracts the K-alpha 2 component, again calculates the peak, and finally calculates the Fourier coefficients normalized to the area of the peak.

Except for the Fourier coefficients all these data are standard information that the X-ray diffractionist often wants to know about a given line. The Fourier coefficients are used to deconvolute a given profile from the line profile of a well annealed specimen that contains no stress and has grains large enough to cause no particle size line broadening [1,2]. If the asymmetric coefficients are small compared to the symmetric coefficients (as they usually are), the true line profile (that is not including instrumental broadening) can be calculated by dividing the observed coefficients by the same coefficients of a well annealed specimen. The quotients are the Fourier coefficients of the line due only to various X-ray active defects such as inhomogeneous stress, small particle size, dislocations, vacancies, and stacking faults. More details can be found in Warren [3].

"Xfoure" is located on track 0, file 0, and the listing is shown in Figure 3. Important lines will be commented on individually.

4 & 5. The computer asks which disk files to use for the angle data and the count data. This data must have been previously stored on the disk under the appropriate file name. If operation of the tape cassette is desired, lines 4 through 9 should be replaced by commands to load the angle data into vector A and the counts into vector C. File names cannot be used so the program changes must be made before the program is run.

10 to 16. The data is formatted and output for the operator to verify.

18. The computer asks the operator to examine the output data and determine where the line begins and ends. It assumes that the angles are entered in increasing 2-theta values; "L" is the lefthand value where the line begins, and "R" is the righthand value as though one were looking at a strip chart.

22. A linear fit is made to the background.

23. Any negative count values resulting from statistical fluctuations in the line tails are set equal to zero. This is the only explicit smoothing in the program. A standard multipoint smooth was not used because it reduces angular resolution, causes periodicities that may appear in the Fourier coefficients, and some smoothing occurs during deconvolution in any case.

25. If this line is removed, the background subtracted line will be printed out.

28. The correction for the Lorentz and polarization factors starts here. The Lorentz factor is a geometric factor caused by the size of the diffracted cone of X-rays, and the polarization factor exists because electrons scatter X-rays preferentially in the forward direction so parts of a line profile on the low angle side are less than on the high angle side.

32. This line is only correct for a copper X-ray tube and a graphite monochromator. If some other conditions are used, ".75 cos A[I]" should be replaced by "$\cos^2 2\alpha \cos$ A[I]" where $2\alpha$ is 180 degrees minus the diffraction angle of the monochromator. If no monochromator at all is used this line should be replaced by

$$\frac{(1 + \cos^2 A[I]}{\sin^2 \frac{A[I]}{2} \cos \frac{A[I]}{2}} \rightarrow Q$$

35. If this line is removed, the Lorentz-polarization factor corrected line will be printed out. In this program the LP correction is made before the Fourier coefficients are calculated. At large values of theta the main cause of broadening in the line of an annealed specimen is spectral breadth of the X-ray source, while at small theta values the main cause of broadening is due to instrumental misalignments. If the broadening caused by misalignments is dominant, the LP correction should be made after the Fourier coefficients are calculated [4]. In any case the differences are small.

40. The Atomic Scattering factor correction subroutine is called.

47. Q is the corrected sum of all the counts in the line. This is the integrated intensity. When comparing the integrated intensities of different lines, the angular interval between points must be corrected for. This interval is printed out by line 48.

51. The numbers of three equally spaced points that span the peak are asked for and must be entered.

53 to 55. The corrected number of counts that occur at these points are printed out. For best accuracy these points should be 85 percent of the peak above background [5].

59. A parabola is fit through these three points and the peak of the parabola is calculated [6]. Experience has shown that the peak position is not very sensitive to which three points are chosen. Typically, the peak can be repeated to ±0.002 degrees if the 85 percent rule is observed. Naturally, the

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statistically uncertainty of the data must be very small for such accuracy. This can be assured by long counting times and is not usually a problem near the peak where the count rate should be high. Another source of statistical inaccuracy comes from using samples with too large a grain size to give a truly random distribution of particle orientations. Usually the particles should be less than 15 μm for cubic crystals and smaller for materials with a lower degree of symmetry [7].

62. The K-alpha 2 component of the X-ray line will now be removed.

64. r1 and r2 are the wavelengths in angstroms of the K-alpha 1 and K-alpha 2 radiation. The numbers entered in the program are for copper radiation. If another tube is used the appropriate values must be entered.

