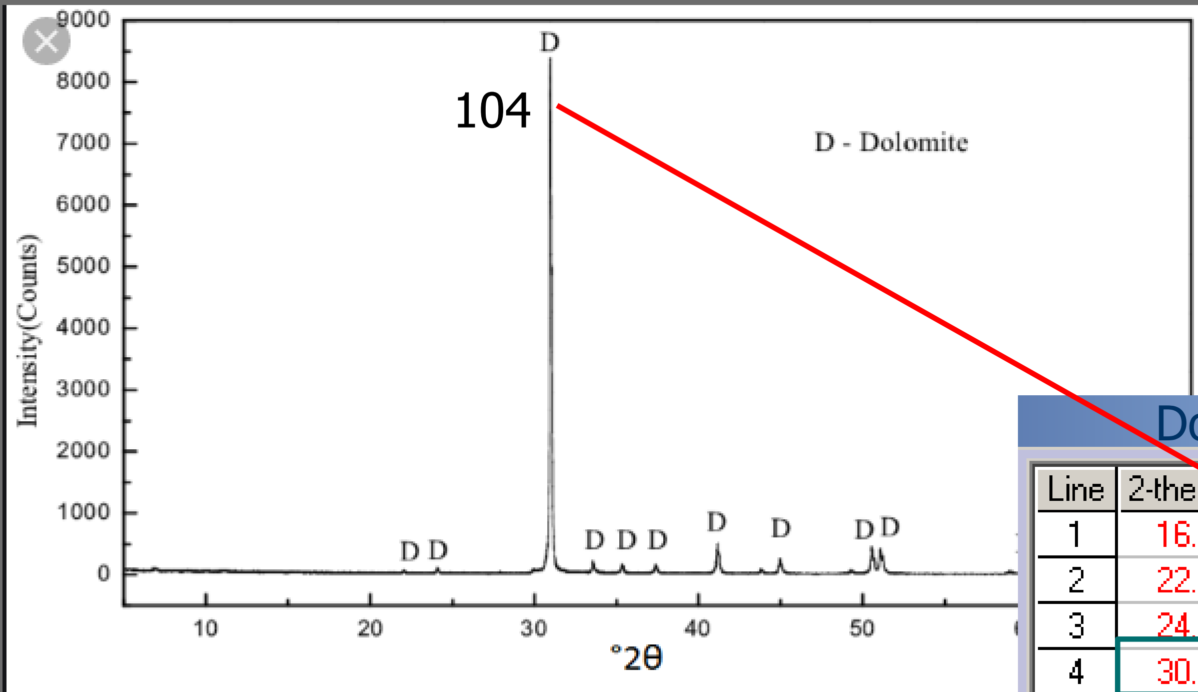
Manual identification and quantification of mineral phases – XRD exercises

Introduction

This document will show the necessary steps for a manual identification and quantification of mineral phases using (1) tables to convert °2θ values to d_{hkl}, (2) reference mineral files, and (3) a table with the experimental reflective power of various minerals. The following image (see below) demonstrates the relationship between the crystallographic planes of a mineral and the peaks of a diffractogram. In the case of dolomite, the radiation emitted coherently by the atoms in the planes parallel to the 104 face generates the most intense peak (d_{104}) of the diffraction pattern. The distance between the planes is 2.887 Å.

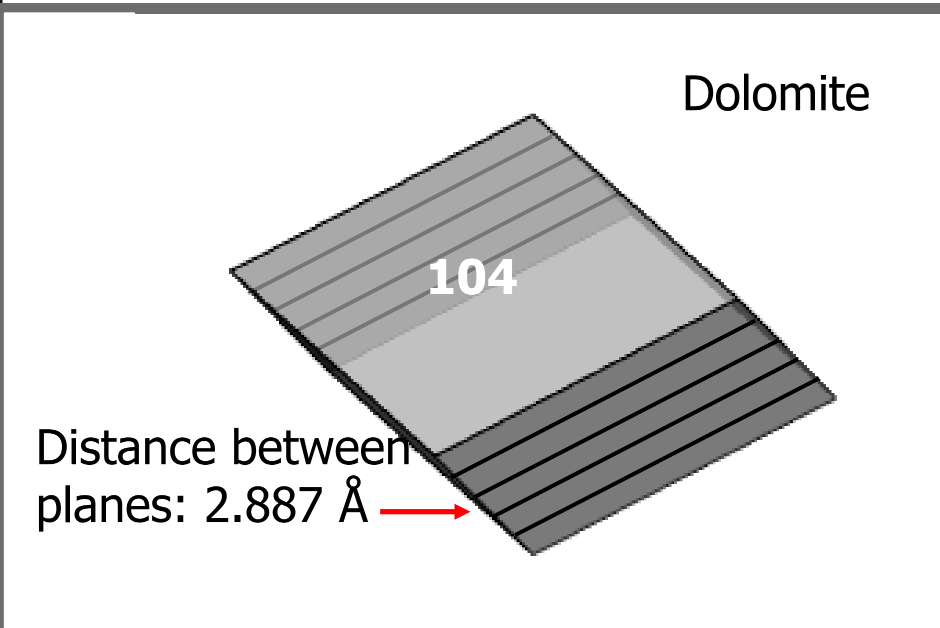
The table with the experimental reflective power of various minerals is included in Annex I. Reference mineral files and conversion tables (°2θ values to d_{hkl}) can be found in Annex II and III, respectively.



°2θ

d-spacing in Ångstrom (Å)

Miller Indices

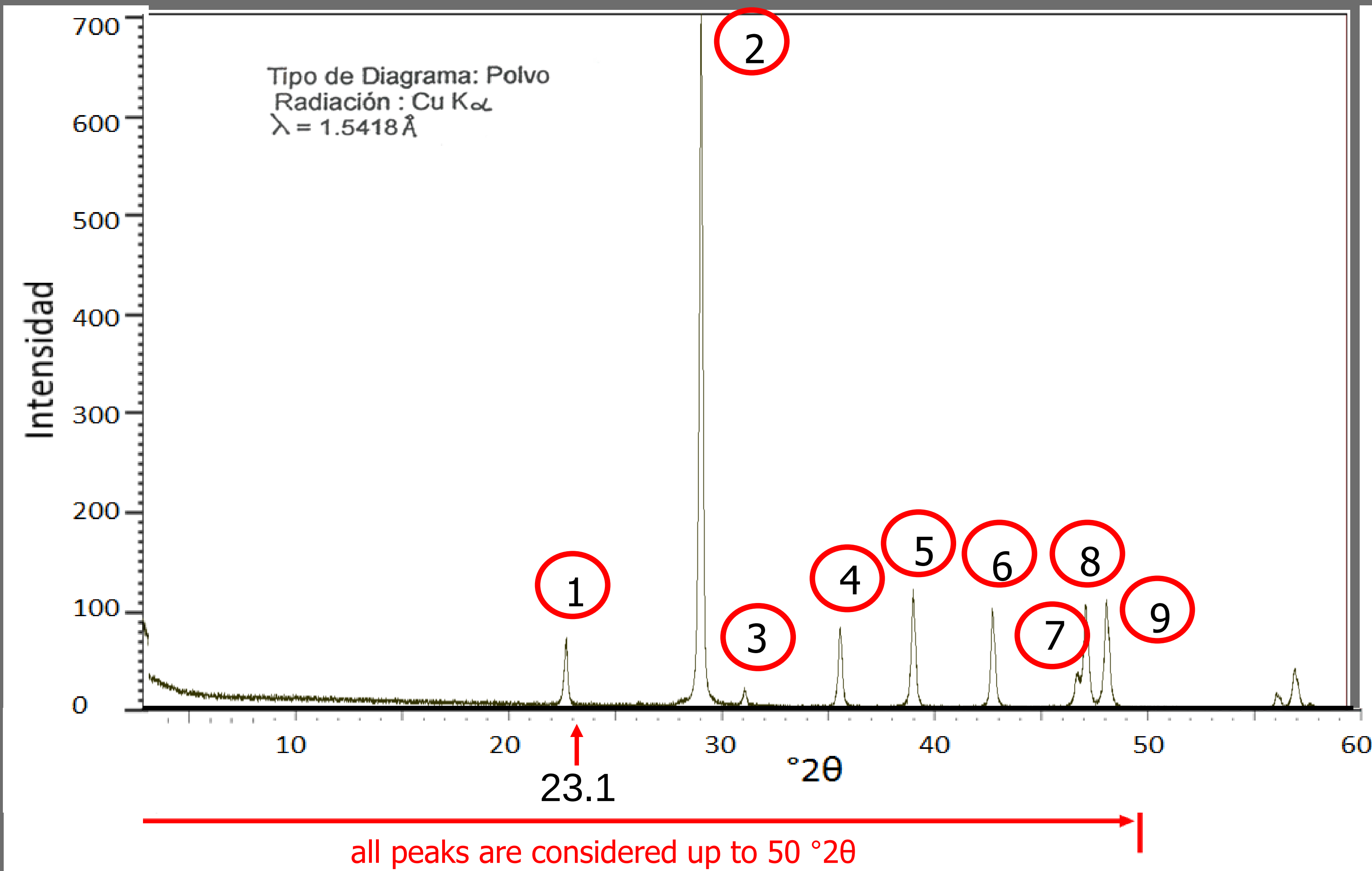


Dolomite Reference File

Line	2-theta angle	d-spacing	Intensity	H K L
1	16.58969	5.339	.1001001	0 0 3
2	22.03488	4.031	2.502502	1 0 1
3	24.06545	3.695	2.802803	0 1 2
4	30.95415	2.887	100	1 0 4
5	33.54045	2.670	4.304304	0 0 6
6	35.31829	2.539	5.105105	0 1 5
7	37.36911	2.404	11.51151	1 1 0
8	41.13905	2.192	22.42242	1 1 -3
9	43.80524	2.065	3.903904	0 2 1
10	44.94209	2.015	13.11311	2 0 2
11	49.28332	1.847	4.104104	0 2 4
12	50.53759	1.805	16.31632	0 1 8
13	51.07982	1.787	18.01802	1 1 -6
14	51.29095	1.780	9.90991	0 0 9
15	52.3603	1.746	.2002002	2 0 5
16	58.90623	1.567	3.803804	1 2 -1
17	59.83002	1.545	8.808809	2 1 -2
18	60.02019	1.540	4.704705	0 2 7

