Clays and Clay Minerals, Vol. 24, pp. 208–210. Pergamon Press 1976. Printed in Great Britain

NOTES

FORTRAN IV PROGRAM FOR COMPUTING *d*-SPACINGS AT 0.01° (2θ) INTERVALS

(*Received* 1 *April* 1976)

It is often desirable to obtain *d*-spacings at closer 2θ intervals than those normally found in published tables (most tables are in tenths of a degree 2θ). In many instances examination of X-ray powder diffraction peaks with a plastic overlay is sufficient for resolving constituent minerals. However, in some cases it is desirable or necessary to obtain a more precise determination for *d*-spacings. Such circumstances commonly result in larger distances between degree marks thereby allowing measurement to 0.01° 2θ. It is an elementary task to interpolate between *d*-spacings published at tenths of a degree 2θ in order to obtain the desired value. However, this becomes quite time-consuming, especially if several spacings are to be determined for each pattern and there are numerous patterns to interpret.

The availability of a table for *d*-spacings at 0.01° 2θ intervals is apparently lacking. Therefore, it is the purpose of this note to make available a simple program which computes and prints *d*-spacings at 0.01° 2θ intervals for any given radiation.

The program as it is reproduced here (Fig. 1) uses the wavelength for $CuK_{\alpha 1}$ radiation ($\lambda = 1.54056$, Klug and Alexander, 1974). Consequently, the *d*-spacings (in angström units) are only appropriate for $CuK_{\alpha 1}$ radiation. Wavelengths (WAVEL) for other sources of radiation may be substituted for 0.77028 Å. Approximately 250K is needed for storage on an IBM 360/370 system. Close to 2800 lines of *d*-spacings are printed at 0.01° 2θ intervals from 1.00° 2θ to 180.99° 2θ.

A sample of the output is given in Fig. 2. This section of print-out was chosen because it is frequently necessary to distinguish kaolinite in the presence of chlorite or *vice versa* without chemical treatment. As described by Biscaye (1964, 1965) the fast scan (2° 2θ/min) ~3.50 Å doublet can often be resolved into the 3.54 Å (004) peak of chlorite (25.12° 2θ = 25.14° 2θ) and the 3.58 Å (002) peak of kaolinite (24.84° 2θ = 24.87° 2θ) at slower goniometer speeds. Therefore, with this table it is an easy and quick task to determine *d*-spacings from peaks which may cluster around 25.0° 2θ.

Use of this table is quite simple. To find a *d*-spacing from an angle measured to tenths or hundredths merely scan the left hand margin of the table until the desired 2θ degree (in tenths) is reached, read the second column under "0.00" for resolution to tenths. If the angle was measured to hundredths of a degree 2θ continue to read across the table until the desired hundredths column is found, read the corresponding *d*-spacing. For example 24.86° 2θ ($CuK_{\alpha 1}$ radiation) has a *d*-spacing of 3.57859 Å.

Mr. Donald Murphy offered many helpful comments in simplifying output formats.