65. The angular separation of the components of the doublet is calculated at the low angle side of the line and for a weighted average of the wavelengths from the tube.

66. This angular separation is printed out.

67. The data occurs in discrete step intervals which are not likely to be even submultiples of the angular separation so some interpolation between steps will be necessary. This line calculates the whole number of steps in the angular separation and outputs this number in line 68.

71. The angular separation is calculated for each angle across the line. This gives slightly higher accuracy than the standard Rachinger correction which usually calculates the separation once for the peak and assumes that this separation is constant across the line [8]. To obtain three decimal place accuracy from data taken at intervals of 0.01 degrees, this higher precision method is necessary. The assumption is still being made, however, that the K-alpha 1 and K-alpha 2 peaks have the same shape, which is not strictly true.

73. Here is the actual Rachinger correction to the number of counts. For interpolation purposes the line is assumed to be linear between data points, and the K-alpha 1 line is assumed to be twice the size of the K-alpha 2 line. The linearity assumption is quite good for the small step sizes (0.01 degree) usually used. The assumption about the ratio of the peaks is also good if a low resolution/high reflectivity monochromating crystal such as the Philips graphite crystal is used. A sharper monochromating crystal may alter this ratio. If it is desired to use a different ratio, the factor "0.5" which occurs twice in this line should be replaced by the correct ratio.

78. If this line is removed, the K-alpha 1 line will be printed out.

94. The K-alpha 1 peak is printed out using a three point parabolic fit.

96. N is the number of Fourier coefficients that will be calculated. Here it is set to 12 but can be easily changed.

97 & 98. The line is moved so that the peak occurs at the origin. This is not strictly necessary for the Fourier analysis but it simplifies writing the Fourier analysis subroutine.

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102. The Fourier analysis subroutine requires an odd number of equally spaced points in the line. This line determines if there is an odd number of points in the line and adds a point with 0 counts on the high angle of the line if needed.

104. The vector Y now contains the count information for the K-alpha 1 line.

106. If this line is removed the vector Y is printed out.

114. The constant term in the Fourier analysis is printed out as A (0).

115 to
118.  Formatting for the Fourier coefficients. In line 117 the coefficients are normalized by the constant term. The constant term, A (0), is the area under the curve which is not relevant for line broadening analysis. By normalizing the coefficients the shapes of lines collected at different X-ray beam currents and for different time intervals can be compared. The sin and cos coefficients are output with a prime (') to indicate this normalization. A' is the cosine coefficient and B' is the sine coefficient. X-ray lines are nearly symmetric so B' is much smaller than A' coefficient. The B' coefficients are not very accurate because these coefficients are sensitive to changes in the peak position as small as 0.002 degree. This is not surprising since the line asymmetry is small to start with and any change in asymmetry is likely to have a large effect.

120. The calculation of Fourier coefficients using Simpson's rule to evaluate the integrals begins here.

123. X and Y are the current value of the angle and the count.

124. Except at the end points of the evaluation, M alternates between 2 and 4 in Simpson's rule.

127. The values that go into the summation in Simpson's rule are calculated here.

129 to
132.  The constant term A (0) is calculated.

135. The atomic scattering factor correction is started here. This correction arises because atoms scatter X-rays most efficiently in the direction of the X-ray beam. The scattering cross section varies inversely with the sine of the scattering angle. Since this factor is angle dependent, the shape of the line is changed and must be corrected for. The atomic scattering factor depends in a rather complicated way on the wavelength of the radiation and on the atomic number of the atom that is doing the scattering. Values of the atomic scattering factor are available and can be used for an alloy assuming an average atomic number for the alloy. If the components in the alloy are close in atomic number, this averaging is a good approximation. If the components of the alloy are widely separated in the periodic table, the various atomic scattering factors of the individual elements must be averaged rather than the atomic number. This program was written for copper nickel alloys where the atomic number averaging is a good approximation. If the atomic numbers of the constituents of the alloy are not close together, the correction to the program is not simple and it may be best to skip this correction. The correction is never large for narrow lines and usually only makes minor changes in the line shape. The correction can be skipped by removing line 40.