Manual identification

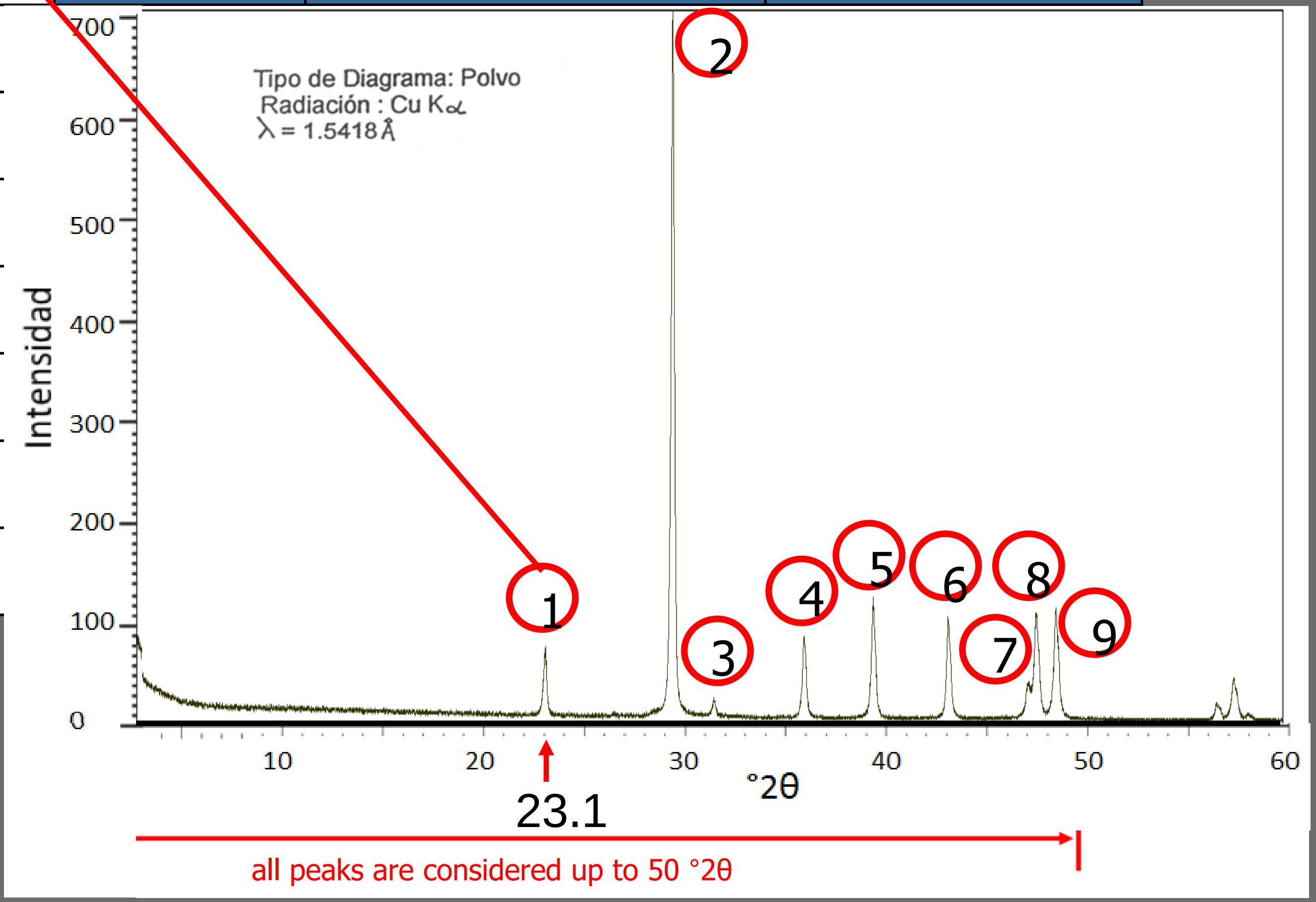
The peaks are first numbered and the value °2θ has to be determined for each peak.



Manual identification

Determination of the °2θ value of each peak

Peak	°2θ	d_{hkl} (Å)	Absolute Intensity (mm^2)	Relative intensity (%)
1	23.1			
2	29.5			
3	31.6			
4	36.0			
5	39.5			
6	43.2			
7	47.2			
8	47.6			
9	48.6			



Manual identification

Conversion of °2θ to d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1.541838

40.10 → 2.2486 → 2.25 Å

°2θ	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
40.00	2.2540	2.2529	2.2519	2.2508	2.2497	2.2486	2.2476	2.2465	2.2454	2.2443
.20	2.2433	2.2422	2.2411	2.2401	2.2390	2.2379	2.2369	2.2358	2.2347	2.2337
.40	2.2326	2.2316	2.2305	2.2294	2.2284	2.2273	2.2263	2.2252	2.2242	2.2231
.60	2.2221	2.2210	2.2200	2.2189	2.2179	2.2169	2.2158	2.2148	2.2137	2.2127
.80	2.2116	2.2106	2.2096	2.2085	2.2075	2.2065	2.2054	2.2044	2.2034	2.2023
41.00	2.2013	2.2003	2.1993	2.1982	2.1972	2.1962	2.1952	[illegible]	[illegible]	2.1921
.20	2.1911	2.1901	2.1891	2.1880	2.1870	2.1860	2.1850	[illegible]	[illegible]	2.1820
.40	2.1810	2.1800	2.1790	2.1780	2.1770	2.1760	2.1749	2.1739	2.1729	2.1719
.60	2.1709	2.1700	2.1690	2.1680	2.1670	2.1660	2.1650	2.1640	2.1630	2.1620
.80	2.1610	2.1600	2.1591	2.1581	2.1571	2.1561	2.1551	2.1541	2.1532	2.1522
42.00	2.1512	2.1502	2.1492	2.1483	2.1473	2.1463	2.1453	2.1444	2.1434	2.1424
.20	2.1415	2.1405	2.1395	2.1386	2.1376	2.1366	2.1357	[illegible]	[illegible]	2.1328
.40	2.1318	2.1309	2.1299	2.1289	2.1280	2.1270	2.1261	[illegible]	[illegible]	2.1232
.60	2.1223	2.1213	2.1204	2.1194	2.1185	2.1175	2.1166	[illegible]	2.1147	2.1138
.80	2.1128	2.1119	2.1109	2.1100	2.1091	2.1081	2.1072	2.1063	2.1053	2.1044
43.00	2.1035	2.1025	2.1016	2.1007	2.0997	2.0988	2.0979	[illegible]	[illegible]	2.0951
.20	2.0942	2.0933	2.0923	2.0914	2.0905	2.0896	2.0887	[illegible]	[illegible]	2.0859
.40	2.0850	2.0841	2.0832	2.0823	2.0813	2.0804	2.0795	[illegible]	[illegible]	2.0768
.60	2.0759	2.0750	2.0741	2.0732	2.0723	2.0714	2.0705	2.0696	2.0687	2.0678
.80	2.0669	2.0660	2.0651	2.0642	2.0633	2.0624	2.0615	2.0606	2.0597	2.0588
44.00	2.0579	2.0571	2.0562	2.0553	2.0544	2.0535	2.0526	2.0517	2.0509	2.0500
.20	2.0491	2.0482	2.0473	2.0465	2.0456	2.0447	2.0438	2.0429	2.0421	2.0412
.40	2.0403	2.0395	2.0386	2.0377	2.0368	2.0360	2.0351	2.0342	2.0334	2.0325
.60	2.0316	2.0308	2.0299	2.0291	2.0282	2.0273	2.0265	2.0256	2.0248	2.0239
.80	2.0230	2.0222	2.0213	2.0205	2.0196	2.0188	2.0179	2.0171	2.0162	2.0154
45.00	2.0145	2.0137	2.0128	2.0120	2.0111	[illegible]	[illegible]	2.0086	2.0077	2.0069
.20	2.0061	2.0052	2.0044	2.0035	2.0027	[illegible]	[illegible]	2.0002	1.9994	1.9985
.40	1.9977	1.9969	1.9960	1.9952	1.9944	[illegible]	[illegible]	1.9919	1.9910	1.9902
.60	1.9894	1.9886	1.9877	1.9869	1.9861	1.9853	1.9844	1.9836	1.9828	1.9820
.80	1.9812	1.9803	1.9795	1.9787	1.9779	1.9771	1.9763	1.9755	1.9746	1.9738

41.50 → 2.1760

42.70 → 2.1175

43.90 → 2.0624

45.05 → 2.0128 / 2.0120

Important: The wavelength of the incident radiation in the conversion table and that used for the analysis of our sample have to be identical (usually Cu Kα).

Manual identification

Conversion of °2θ to d_{hkl}

Peak	°2θ	d_{hkl} (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85		
2	29.5			
3	31.6			
4	36.0			
5	39.5			
6	43.2			
7	47.2			
8	47.6			
9	48.6			

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14
20.00	4.4395	4.4352	4.4308	4.4264	4.4220	4.4177	4.4133	4.4090
.20	4.3960	4.3917	4.3874	4.3832	4.3789	4.3746	4.3704	4.3661
.40	4.3534	4.3492	4.3450	4.3408	4.3366	4.3324	4.3282	4.3240
.60	4.3116	4.3074	4.3033	4.2992	4.2951	4.2910	4.2869	4.2828
.80	4.2706	4.2665	4.2625	4.2584	4.2544	4.2504	4.2463	4.2423
21.00	4.2303	4.2264	4.2224	4.2184	4.2145	4.2105	4.2066	4.2026
.20	4.1909	4.1870	4.1831	4.1792	4.1753	4.1714	4.1676	4.1637
.40	4.1522	4.1483	4.1445	4.1407	4.1369	4.1331	4.1293	4.1255
.60	4.1142	4.1104	4.1067	4.1029	4.0992	4.0954	4.0917	4.0880
.80	4.0769	4.0732	4.0695	4.0658	4.0622	4.0585	4.0548	4.0512
22.00	4.0403	4.0366	4.0330	4.0294	4.0258	4.0222	4.0186	4.0150
.20	4.0043	4.0008	3.9972	3.9937	3.9901	3.9866	3.9831	3.9795
.40	3.9690	3.9655	3.9620	3.9585	3.9551	3.9516	3.9481	3.9447
.60	3.9343	3.9309	3.9275	3.9241	3.9206	3.9172	3.9138	3.9104
.80	3.9003	3.8969	3.8935	3.8902	3.8868	3.8835	3.8801	3.8768
23.00	3.8668	3.8635	3.8602	3.8569	3.8536	3.8503	3.8470	3.8437
.20	3.8339	3.8307	3.8274	3.8242	3.8209	3.8177	3.8145	3.8113
.40	3.8016	3.7984	3.7952	3.7920	3.7888	3.7857	3.7825	3.7793
.60	3.7698	3.7667	3.7636	3.7604	3.7573	3.7542	3.7510	3.7479
.80	3.7386	3.7355	3.7324	3.7294	3.7263	3.7232	3.7201	3.7171

