

NOTE

COMMENTS ON FORTRAN ROUTINE FOR CALCULATING *d*-SPACINGS

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In Vol. 24, pp. 208–210, a program for calculating *d*-spacings at 0.01° (2θ) intervals was published. This program was specifically written to run on a large machine and required large amounts (approx. 250 K) of core storage. The program also used a constant increment for the calculation. Since pi is irrational, this constant could lead to an accumulative error in the calculations.

The two programs below read the radiating wave length, starting angle and the number of pages from the input keyboard (or other input device), and calculate and print one line at a time. This results in very low core storage

requirements, allowing the routines to run in mini-computer type machines. The routines also recalculate the index at the beginning of each line, avoiding the possible accumulative error.

Users should be cautioned that all FORTRAN compilers and Basic executors have some peculiarities that may require some rewriting, particularly in input/output.

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BASIC

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10 OPEN #0, "$LPT"
20 DIM S1$(20)
30 DIM #%, D1[10]
40 LET K=360/(2*3.14159265)
50 INPUT "/215/RADIATING WAVE LENGTH ? "W2
60 INPUT "/215/STARTING 2 THETA (IN DEGREES) ? "T4
70 INPUT "/215/NUMBER OF PAGES ? "J6
80 PRINT
90 PRINT #0, "/214/"
100 LET W1=W2/2
110 LET DO=T4
120 FOR J1=1 TO J6
130 PRINT #0; "/214/"
140 PRINT #0; " RADIATING WAVE LENGTH "; TAB (30); W2
150 LET S1$=" ##"
160 LET J8=19
170 FOR D9=0 TO 9E-02 STEP 1E-02
180 PRINT #0; USING S1$; (J8); D9;
190 LET J8=J8+10
200 NEXT D9
210 PRINT #0; " "
220 PRINT #0; " "
230 LET S1 $=" ## #####"
240 FOR J9=1 TO 5
250 FOR J2=1 TO 10
260 LET D2=DO
270 FOR J3=1 TO 10
280 LET T1=(D2/2)/K
290 LET D1[J3]=W1 / SIN (T1)
300 LET D2=D2+1E-02
310 NEXT J3
320 PRINT #0; DO;
330 LET J5=17
340 FOR J4=1 TO 10
350 PRINT #0; USING S1$; TAB (J5); D1[J4];
360 LET J5=J5+10
370 NEXT J4
380 PRINT #0; " "
390 LET DO=DO+.1
400 NEXT J2
410 PRINT #0; " "
420 NEXT J9
430 Next J1
    
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FORTRAN

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COMPILER DOUBLE PRECISION
THIS ROUTINE CALCULATES D SPACING AT .01 DEGREE
(2 THETA) INCREMENTS FROM THE RADIATING
WAVELENGTH INPUT FROM THE KEYBOARD
FROM A SPECIFIED STARTING THETA FOR A SPECIFIED
NUMBER OF PAGES
THERE ARE 50 LINES TO A PAGE SEPARATED
BY SPACES EVERY 10 LINES (FOR EASE IN READING)

DIMENSION D1 (10)
RK=360 / (2.*3.14159265)
ACCEPT "RADIATING WAVE LENGTH ? ", W2
ACCEPT "STARTING 2 THETA (IN DEGREES) ? ", T4
ACCEPT "NUMBER OF PAGES ", J6
W1=W2/2
DO=T4
DO 50 J1=1, J6
WRITE (12, 100)
WRITE (12, 101), W2
DO 10 J=1, 10
D1 (J)=(J-1) /100.
WRITE (12,102)(D1(J)J=1,10)
WRITE (12,103)
DO 20 J9=1,5
DO 30 J2=1,10
D2=DO
DO 40 J3=1, 10
T1=(D2/2.) / RK
D1(J3)=W1 /DSIN(T1)
D2=D2+.01
40 CONTINUE
WRITE (12,104)DO,(D1(J)J=1,10)
DO=DO+.1
30 CONTINUE
WRITE (12,105)
20 CONTINUE
50 CONTINUE
100 FORMAT (1H1)
101 FORMAT (" RADIATING WAVE LENGTH ",F10.6)
102 FORMAT (" ",17X,F5.2,9(5X,F5.2))
103 FORMAT (//)
104 FORMAT (" ",F5.1,10X,10(F9.5,1X))
105 FORMAT (" ")
END
    
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