There are two other line shape corrections that are sometimes mentioned in the literature. If the path length of the X-rays in the sample depends on theta, differential absorption of X-rays takes place as a line is scanned. For the Bragg focusing geometry used in a diffractometer, absorption in the specimen attenuates all lines uniformly so no absorption correction is needed. Another correction is the temperature factor which changes line shape because planes with narrower spacing (that is greater Bragg angles) are more affected by thermal vibrations than are widely spaced planes where the spacing is large compared to the thermal vibrations. This correction is usually the smallest and its calculation is difficult for alloys. It has not yet been incorporated into this program.

137 to 143. These are the atomic scattering factors [9] of pure copper for one-tenth integer values of sin $\theta/\lambda$.

145. The atomic scattering factor is calculated for an alloy of copper and nickel by averaging the atomic number of the alloy.

149. The one-tenth integer value of sin $\theta/\lambda$ is calculated for the alloy. This value is needed because the table of atomic scattering factors in lines 137 to 143 gives the factors for discrete values of sin $\theta/\lambda$. If some other radiation than copper is used, the factor 1.5417 should be replaced by the wavelength of the radiation in angstroms.

150. This is a linear interpolation between entries in the values in the atomic scattering list. "H" is the final correction factor.

152. If this line is removed, the corrected value of the line will be printed out.

## "pkfd"

This program is located on track 0, file 2 and fits a parabola to three pairs of angles and counts that are manually entered. The peak of the parabola is calculated and output as the peak value of the line. The three angles must be equally spaced. The program is shown in ring 4.

8 to 13. The Lorentz Polarization Correction is made in exactly the same way that it is made in the program "Xfoure". See the documentation for that program for details.

14 to 35. The values for the atomic scattering factor of both copper and nickel are entered for discrete values of sin $\theta/\lambda$.

36. The atomic scattering factor of the alloy corresponding to the nearest discrete value of sin $\theta/\lambda$ is calculated. This calculation is slightly more accurate than the calculation made in "Xfoure" because the assumption of a constant value of the copper to nickel atomic absorption factor ratio is not made.

37, 40, and 43. The final values of the atomic scattering factor corrections are calculated using linear interpolation between the discrete values calculated in line 36. These factors are for each of the three entered angles.

44 to 46. The values of the corrected counts are printed out so that the operator can verify that they are sufficiently close to the peak that the parabola is a good approximation.

## "mpkf"

This program is located on track 0, file 3 and reads pairs of angles and counts directly from the diffractometer  and chooses several sets of three equally spaced points to calculate and output the peak from each of these three sets of values.  The listing is shown in Figure 5.

1 to 14. The data are read in exactly the same way that it is read in the program "datrd".  Angles are stored in the vector A, and counts are stored in the vector C.

15. T is the loop counter which determines the number of sets of points that will be used to calculate parabolas.  As the program is written, four sets will be chosen but any number less than L/2 can be chosen, where L is the number of data points entered.

16. The center point of the parabola is chosen to be "H" which is the largest value of the count vector.

The remainder of the program proceeds exactly the same as "pkfd".

## CONCLUSIONS AND RECOMMENDATIONS

These programs greatly simplify the collection and analysis of data taken from the X-ray diffractometer.  In addition, a versatile instrument system has been established that an engineer can program to his/her specific needs.

A number of additional features can be incorporated into the present data analysis programs such as:

1) An automatic decision making program that locates the start and finish of the peak.

2) Calculation of the peak centroid.

3) A peak location algorithm based on minimization of the asymmetric Fourier coefficients.

4) A quick measure of the peak breadth such as calculation of the peak breadth at half height.

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```
A 003457 B 000200 C 004329 D 020000
A 003494 B 000200 C 004329 D 020000
A 003483 B 000200 C 004330 D 020000
A 003508 B 000200 C 004331 D 020000
A 003500 B 000200 C 004332 D 020000
A 003449 B 000200 C 004333 D 020000
A 003399 B 000200 C 004334 D 020000
A 003300 B 000200 C 004335 D 020000
A 003262 B 000200 C 004336 D 020000
A 003141 B 000200 C 004337 D 020000
A 003072 B 000200 C 004338 D 020000
```

Figure 1.  Output from DEC writer.

```
0: dsp "This program read angles and counts and stores them on disk."
1: enp "How many data points?",M
2: dim A[M];dim C[M]
3: for I=1 to M
4: red 11,D
5: red 11,C[I]
6: prt "C[I]=",C[I]
7: red 11,B
8: red 11,A[I]
9: .01A[I]:A[I]
10: prt "A[I]=",A[I]
11: prt "I=",I
12: prt "   "
13: next I
14: files Atest,Ctest
15: sprt 1,A[*]
16: sprt 2,C[*]
17: end
*2736
```

Figure 2.  Program listing for "datrd".