Manual identification

Conversion of °2θ to d_{hkl} using the Bragg formula

Bragg formula:

$$n\lambda = 2d_{hkl} \text{ sen } \theta$$

The Bragg formula is rearranged to calculate d_{hkl}, considering a wavelength of Cu Kα = 1.5418 Å:

$$d_{hkl} = 1.5418/(2 \text{ sen } \theta)$$

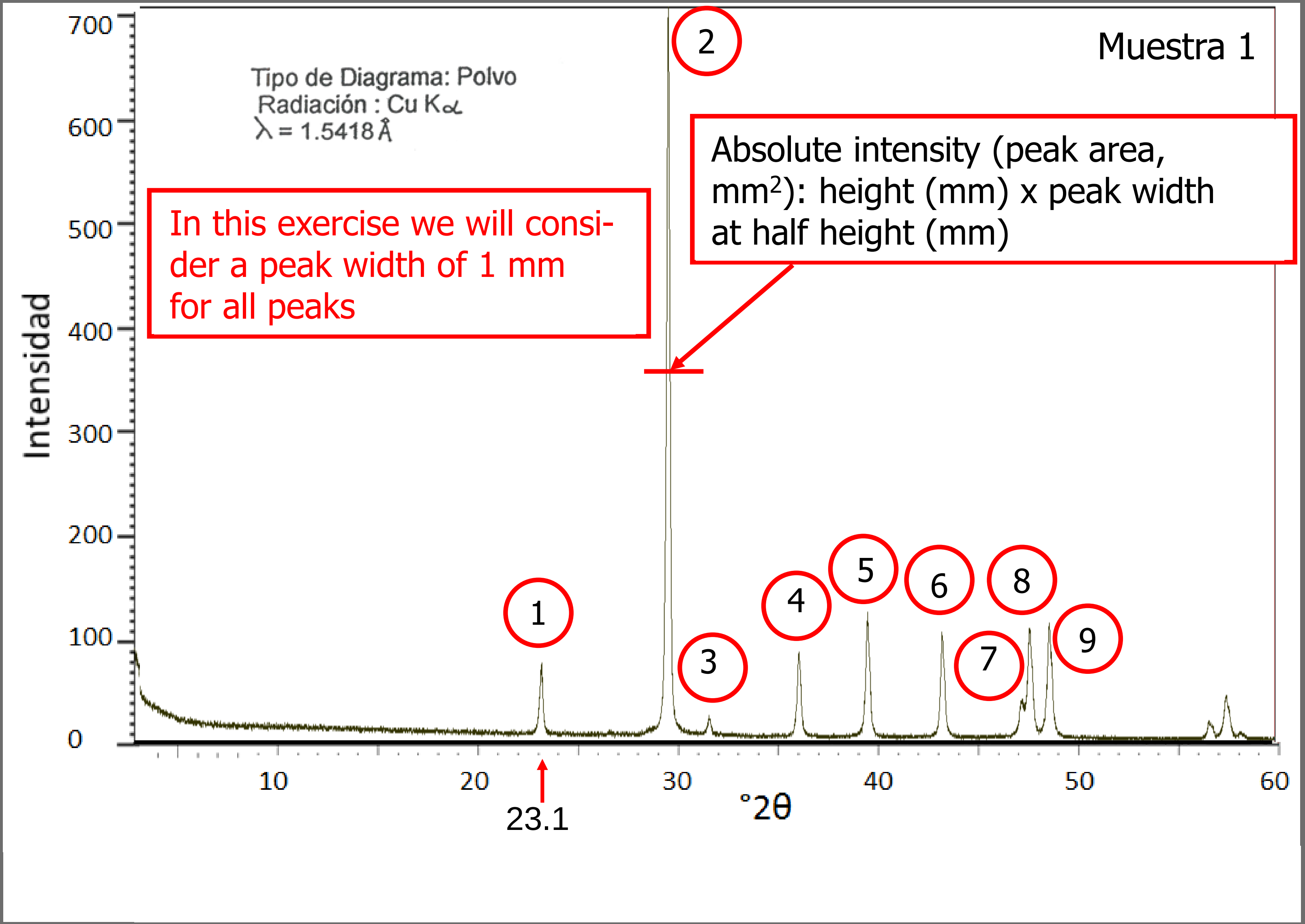
Manual identification

Conversion of °2θ to d_{hkl}

Peak	°2θ	d_{hkl} (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85		
2	29.5	3.03		
3	31.6	2.83		
4	36.0	2.49		
5	39.5	2.28		
6	43.2	2.09		
7	47.2	1.93		
8	47.6	1.91		
9	48.6	1.87		