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      DOUBLE PRECISION D(180,100),THET,WAVEL
      DIMENSION DD(10), SYM(101)
C   WRITTEN BY MORTON E. WAKELAND, JR., MARINE SCIENCES INSTITUTE, UCONN
C   PROGRAM COMPUTES "D" SPACINGS FROM 1.00 TO 180.99 DEGREES 2-THETA
C   THIS PROGRAM IS FOR CU K-ALPHA RADIATION ONLY
C   D(I,J) IS THE STORED ARRAY FOR "D" SPACINGS
C   DD(J) IS USED FOR PRINTING TENTHS OF A DEGREE IN LEFT MARGIN OF PRINT OUT
C   READ IN SYM(I) TO SEPARATE 2-THETA ANGLES AND D-SPACINGS
C   ANY SYMBOL MAY BE SUBSTITUTED FOR THE STAR (*), USE ALPHANUMERIC FORMAT
      READ(5,104) (SYM(I), I = 1,101)
  104 FORMAT(80A1)
      DD(1) = .00
      DO 400 J = 2,10
      JJ = J - 1
      DD(J) = DD(JJ) + .1
  400 CONTINUE
C   BEGIN "D" SPACINGS AT 1 DEGREE 2-THETA
C   RADIANS MUST BE USED FOR THE ARGUMENT ON IBM SYSTEMS, THEREFORE
C   .5 DEGREES = .0087266 RADIANS
C   FOR COMPUTATION USE .5 DEGREES SINCE SIN(THETA) IS NEEDED NOT SIN(2-THETA)
      THET = .0087266
C   COMPUTE "D" SPACINGS USING THE BRAGG EQUATION FOR CU RADIATION
C   WAVELENGTH FOR CU IS 1.54056 A,  THEREFORE WAVEL/2 = .77028
C   WAVEL IS THE VARIABLE NAME  FOR THE DESIRED RADIATION WAVELENGTH
      DO 50 I = 1,180
      DO 55 J = 1,100
C   VALUES FOR OTHER TARGETS SHOULD BE SUBSTITUTED FOR WAVEL
      WAVEL = .77028
      D(I,J) = WAVEL/(DSIN(THET))
C   INCREMENT BY .01 DEGREE 2-THETA
      THET = THET + .000174533/2.
   55 CONTINUE
   50 CONTINUE
      WRITE(6,101)
      WRITE(6,107) (SYM(I), I = 1,101)
      II = 1
      III = 4
      GO TO 150
  140 II = II + 4
      IF(II - 181) 145,999,998
  145 III = III + 4
C   WRITE OUT COLUMN HEADINGS FOR HUNDREDTHS OF A DEGREE
      WRITE(6,101)
      WRITE(6,107) (SYM(I), I = 1,101)
  101 FORMAT(1H1,///////    ,17X,'.00',7X,'.01',7X,'.02',7X,'.03',7X,'.04
     1',7X,'.05',7X,'.06',7X,'.07',7X,'.08',7X,'.09')
  107 FORMAT(12X,101A1)
  150 DO 301 I = II,III
      JJ = 1
      JJJ = 10
      IT = I
C   WRITE OUT A BLOCK OF "D" SPACINGS AT .01 DEGREE 2-THETA INTERVALS
      DO 210 K = 1,10
      WRITE(6,102) IT,DD(K),SYM(1),(D(I,J),J = JJ,JJJ)
  102 FORMAT(1H ,4X,I3,F3.2,1X,A1,10F10.5)
  100 JJ = JJ + 10
      IF(JJ - 101) 105,300,998
  105 JJJ = JJJ + 10
  210 CONTINUE
  300 WRITE(6,103)
  103 FORMAT(1H ,/)
  301 CONTINUE
      GO TO 140
  998 STOP 998
  999 STOP 1
      END
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Fig. 1. Computer program for computing and printing *d*-spacings at 0.01° 2θ intervals ($CuK_{\alpha 1}$ radiation).

https://doi.org/10.1346/CCMN.1976.0240409 Published online by Cambridge University Press