```
0: enp "How many 2 theta values?",M
1: dim A$[6];dim C$[6]
2: deg
3: dim A[M];dim C[M]
4: enp "Which angle file?",A$
5: enp "Which count file?",C$
6: asgn C$,2
7: asgn A$,1
8: sread 2,C[*]
9: sread 1,A[*]
10: fmt c3,b,5x,c7,/
11: wrt 16,"2",16,"counts"
12: for I=1 to M
13: fmt f3.0,f6.2,f6.0
14: wrt 16,I,A[I],C[I]
15: next I
16: dsp "We are now starting the background subtraction"
17: beep
18: enp "Numbers where line begins and ends",L,R
19: dsp "R-L must be even"
20: C[L];0
21: for I=L to R
22: C[I]-0+(I-L)/(R-L)*(0-C[R]);C[I]
23: if C[I]<0;0)C[I]
24: fmt f3.0,f6.0,f6.2
25: gto 27
26: wrt 16,I,C[I],A[I]
27: next I
28: dsp "Starting LP correction"
29: dsp "Cu radiation and graphite mono. only."
30: prt "LP CORRECTED PEAK IS"
31: for I=L to R
32: sin(A[I]/2)^2cos(A[I]/2)/(1+.75cos(A[I])^2);Q
33: Q*C[I];C[I]
34: fmt f3.0,f6.2,/,f8.4
35: gto 38
36: wrt 16,I,A[I],C[I]
37: prt "   "
38: next I
39: beep
40: gsb "ASFCor"
41: prt "The integrated intensity is"
42: 0;Q
43: for I=L to R
44: C[I]+0;0
45: next I
46: fxd 2
47: prt Q
48: prt "The interval is",A[R+1]-A[R],"degrees two theta"
49: dsp "We are now locating the peak"
50: beep
51: enp "Choose three equally spaced  points  spanning peak. R-L even",Q,N,O
52: 0;T
53: prt "C[Q]=",C[Q]
54: prt "C[N]=",C[N]
55: prt "C[O]=",C[O]
```

Figure 3.  Program listing for "Xfoure".

```
56: A[N]-A[Q])r3
57: 1/C[O]-1/C[N])r2
58: 1/C[Q]-1/C[N])r1
59: A[Q]+r3((3*r1+r2)/(2r1+2r2)))P
60: fxd 3
61: prt "The peak is at",P,"degrees two theta"
62: dsp "We are now doing a Rachinger correction"
63: dsp "this is for a Cu tube only"
64: 1.54433)r2;1.54051)r1
65: 3*57.2958*((r2-r1)tan(A[L]/2)/(2r1+r2)))A
66: prt "Delta theta =",A
67: int(2A/(A[P+1]-A[P])))D
68: prt "steps back is",D
69: dsp "Assume alpha 1:2 ratio is 2:1"
70: for I=L+D to R
71: 57.2958*.00382*tan(A[I]/2)/1.54178)A
72: int(2A/(A[P+1]-A[P])))Q
73: C[I]-.5C[I-Q]-.5frc(2A/(A[P+1]-A[P]))(C[I-Q-1]-C[I-Q]))C[I]
74: if C[I]<0;0)C[I]
75: next I
76: for I=R-D to R
77: 0)C[I];next I
78: gto 88
79: prt "The K alpha 1  line is"
80: prt "I Angle Count"
81: fmt f3.0,f6.2
82: for I=L to R-D
83: wrt 16,I,A[I]
84: fxd 5
85: prt "C[I]=",C[I]
86: prt "  "
87: next I
88: dsp "Now find the K alpha 1 peak"
89: T)Q
90: 1/C[O]-1/C[N])r2
91: 1/C[Q]-1/C[N])r1
92: A[Q]+r3((3r1+r2)/(2r1+2r2)))P
93: fxd 3
94: prt "The K alpha 1 peak is at",P,"degrees two theta"
95: fxd 5
96: 12)N
97: for I=1 to M-1;A[I]-P)A[I];next I
98: for I=1 to R-L+1;A[L-1+I])A[I];next I
99: A[1])H
100: A[2]-A[1])W
101: R-L+1-D)K
102: if frc(K/2)=0;K+1)K
103: dim Y[R-L+1]
104: for I=L to R;C[I])Y[I-L+1]
105: next I
106: gto 111
107: for I=1 to R-L+1
108: prt "I=",I
109: prt "Y[I]=",Y[I]
110: next I
111: gsb "FOURE"
```

Figure 3.   (Continued)