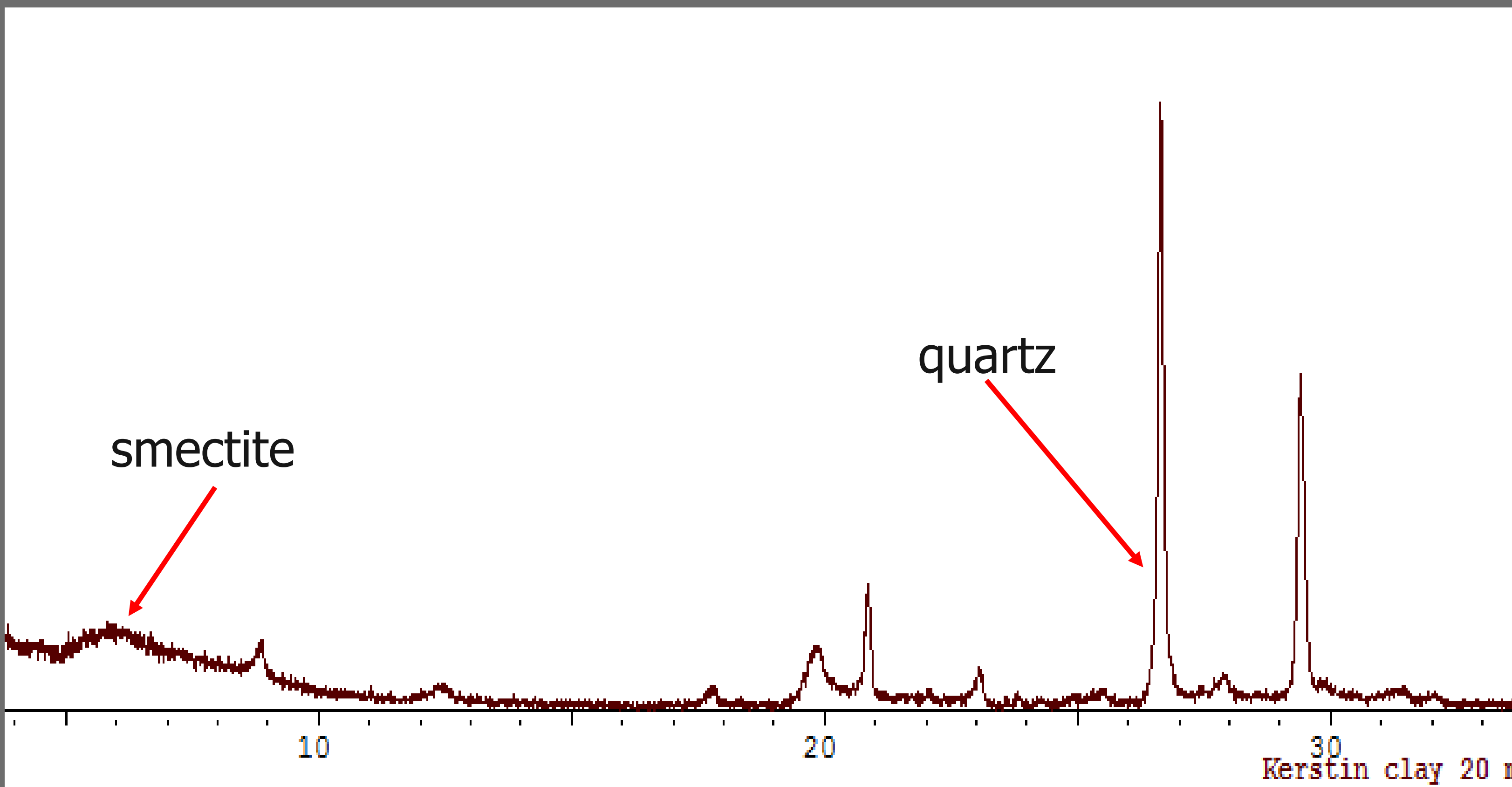
Manual identification

Determination of the absolute intensity



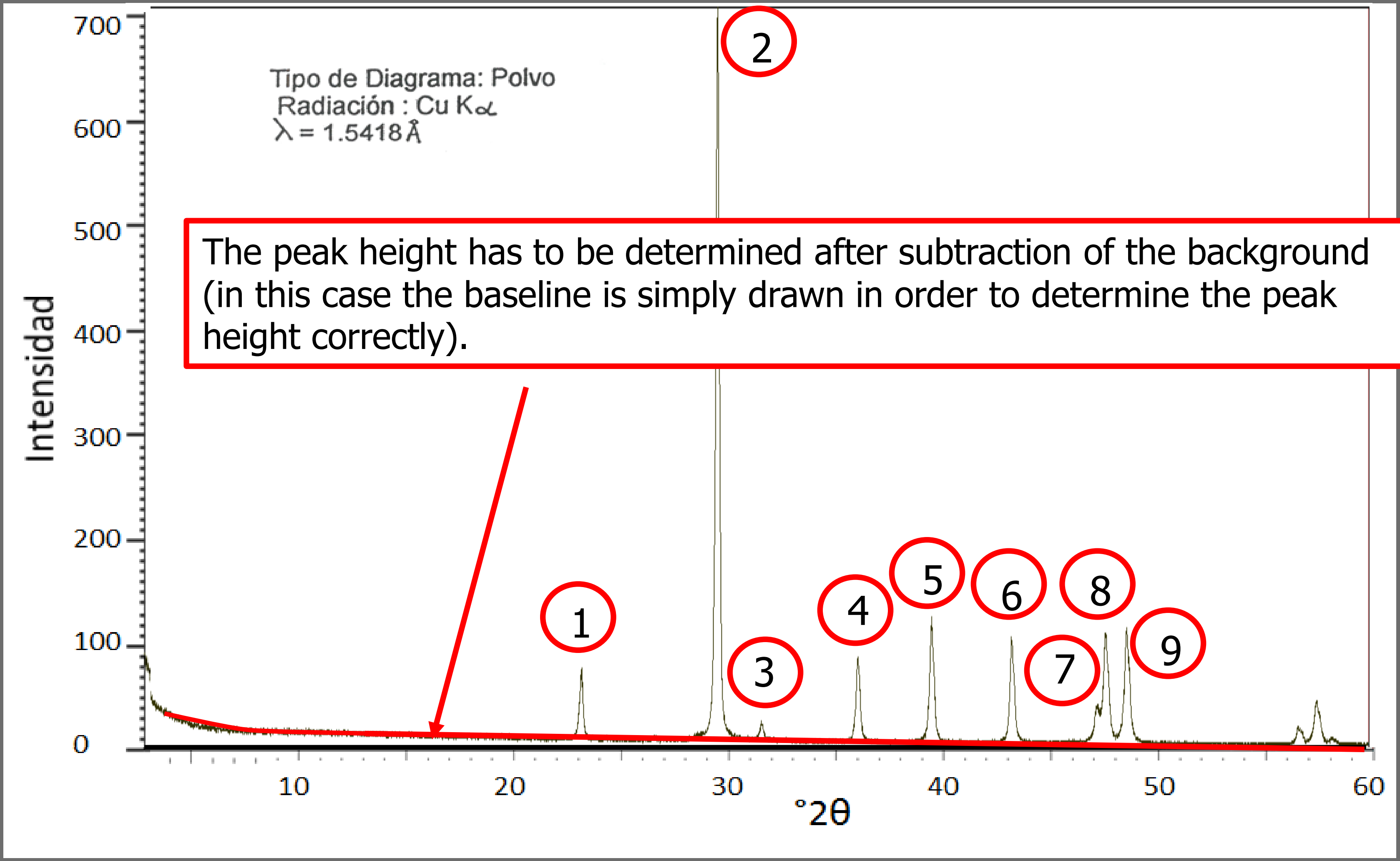
Manual identification

The width of the peaks generally depends on the crystallinity of the mineral. Phases of low crystallinity such as smectites have very broad peaks, while quartz is much more crystalline and usually has narrow peaks.



Manual identification

Background subtraction

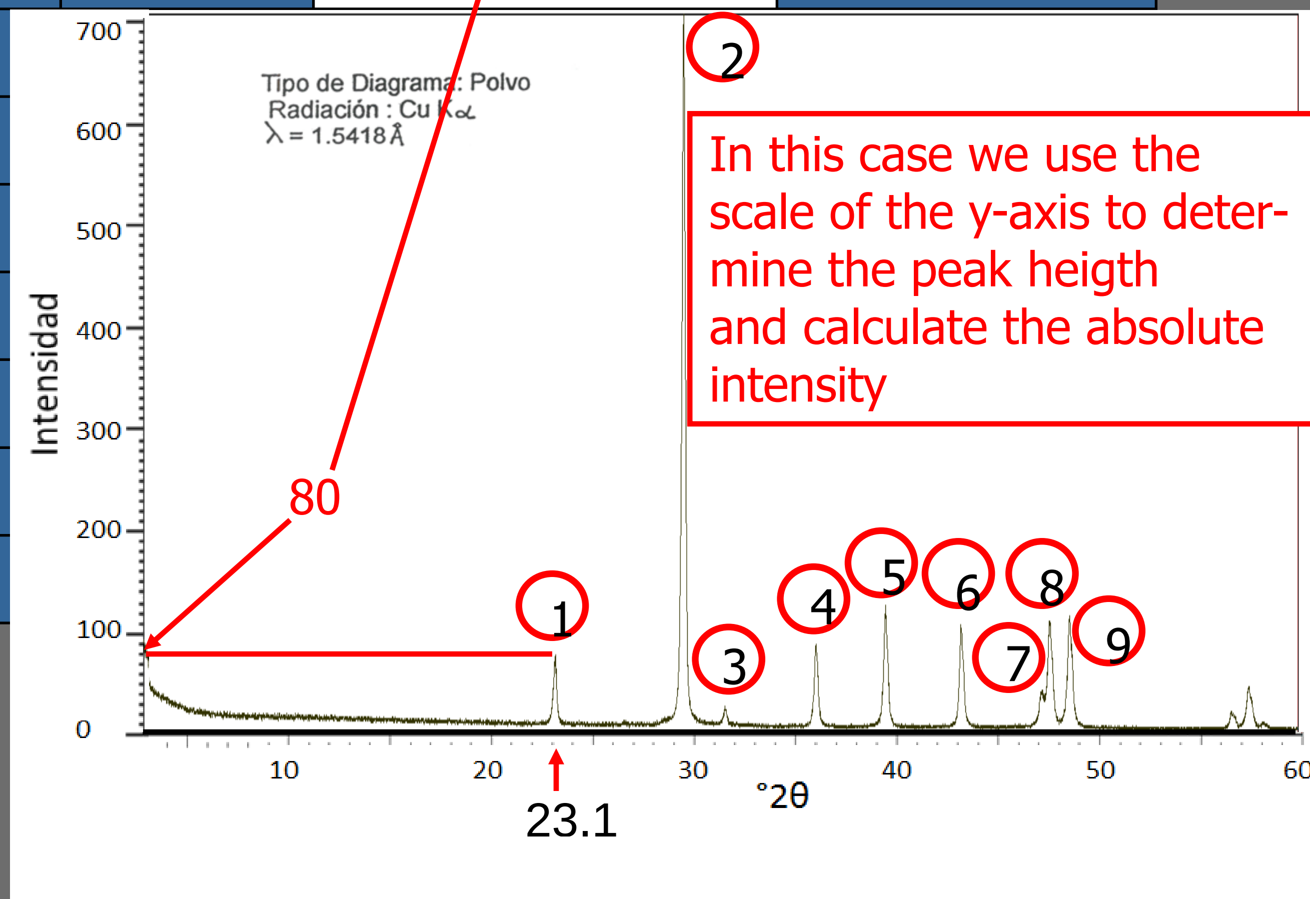


The peak height has to be determined after subtraction of the background (in this case the baseline is simply drawn in order to determine the peak height correctly).

Manual identification

Determination of the peaks absolute intensity

Peak	°2θ	d_{hkl} (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85	80	
2	29.5	3.03		
3	31.6			
4	36.0			
5	39.5			
6	43.2			
7	47.2			
8	47.6			
9	48.6			



Manual identification

Determination of the peaks absolute intensity

Peak	°2ө	d $_{hkl}$ (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85	80	
2	29.5	3.03	700	
3	31.6	2.83	20	
4	36.0	2.49	90	
5	39.5	2.28	130	
6	43.2	2.09	100	
7	47.2	1.93	50	
8	47.6	1.91	110	
9	48.6	1.87	120	

Manual identification

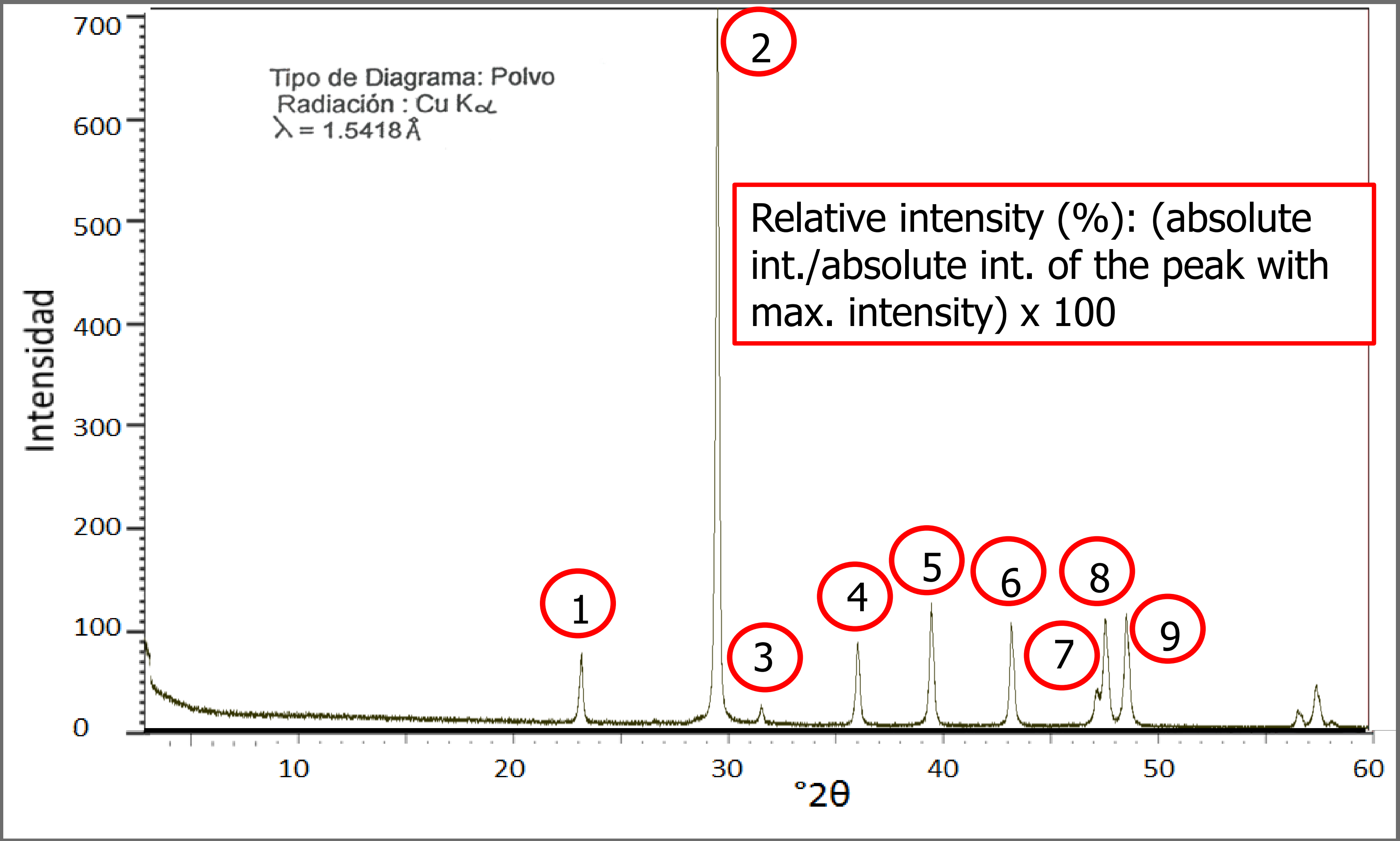
In order to be able to compare the peaks d_{hkl} and intensities of our sample with those of the reference minerals, we have to calculate the peaks relative intensity (%).