	.00	.01	.02	.03	.04	.05	.06	.07	.08	.09
24.0 *	3.70484	3.70332	3.70180	3.70029	3.69877	3.69725	3.69574	3.69423	3.69272	3.69120
24.10 *	3.68970	3.68819	3.68668	3.68518	3.68367	3.68217	3.68067	3.67917	3.67767	3.67617
24.20 *	3.67468	3.67318	3.67169	3.67019	3.66870	3.66721	3.66572	3.66423	3.66275	3.66126
24.30 *	3.65978	3.65830	3.65681	3.65533	3.65386	3.65238	3.65090	3.64943	3.64795	3.64648
24.40 *	3.64501	3.64354	3.64207	3.64060	3.63913	3.63767	3.63620	3.63474	3.63327	3.63181
24.50 *	3.63035	3.62890	3.62744	3.62598	3.62453	3.62307	3.62162	3.62017	3.61872	3.61727
24.60 *	3.61582	3.61438	3.61293	3.61149	3.61004	3.60860	3.60716	3.60572	3.60428	3.60285
24.70 *	3.60141	3.59998	3.59854	3.59711	3.59568	3.59425	3.59282	3.59139	3.58996	3.58854
24.80 *	3.58711	3.58569	3.58427	3.58285	3.58143	3.58001	3.57859	3.57718	3.57576	3.57435
24.90 *	3.57293	3.57152	3.57011	3.56870	3.56729	3.56589	3.56448	3.56308	3.56167	3.56027
25.0 *	3.55887	3.55747	3.55607	3.55467	3.55327	3.55188	3.55048	3.54909	3.54770	3.54631
25.10 *	3.54492	3.54353	3.54214	3.54075	3.53937	3.53798	3.53660	3.53522	3.53383	3.53245
25.20 *	3.53107	3.52970	3.52832	3.52694	3.52557	3.52420	3.52282	3.52145	3.52008	3.51871
25.30 *	3.51734	3.51598	3.51461	3.51325	3.51188	3.51052	3.50916	3.50780	3.50644	3.50508
25.40 *	3.50372	3.50237	3.50101	3.49966	3.49830	3.49695	3.49560	3.49425	3.49290	3.49156
25.50 *	3.49021	3.48886	3.48752	3.48618	3.48483	3.48349	3.48215	3.48081	3.47947	3.47814
25.60 *	3.47680	3.47547	3.47413	3.47280	3.47147	3.47014	3.46881	3.46748	3.46615	3.46482
25.70 *	3.46350	3.46217	3.46085	3.45953	3.45821	3.45689	3.45557	3.45425	3.45293	3.45162
25.80 *	3.45030	3.44899	3.44767	3.44636	3.44505	3.44374	3.44243	3.44112	3.43982	3.43851
25.90 *	3.43721	3.43590	3.43460	3.43330	3.43200	3.43070	3.42940	3.42810	3.42680	3.42551
26.0 *	3.42421	3.42292	3.42163	3.42033	3.41904	3.41775	3.41646	3.41518	3.41389	3.41260
26.10 *	3.41132	3.41003	3.40875	3.40747	3.40619	3.40491	3.40363	3.40235	3.40108	3.39980
26.20 *	3.39852	3.39725	3.39598	3.39471	3.39343	3.39216	3.39090	3.38963	3.38836	3.38709
26.30 *	3.38583	3.38456	3.38330	3.38204	3.38078	3.37952	3.37826	3.37700	3.37574	3.37449
26.40 *	3.37323	3.37198	3.37072	3.36947	3.36822	3.36697	3.36572	3.36447	3.36322	3.36197
26.50 *	3.36073	3.35948	3.35824	3.35700	3.35575	3.35451	3.35327	3.35203	3.35079	3.34956
26.60 *	3.34832	3.34708	3.34585	3.34462	3.34338	3.34215	3.34092	3.33969	3.33846	3.33723
26.70 *	3.33601	3.33478	3.33355	3.33233	3.33111	3.32988	3.32866	3.32744	3.32622	3.32500
26.80 *	3.32378	3.32257	3.32135	3.32014	3.31892	3.31771	3.31650	3.31528	3.31407	3.31286
26.90 *	3.31165	3.31045	3.30924	3.30803	3.30683	3.30562	3.30442	3.30322	3.30202	3.30082
27.0 *	3.29962	3.29842	3.29722	3.29602	3.29483	3.29363	3.29244	3.29124	3.29005	3.28886
27.10 *	3.28767	3.28648	3.28529	3.28410	3.28291	3.28173	3.28054	3.27936	3.27817	3.27699
27.20 *	3.27581	3.27463	3.27345	3.27227	3.27109	3.26991	3.26873	3.26756	3.26638	3.26521
27.30 *	3.26403	3.26286	3.26169	3.26052	3.25935	3.25818	3.25701	3.25584	3.25468	3.25351
27.40 *	3.25235	3.25118	3.25002	3.24886	3.24770	3.24654	3.24538	3.24422	3.24306	3.24190
27.50 *	3.24075	3.23959	3.23844	3.23728	3.23613	3.23498	3.23383	3.23268	3.23153	3.23038
27.60 *	3.22923	3.22809	3.22694	3.22579	3.22465	3.22351	3.22236	3.22122	3.22008	3.21894
27.70 *	3.21780	3.21666	3.21553	3.21439	3.21325	3.21212	3.21098	3.20985	3.20872	3.20758
27.80 *	3.20645	3.20532	3.20419	3.20307	3.20194	3.20081	3.19968	3.19856	3.19743	3.19631
27.90 *	3.19519	3.19407	3.19294	3.19182	3.19070	3.18959	3.18847	3.18735	3.18623	3.18512

Fig. 2. Sample out-put from the computer program, 24.00° 2θ–27.99° 2θ.

https://doi.org/10.1346/CCMN.1976.0240409 Published online by Cambridge University Press