```
112: fxd 4
113: prt "Coefficients"
114: prt "A(0)=",H[0]
115: for I=1 to N
116: fmt c3,f2.0,c2,x,f9.4,/,c3,f2.0,c2,x,f9.4,/
117: wrt 16,"A(",I,")=",H[I]/H[0],"B(",I,")=",B[I]/H[0]
118: next I
119: end
120: "FOURE":rad;cfg 2;dim H[0:N],B[N];1)J;0)I;(K-1)W)D
121: if K/2=int(K/2);sfg 2;dsp "ODD NO OF PTS";ret
122: if (I+1)I))K;gto +8
123: H+(I-1)W)X;Y[I])Y;if I=1 or I=K;1)M;gto +3
124: if M=4;2)M;gto +2
125: 4)M
126: cos(2(X/D)E))S)F;sin(E))2)G
127: MYF+H[J])H[J];MYG+B[J])B[J]
128: if (J+1)J)<=N;SF-ZG)T;ZF+SG)G;T)F;gto -1
129: 1)J;gto -7
130: Y[1]+4Y[2]+Y[K])S;3)I
131: S+2Y[I]+4Y[I+1])S;jmp (I+2)I))K
132: SW/3D)H[0];1)J
133: 2H[J]W/3D)H[J];2B[J]W/3D)B[J];jmp (J+1)J))N
134: ret
135: "ASFCor":enp "What atomic percentage of nickel is in sample?",Q
136: dim F[8]
137: 29)F[1]
138: 25.9)F[2]
139: 21.6)F[3]
140: 17.9)F[4]
141: 15.2)F[5]
142: 13.3)F[6]
143: 11.7)F[7]
144: for I=1 to 7
145: F[I]-.01Q*.0406F[I])F[I]
146: next I
147: prt "ATOMIC SCATTERING FACTOR CORRECTED LINE IS"
148: for I=L to R
149: 1+int(10sin(A[I]/2)/1.54178))r4
150: F[r4]-(F[r4]-F[r4+1])frc(10sin(A[I]/2)/1.54178))H
151: C[I]/H^2)C[I]
152: gto 158
153: fxd 5
154: prt "C[I]=",C[I]
155: prt "A[I]=",A[I]
156: prt "I=",I
157: prt "  "
158: next I
159: ret
*3678
```

Figure 3.   (Concluded)

```
0: dsp "This program uses three points on a parabola to determine the peak"
1: enp "ang. 1",C
2: enp "ang. 2",E
3: enp "ang. 3",I
4: enp "f(1)",G
5: enp "f(2)",H
6: enp "f(3)",J
7: enp "what atomic percentage of nickle is in the sample?",Q
8: sin(C/2)*sin(C/2)*cos(C/2)*G/(1+.75cos(C)*cos(C))>G
9: sin(E/2)*sin(E/2)*cos(E/2)*H/(1+.75cos(E)*cos(E))>H
10: sin(I/2)*sin(I/2)*cos(I/2)*J/(1+.75cos(I)*cos(I))>J
11: sin(C/2)/1.54178>M
12: sin(E/2)/1.54178>R
13: sin(I/2)/1.54178>S
14: dim F[21]
15: 29>F[1]
16: 25.9>F[2]
17: 21.6>F[3]
18: 17.9>F[4]
19: 15.2>F[5]
20: 13.3>F[6]
21: 11.7>F[7]
22: 10.2>F[8]
23: 9.1>F[9]
24: 8.1>F[10]
25: 28>F[11]
26: 25>F[12]
27: 20.7>F[13]
28: 17.2>F[14]
29: 14.6>F[15]
30: 12.7>F[16]
31: 11.2>F[17]
32: 9.8>F[18]
33: 8.7>F[19]
34: 7.7>F[20]
35: 1+int(10*M)>r2
36: F[r2]-.01*Q*(F[r2]-F[r2+10])>F[r2]
37: F[r2]-(F[r2]-F[r2+1])*frc(10M)>K
38: 1+int(10R)>r3
39: F[r3]-.01Q*(F[r3]-F[r3+10])>F[r3]
40: F[r3]-(F[r3]-F[r3+1])*frc(10R)>L
41: 1+int(10S)>r4
42: F[r4]-.01Q*(F[r4]-F[r4+10])>F[r4]
43: F[r4]-(F[r4]-F[r4+1])*frc(10S)>N
44: G/K^2>G
45: H/L^2>H
46: J/N^2>J
47: prt "G=",G
48: prt "H=",H
49: prt "J=",J
50: fxd 3
51: C+((E-C)/2)((4H-3G-J)/(2H-G-J))>P
52: prt "The peak is at "
53: prt P
54: prt "deg. two-theta"
55: end
*8346
```

Figure 4.  Program listing for "pkfd".