Reference mineral file

Line	2-theta angle	d-spacing	Intensity	H K L
1	23.06002	3.854	9.90991	0 1 2
2	29.40495	3.035	100	1 0 4
3	31.43548	2.843	2.102102	0 0 6
4	35.98124	2.494	14.21421	1 1 0
5	39.41959	2.284	17.81782	1 1 3
6	43.17179	2.094	15.01501	2 0 2
7	47.12651	1.927	6.306306	0 2 4
8	47.50888	1.912	17.61762	0 1 8
9	48.5141	1.875	18.41842	1 1 6
10	56.58189	1.625	3.103103	2 1 1
11	57.4174	1.604	8.808809	1 2 2
12	58.08212	1.587	.8008008	1 0 10

Manual identification

Determination of the peaks relative intensity



Manual identification

Determination of the peaks relative intensity

Peak	°2θ	d_{hkl} (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85	80	11
2	29.5	3.03	700	
3	31.6	2.83	20	
4	36.0	2.49	90	
5	39.5	2.28	130	
6	43.2	2.09	100	
7	47.2	1.93	50	
8	47.6	1.91	110	
9	48.6	1.87	120	

(80/700)*100 = 11

Manual identification

Identification of the mineral considering the peak of max. relative intensity (100%) and verification considering the positions and intensities of the remaining peaks.

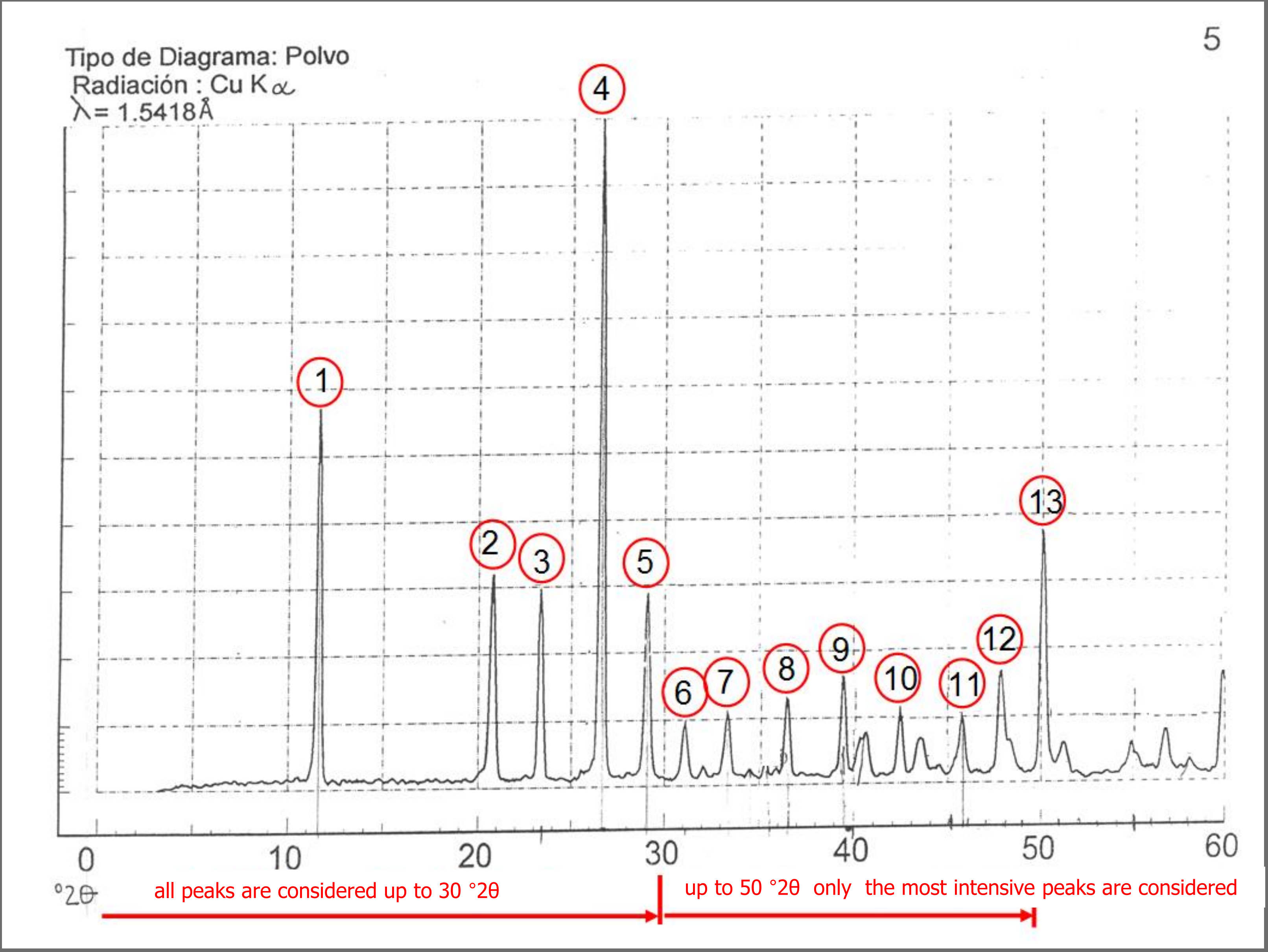
Peak	°2θ	d $_{hkl}$ (Å)	Absolute intensity (mm^2)	Relative intensity (%)
1	23.1	3.85	80	11
2	29.5	3.03	700	100
3	31.6	2.83	20	3
4	36.0	2.49	90	13
5	39.5	2.28	130	19
6	43.2	2.09		14
7	47.2	1.93		7
8	47.6	1.91		16
9	48.6	1.87		17

Calcite Reference File

Line	2-theta angle	d-spacing	Intensity	H K L
1	23.06002	3.854	9.90991	0 1 2
2	29.40495	3.035	100	1 0 4
3	31.43548	2.843	2.102102	0 0 6
4	35.98124	2.494	14.21421	1 1 0
5	39.41959	2.284	17.81782	1 1 3
6	43.17179	2.094	15.01501	2 0 2
7	47.12651	1.927	6.306306	0 2 4
8	47.50888	1.912	17.61762	0 1 8
9	48.5141	1.875	18.41842	1 1 6

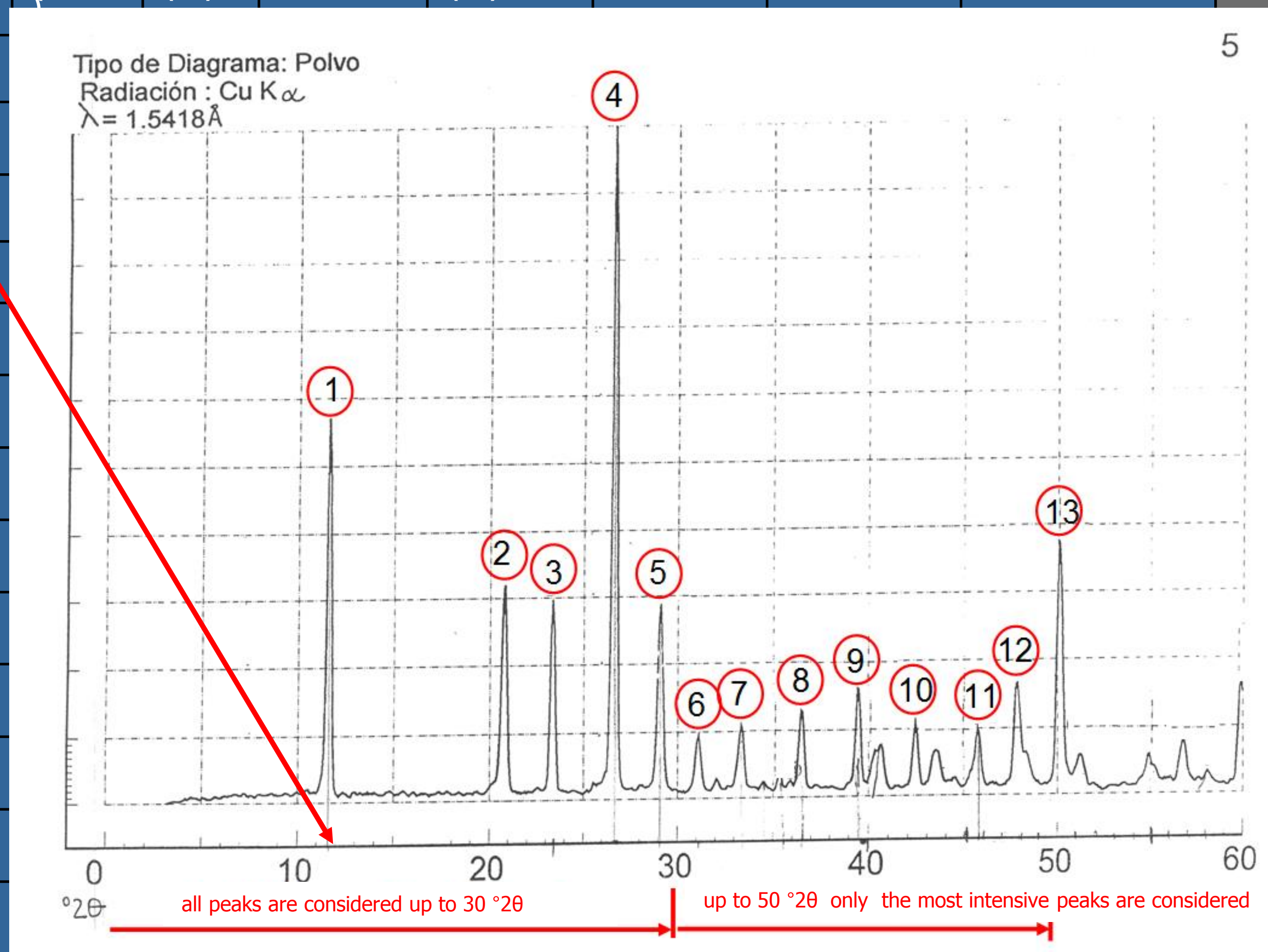
Manual identification and quantification