```
0: dim F[21]
1: enp "How many data points?",L
2: enp "What atomic percent of nickel?",Q
3: dim A[L];dim C[L]
4: for I=1 to L
5: red 11,D
6: red 11,C[I]
7: prt "C[I]=",C[I]
8: red 11,B
9: red 11,A[I]
10: .01A[I])A[I]
11: prt "A[I]=",A[I]
12: prt "I=",I
13: prt "    "
14: next I
15: for T=1 to 4
16: max(C[*])>H
17: for I=1 to L
18: if C[I]=H;gto "LABEL"
19: next I
20: "LABEL":A[I])E
21: max(C[*])>H
22: C[I-T])G
23: C[I+T])J
24: A[I-T])C
25: A[I+T])I
26: sin(C/2)*sin(C/2)+cos(C/2)*G/(1+.75cos(C)*cos(C)))G
27: sin(E/2)*sin(E/2)+cos(E/2)*H/(1+.75cos(E)*cos(E)))H
28: sin(I/2)*sin(I/2)+cos(I/2)*J/(1+.75cos(I)*cos(I)))J
29: sin(C/2)/1.54178)M
30: sin(E/2)/1.54178)R
31: sin(I/2)/1.54178)S
32: 29)F[1]
33: 25.9)F[2]
34: 21.6)F[3]
35: 17.9)F[4]
36: 15.2)F[5]
37: 13.3)F[6]
38: 11.7)F[7]
39: 10.2)F[8]
40: 9.1)F[9]
41: 8.1)F[10]
42: 28)F[11]
43: 25)F[12]
44: 20.7)F[13]
45: 17.2)F[14]
46: 14.6)F[15]
47: 12.7)F[16]
48: 11.2)F[17]
49: 9.8)F[18]
50: 8.7)F[19]
51: 7.7)F[20]
52: 1+int(10*M))r2
53: F[r2]-.01*Q*(F[r2]-F[r2+10]))F[r2]
54: F[r2]-(F[r2]-F[r2+1])*frc(10M))K
55: 1+int(10R))r3
56: F[r3]-.01Q*(F[r3]-F[r3+10]))F[r3]
```

Figure 5.  Program listing for "mpkf".

15

```
57: F[r3]-(F[r3]-F[r3+1])frc(10R))L
58: 1+int(10S))r4
59: F[r4]-.01Q*(F[r4]-F[r4+10]))F[r4]
60: F[r4]-(F[r4]-F[r4+1])frc(10S))N
61: G/K^2)G
62: H/L^2)H
63: J/N^2)J
64: prt "G=",G
65: prt "H=",H
66: prt "J=",J
67: fxd 3
68: C+((E-C)/2)((4H-3G-J)/(2H-G-J)))P
69: prt "The peak is at"
70: prt P
71: prt "deg. two-theta"
72: prt "   "
73: next T
74: end
*27620
```
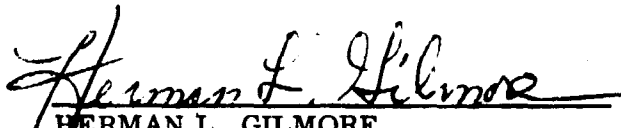
Figure 5.   (Concluded)

APPROVAL


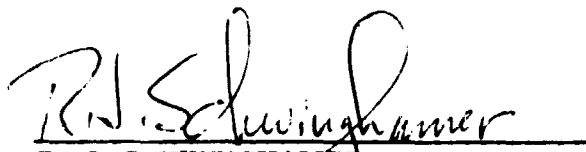COMPUTER PROGRAM FOR X-RAY DATA REDUCTION


by

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