Identification and quantification of a mixture of minerals



Determination of °2θ

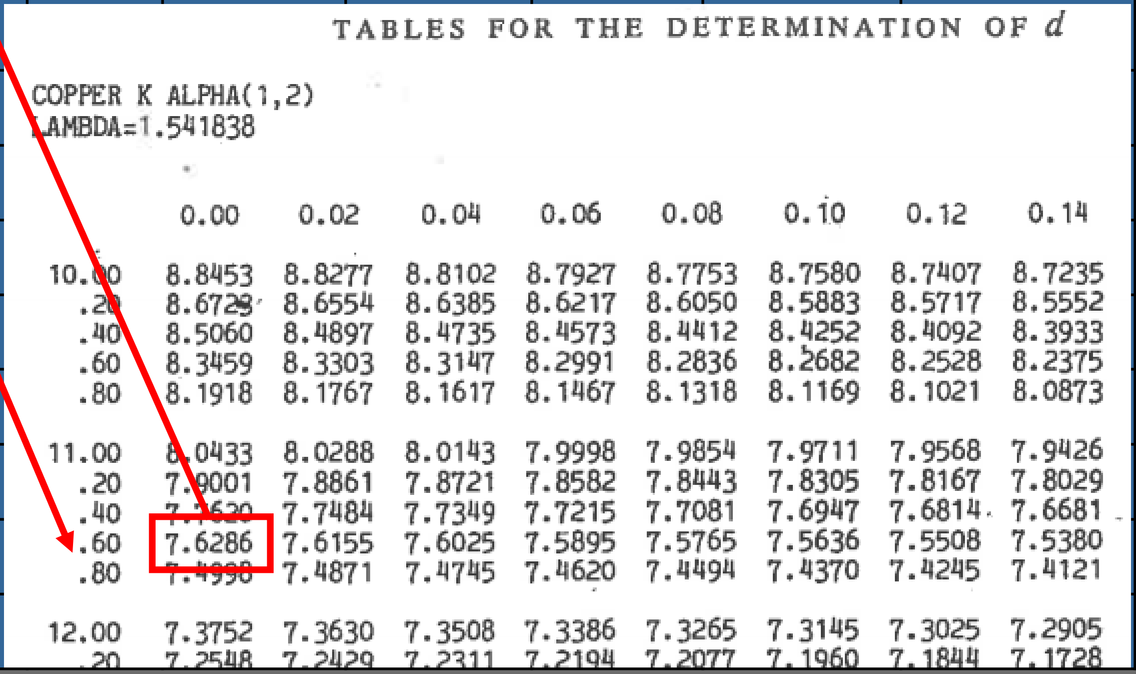
Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	A.I./R.P.	wt%
1	11.6								
2	20.9								
3	23.4								
4	26.7								
5	29.0								
6	31.2								
7	33.4								
8	36.5								
9	39.5								
10	42.5								
11	45.7								
12	47.9								
13	50.1								



d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Conversion of °2θ to d_{hkl}

Identification								Quantification	
Peak	°2θ	d hkl (Å)	A.I. (mm²)	R.I. (%)	Phase1	R.I. Ph2 (%)	Phase2	I.a./P.R.	wt%
1	11.6	7.63							
2	20.9	4.25							
3	23.4	3.80							
4	26.7	3.34							
5	29.0	3.08							
6	31.2	2.87							
7	33.4	2.68							
8	36.5	2.46							
9	39.5	2.28							
10	42.5	2.13							
11	45.7	1.99							
12	47.9	1.90							
13	50.1	1.82							



TABLES FOR THE DETERMINATION OF *d*

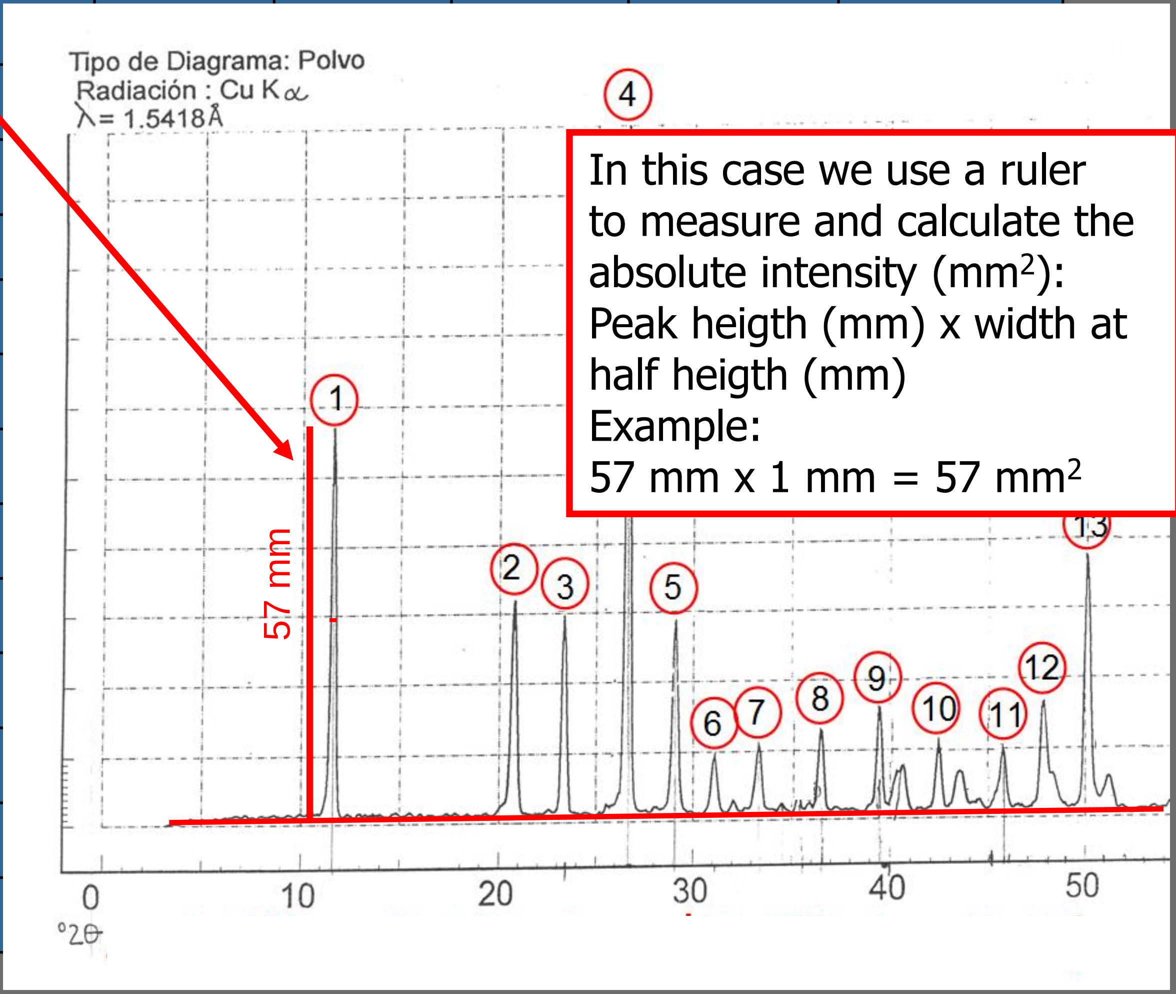
COPPER K ALPHA(1,2)
LAMBDA=1.541838

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14
10.00	8.8453	8.8277	8.8102	8.7927	8.7753	8.7580	8.7407	8.7235
.20	8.6728	8.6554	8.6385	8.6217	8.6050	8.5883	8.5717	8.5552
.40	8.5060	8.4897	8.4735	8.4573	8.4412	8.4252	8.4092	8.3933
.60	8.3459	8.3303	8.3147	8.2991	8.2836	8.2682	8.2528	8.2375
.80	8.1918	8.1767	8.1617	8.1467	8.1318	8.1169	8.1021	8.0873
11.00	8.0433	8.0288	8.0143	7.9998	7.9854	7.9711	7.9568	7.9426
.20	7.9001	7.8861	7.8721	7.8582	7.8443	7.8305	7.8167	7.8029
.40	[illegible]	7.7484	7.7349	7.7215	7.7081	7.6947	7.6814	7.6681
.60	7.6286	7.6155	7.6025	7.5895	7.5765	7.5636	7.5508	7.5380
.80	[illegible]	7.4871	7.4745	7.4620	7.4494	7.4370	7.4245	7.4121
12.00	7.3752	7.3630	7.3508	7.3386	7.3265	7.3145	7.3025	7.2905
.20	7.2548	7.2429	7.2311	7.2194	7.2077	7.1960	7.1844	7.1728

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Determination of the absolute intensity

Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	I.a./P.R.	wt%
1	11.6	7.62	57						
2	20.9	4.25	33						
3	23.4	3.80	30						
4	26.7	3.34	100						
5	29.0	3.08	28						
6	31.2	2.87	10						
7	33.4	2.68	11						
8	36.5	2.46	13						
9	39.5	2.28	16						
10	42.5	2.13	12						
11	45.7	1.99	10						
12	47.9	1.90	16						
13	50.1	1.82	37						



In this case we use a ruler to measure and calculate the absolute intensity (mm^2): Peak heigth (mm) x width at half heigth (mm)

Example:

57 mm x 1 mm = 57 mm^2

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Determination of the relative intensity

Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	I.a./P.R.	wt%
1	11.6	7.62	57	57					
2	20.9	4.25	33	33					
3	23.4	3.80	30	30					
4	26.7	3.34	100	100					
5	29.0	3.08	28	28					
6	31.2	2.87	10	10					
7	33.4	2.68	11	11					
8	36.5	2.46	13	13					
9	39.5	2.28	16	16					
10	42.5	2.13	12	12					
11	45.7	1.99	10	10					
12	47.9	1.90	16	16					
13	50.1	1.82	37	37					

In order to use the mineral reference files to identify the mineral phases in our samples we have to calculate the relative intensity (%) of all peaks

Relative intensity (%) = (Absolute intensity (mm^2)/ absolute intensity of the peak with max. absolute intensity (mm^2)) x 100

Example:
($57\ mm^2/100\ mm^2$) x 100% = 57%

In this case both have the same value because the absolute intensity of the peak with the max. intensity = 100 mm^2

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

We consider the peak with the max. relative intensity (100%) in order to identify the first phase in our sample and compare all other peaks of the reference mineral file with the remaining peaks of our sample.

Identification						Quantification			
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1				
1	11.6	7.62	57	57					
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30					
4	26.7	3.34	100	100	Quartz				
5	29.0	3.08	28	28					
6	31.2	2.87	10	10					
7	33.4	2.68	11	11					
8	36.5	2.46	13	13	Quartz				
9	39.5	2.28	16	16	Quartz				
10	42.5	2.13	12	12	Quartz				
11	45.7	1.99	10	10	Quartz				
12	47.9	1.90	16	16					
13	50.1	1.82	37	37	Quartz				

Quartz

Line	2-theta angle	d-spacing	Intensity	H K L
1	20.83469	4.260	35	1 0 0
2	26.64311	3.343	100	1 0 1
3	36.52569	2.458	12	1 1 0
4	39.45487	2.282	12	1 0 2
5	40.28256	2.237	6	1 1 1
6	42.44291	2.128	9	2 0 0
7	45.78835	1.980	6	2 0 1
8	50.16585	1.817	17	1 1 2
9	50.64283	1.801	1	0 0 3
10	54.86377	1.672	7	2 0 2
11	55.33035	1.659	3	1 0 3
12	57.24412	1.608	1	2 1 0
13	59.98111	1.541	15	2 1 1

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.F2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Determination of the relative intensity of the remaining peaks

Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm²)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	I.a./P.R.	wt%
1	11.6	7.62	57	57		100			
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30		53			
4	26.7	3.34	100	100	Quartz				
5	29.0	3.08	28	28		49			
6	31.2	2.87	10	10		18			
7	33.4	2.68	11	11		19			
8	36.5	2.46	13	13	Quartz				
9	39.5	2.28	16	16	Quartz				
10	42.5	2.13	12	12	Quartz				
11	45.7	1.99	10	10	Quartz				
12	47.9	1.90	16	16		28			
13	50.1	1.82	37	37	Quartz				

In order to identify the additional mineral phases of our sample, we have to re-scale the most intense peak of the remaining peaks to 100% and calculate the relative intensity of all remaining peaks.

Example: 100%/57% = 1.75

30% x 1.75 = 53%

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Identification of the second phase of our sample considering the max. relative intensity (100%) of the remaining peaks and verification by comparing the position and intensities of all peaks of the reference mineral file.

Identification								Quantification
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	
1	11.6	7.62	57	57		100	Yeso	
2	20.9	4.25	33	33	Quartz			
3	23.4	3.80	30	30		53	Yeso	
4	26.7	3.34	100	100	Quartz			
5	29.0	3.08	28	28		49	Yeso	
6	31.2	2.87	10	10		18	Yeso	
7	33.4	2.68	11	11		19	Yeso	
8	36.5	2.46	13	13	Quartz			
9	39.5	2.28	16	16	Quartz			
10	42.5	2.13	12	12	Quartz	21	Yeso	
11	45.7	1.99	10	10	Quartz	18	Yeso	
12	47.9	1.90	16	16		28	Yeso	
13	50.1	1.82	37	37	Quartz	65	Yeso	

Gypsum

Line	2-theta angle	d-spacing	Intensity
1	11.6959	7.560	100
2	20.78535	4.270	50
3	23.45299	3.790	20
4	28.18975	3.163	4
5	29.16983	3.059	55
6	31.1704	2.867	25
7	32.10075	2.786	6
8	33.4197	2.679	28
9	34.58989	2.591	4
10	35.45118	2.530	1
11	35.96536	2.495	6
12	36.64919	2.450	4
13	37.44077	2.400	4
14	40.68109	2.216	6
15	42.21418	2.139	2
16	43.47157	2.080	10
17	43.62587	2.073	8
18	45.54528	1.990	4
19	46.45819	1.953	2
20	47.88728	1.898	16
21	48.40232	1.879	10
22	48.8171	1.864	4
23	49.41033	1.843	2
24	50.3139	1.812	10
25	50.79382	1.796	4

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R ... ,
A.I./R.P. = Absolute intensity divided by the reflective power

Identification of the second phase of our sample considering the max. relative intensity (100%) of the remaining peaks and verification by comparing the position and intensities of all peaks of the reference mineral file.

Identification								Quantification
Peak	°2θ	d_{hkl} (Å)	A.I. (mm²)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phas	
1	11.6	7.62	57	57		100	Yeso	
2	20.9	4.25	33	33	Quartz			
3	23.4	3.80	30	30		53	Yeso	
4	26							
5	29						Yeso	
6	31						Yeso	
7	33						Yeso	
8	36						Yeso	
9	39							
10	42						Yeso	
11	45.7	1.99	10	10	Quartz	18	Yeso	
12	47.9	1.90	16	16		28	Yeso	
13	50.1	1.82	37	37	Quartz	65	Yeso	

In some cases small variations in the second decimal of the d_{hkl} values might be observed due to experimental errors or changes in the lattice parameters, for example due to isomorphic substitutions. Variations in intensity might be more severe and are due to the preferred orientation of the crystals in our sample.

Gypsum

Line	2-theta angle	d-spacing	Intensity
1	11.6959	7.560	100
2	20.78535	4.270	50
3	23.45299	3.790	20
4	28.18975	3.163	4
5	29.16903	3.059	55
6	31.1704	2.867	25
7	32.10075	2.786	6
8	33.4197	2.679	28
9	34.58989	2.591	4
10	35.45118	2.530	1
11	35.96536	2.495	6
12	36.64919	2.450	4
13	37.44077	2.400	4
14	40.68109	2.216	6
15	42.21418	2.139	2
16	43.47157	2.080	10
17	43.62587	2.073	8
18	45.54528	1.990	4
19	46.45819	1.953	2
20	47.88726	1.898	16
21	48.40232	1.879	10
22	48.8171	1.864	4
23	49.41033	1.843	2
24	50.3139	1.812	10
25	50.79382	1.796	4

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; … 2,
A.I./R.P. = Absolute intensity divided by the reflective power

Identification of the second phase of our sample considering the max. relative intensity (100%) of the remaining peaks and verification by comparing the position and intensities of all peaks of the reference mineral file.

Identification								Quantification	
Peak	°2ϴ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	I.a./P.R.	wt%
1	11.6	7.62	57	57		100	Yeso		
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Quartz				
5	29.0	3.08	28	28		49	Yeso		
6	31.2	2.87	10	10		18	Yeso		
7	33.4	2.68	11	11		19	Yeso		
8	36.5	2.46	13	13	Quartz				
9	39.5	2.28	16	16	Quartz				
10	42.5	2.13	12	12	Quartz	21	Yeso		
11	45.7	1.99	10	10	Quartz	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Quartz	65	Yeso		

Some peaks may have intensity contribution of two or more phases. Hence, their intensity is higher than that shown in the reference pattern files.

d_{hkl} = d-spacing; A.I. = Absolute intensity; R.I. = Relative intensity; R.I.Ph2 = Relative intensity of phase 2, A.I./R.P. = Absolute intensity divided by the reflective power

Manual quantification

For the manual quantification we have to divide the value of the max. absolute intensity (the d_{hkl} of the corresponding peak is indicated in the table) of each phase by the corresponding reflective power (R.P.). In our case it would be the R.P. of quartz and gypsum. Note: Mineral names are included in English because XRD analysis software use English names.

Fase	P.R.	d_{hkl} (Å)
Quartz	1.43	3.34
Calcite	1.05	3.03
Dolomite	1.03	2.88
Gypsum	0.70	7.56
Feldspars	0.98	~3.20
Strontianite	0.60	3.53
Celestite	0.52	2.97
Fluorite	2.00	3.16
Galena	1.50	2.96
Clays (mica, illite, kaolinite, smectite)	0.09	~4.50

Manual quantification

Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm^2)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	A.I../P.R.	wt%
1	11.6	7.62	57	57		100	Yeso	57/0.7 = 81.4	
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Quartz			100/1.43= 69.9	
5	29.0	3.08	28	28		49	Yeso		
6	31.2	2.87	10	10		18	Yeso		
9	39.5	2.28	16	16	Cuarzo				
10	42.5	2.13	12	12	Quartz	21	Yeso		
11	45.7	1.99	10	10	Quartz	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Quartz	65	Yeso		
								sum.:151.4	

For the quantification we have to divide the max. absolute intensity of both phases by the corresponding reflective power. Both results are integrated.

Manual quantification

Identification								Quantification	
Peak	°2θ	d_{hkl} (Å)	A.I. (mm²)	R.I. (%)	Phase1	R.I.Ph2 (%)	Phase2	A.I./P.R.	w%
1	11.6	7.62	57	57		100	Yeso	57/0.7 = 81.4	(81.4/151.4) x 100 wt% = 54 wt%
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Quartz			100/1.43 = 69.9	(69.9/151.4) x 100 wt% = 46 wt%
5	29.0	3.08	28	28		49	Yeso		
6	3[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	Yeso		
7	3[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	Yeso		
8	3[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]			
9	39.5	2.28	16	16	Quartz				
10	42.5	2.13	12	12	Quartz	21	Yeso		
11	45.7	1.99	10	10	Quartz	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Quartz	65	Yeso		
								sum.:151.4	

Both results are divided by the sum and multipied by 100 in order to obtain a quantification in weight % (wt%).

Manual quantification

Identification								Quantification	
Peak	°2θ	d hkl (Å)	I.a. (mm²)	I.r.T (%)	Phase1	R.I.Ph2 (%)	Phase2	A.I./P.R.	wt%
1	11.6	7.62	57	57		100	Yeso	57/0.7 = 81.4	(81.4/151.4) x 100 wt%= 54 wt%
2	20.9	4.25	33	33	Quartz				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Quartz			100/1.43= 69.9	(69.9/151.4) x 100 wt%= 46 wt%
5	29.0	3.08	28	28		49	Yeso		
6	31.2	2.87	10	10		18	Yeso		
7	33.4	2.68	11	11		19	Yeso		
8	36.5	2.46	13	13	Quartz				
9	39.5	2.28	16	16	Quartz				
10	42.5	2.13	12	12	Quartz	21	Yeso		
11	45.7	1.99	10	10	Quartz	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Quartz	65	Yeso		
								sum.:151.4	

Annex I

Reflective power (R.P.) of various minerals and d_{hkl} of the most intensive peaks

Fase	P.R.	d_{hkl} (Å)
Quartz	1.43	3.34
Calcite	1.05	3.03
Dolomite	1.03	2.88
Gypsum	0.70	7.56
Feldspars	0.98	~3.20
Strontianite	0.60	3.53
Celestite	0.52	2.97
Fluorite	2.00	3.16
Galena	1.50	2.96
Clays (mica, illite, kaolinite, smectite)	0.09	~4.50

Annex II

Reference mineral file

Calcite

Reference Pattern: 01-086-2334

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	1	2	3.85379	23.060	9.9
2	1	0	4	3.03507	29.405	100.0
3	0	0	6	2.84350	31.435	2.1
4	1	1	0	2.49400	35.981	14.2
5	1	1	3	2.28402	39.420	17.8
6	2	0	2	2.09380	43.172	15.0
7	0	2	4	1.92690	47.126	6.3
8	0	1	8	1.91228	47.509	17.6
9	1	1	6	1.87498	48.514	18.4
10	2	1	1	1.62528	56.582	3.1
11	1	2	2	1.60360	57.417	8.8
12	1	0	10	1.58682	58.082	0.8
13	2	1	4	1.52481	60.686	4.9
14	2	0	8	1.51753	61.008	2.0
15	1	1	9	1.50919	61.382	2.3
16	1	2	5	1.47279	63.070	1.9
17	3	0	0	1.43991	64.683	5.7
18	0	0	12	1.42175	65.612	2.8
19	2	1	7	1.35647	69.204	1.0
20	0	2	10	1.33880	70.250	1.6
21	1	2	8	1.29640	72.909	2.4
22	3	0	6	1.28460	73.688	0.6
23	2	2	0	1.24700	76.300	1.1
24	1	1	12	1.23515	77.166	1.4
25	2	2	3	1.21806	78.455	0.1
26	1	3	1	1.19514	80.260	0.1
27	3	1	2	1.18643	80.971	0.5
28	2	1	10	1.17959	81.540	1.8
29	0	1	14	1.17286	82.108	0.2
30	1	3	4	1.15344	83.799	3.8
31	2	2	6	1.14201	84.832	1.6
32	3	1	5	1.13042	85.911	0.1
33	1	2	11	1.12450	86.474	0.4

Annex II

Reference mineral file

Quartz

Reference Pattern: 00-005-0490

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	0	0	4.26000	20.835	35.0
2	1	0	1	3.34300	26.644	100.0
3	1	1	0	2.45800	36.527	12.0
4	1	0	2	2.28200	39.456	12.0
5	1	1	1	2.23700	40.284	6.0
6	2	0	0	2.12800	42.444	9.0
7	2	0	1	1.98000	45.790	6.0
8	1	1	2	1.81700	50.167	17.0
9	0	0	3	1.80100	50.644	1.0
10	2	0	2	1.67200	54.865	7.0
11	1	0	3	1.65900	55.332	3.0
12	2	1	0	1.60800	57.246	1.0
13	2	1	1	1.54100	59.983	15.0
14	1	1	3	1.45300	64.030	3.0
15	3	0	0	1.41800	65.807	1.0
16	2	1	2	1.38200	67.750	7.0
17	2	0	3	1.37500	68.142	11.0
18	3	0	1	1.37200	68.311	9.0
19	1	0	4	1.28800	73.462	3.0
20	3	0	2	1.25600	75.656	4.0
21	2	2	0	1.22800	77.699	2.0
22	2	1	3	1.19970	79.894	5.0
23	2	2	1	1.19730	80.086	2.0
24	1	1	4	1.18380	81.189	4.0
25	3	1	0	1.18020	81.489	4.0
26	3	1	1	1.15300	83.838	2.0
27	2	0	4	1.14080	84.944	1.0
28	3	0	3	1.11440	87.454	1.0
29	3	1	2	1.08160	90.826	4.0
30	4	0	0	1.06360	92.811	1.0
31	1	0	5	1.04770	94.653	2.0
32	4	0	1	1.04370	95.131	2.0
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Annex II

Reference mineral file

Gypsum

Reference Pattern: 00-006-0046

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	2	0	7.56000	11.696	100.0
2	-1	2	1	4.27000	20.786	50.0
3	0	3	1	3.79000	23.454	20.0
4	-1	1	2	3.16300	28.190	4.0
5	-1	4	1	3.05900	29.170	55.0
6	0	0	2	2.86700	31.171	25.0
7	-2	1	1	2.78600	32.102	6.0
8	0	2	2	2.67900	33.421	28.0
9	-2	0	2	2.59100	34.591	4.0
10	0	6	0	2.53000	35.452	1.0
11	2	0	0	2.49500	35.966	6.0
12	-2	2	2	2.45000	36.650	4.0
13	1	4	1	2.40000	37.442	4.0
14	-1	5	2	2.21600	40.682	6.0
15	-2	4	2	2.13900	42.215	2.0
16	-1	2	3	2.08000	43.473	10.0
17	-2	5	1	2.07300	43.627	8.0
18	1	7	0	1.99000	45.546	4.0
19	2	1	1	1.95300	46.459	2.0
20	0	8	0	1.89800	47.889	16.0
21	-1	4	3	1.87900	48.404	10.0
22	-3	1	2	1.86400	48.818	4.0
23	2	3	1	1.84300	49.412	2.0
24	-2	6	2	1.81200	50.315	10.0
25	-3	2	1	1.79600	50.795	4.0
26	2	6	0	1.77800	51.347	10.0
27	-2	5	3	1.71100	53.514	2.0
28	-3	2	3	1.68400	54.442	2.0
29	-3	4	1	1.66400	55.151	4.0
30	-1	6	3	1.64500	55.844	2.0
31	1	8	1	1.62100	56.745	6.0
32	-3	5	2	1.59900	57.598	1.0

Annex II

Reference mineral file

Dolomite

Reference Pattern: 00-011-0078

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	0	1	4.03000	22.039	3.0
2	0	1	2	3.69000	24.099	5.0
3	1	0	4	2.88600	30.961	100.0
4	0	0	6	2.67000	33.537	10.0
5	0	1	5	2.54000	35.308	8.0
6	1	1	0	2.40500	37.361	10.0
7	1	1	3	2.19200	41.148	30.0
8	0	2	1	2.06600	43.782	5.0
9	2	0	2	2.01500	44.950	15.0
10	0	2	4	1.84800	49.269	5.0
11	0	1	8	1.80400	50.554	20.0
12	1	1	6	1.78600	51.100	30.0
13	0	0	9	1.78100	51.254	30.0
14	2	1	1	1.56700	58.888	8.0
15	1	2	2	1.54500	59.812	10.0
16	1	0	10	1.49600	61.982	1.0
17	2	1	4	1.46500	63.444	5.0
18	2	0	8	1.44500	64.427	4.0
19	1	1	9	1.43100	65.135	10.0
20	1	2	5	1.41300	66.070	4.0
21	3	0	0	1.38900	67.362	15.0
22	0	0	12	1.33500	70.480	8.0
23	2	1	7	1.29700	72.870	2.0
24	0	2	10	1.26900	74.748	2.0
25	1	2	8	1.23800	76.956	5.0
26	2	2	0	1.20200	79.710	3.0
27	1	1	12	1.16800	82.524	4.0
28	3	1	2	1.14400	84.650	2.0
29	2	1	10	1.12300	86.618	5.0
30	2	2	6	1.09600	89.309	3.0
31	0	0	15	1.06800	92.316	1.0
32	4	0	4	1.00800	99.669	4.0

Annex II

Reference mineral file

Galena

Reference Pattern: 00-005-0592

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	1	1	3.42900	25.964	84.0
2	2	0	0	2.96900	30.075	100.0
3	2	2	0	2.09900	43.059	57.0
4	3	1	1	1.79000	50.978	35.0
5	2	2	2	1.71400	53.412	16.0
6	4	0	0	1.48400	62.540	10.0
7	3	3	1	1.36200	68.883	10.0
8	4	2	0	1.32700	70.969	17.0
9	4	2	2	1.21200	78.923	10.0
10	5	1	1	1.14240	84.797	6.0
11	4	4	0	1.04890	94.511	3.0
12	5	3	1	1.00340	100.294	5.0
13	6	0	0	0.98930	102.271	6.0
14	6	2	0	0.93860	110.308	4.0
15	5	3	3	0.90500	116.676	2.0
16	6	2	2	0.89520	118.740	4.0
17	4	4	4	0.85680	128.065	1.0
18	7	1	1	0.83120	135.862	3.0
19	6	4	0	0.82320	138.695	3.0

Annex II

Reference mineral file

Celestite

Reference Pattern: 00-001-0885

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	1	1	4.22000	21.035	14.0
2	0	0	2	3.42000	26.033	14.0
3	2	1	0	3.29000	27.081	29.0
4	1	0	2	3.16000	28.218	21.0
5	2	1	1	2.97000	30.064	100.0
6	0	2	0	2.70000	33.153	72.0
7	2	1	2	2.37000	37.934	14.0
8	2	2	0	2.26000	39.856	14.0
9	0	2	2	2.12000	42.612	14.0
10	1	1	3	2.03000	44.600	43.0
11	4	0	1	2.00000	45.306	21.0
12	4	1	0	1.94000	46.789	14.0
13	2	2	2	1.88000	48.376	14.0
14	3	2	1	1.84000	49.498	14.0
15	3	0	3	1.76000	51.911	14.0
16	1	0	4	1.67000	54.936	14.0
17	2	0	4	1.59000	57.955	14.0
18	5	1	1	1.55000	59.599	14.0
19	3	3	1	1.47000	63.204	14.0
20	1	2	4	1.42000	65.703	14.0

Annex II

Reference mineral file
Strontianite

Reference Pattern: 00-005-0418

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	1	0	4.36700	20.319	14.0
2	0	2	0	4.20700	21.101	6.0
3	1	1	1	3.53500	25.172	100.0
4	0	2	1	3.45000	25.803	70.0
5	0	0	2	3.01400	29.615	22.0
6	1	2	1	2.85900	31.261	5.0
7	0	1	2	2.83800	31.498	20.0
8	1	0	2	2.59600	34.522	12.0
9	2	0	0	2.55400	35.108	23.0
10	1	1	2	2.48100	36.176	34.0
11	1	3	0	2.45800	36.527	40.0
12	0	2	2	2.45110	36.633	33.0
13	2	1	1	2.26460	39.772	5.0
14	2	2	0	2.18310	41.323	16.0
15	0	4	0	2.10350	42.963	7.0
16	2	2	1	2.05260	44.083	50.0
17	0	4	1	1.98600	45.643	26.0
18	2	0	2	1.94890	46.563	21.0
19	1	3	2	1.90530	47.694	35.0
20	1	4	1	1.85140	49.173	3.0
21	1	1	3	1.82530	49.923	31.0
22	0	2	3	1.81340	50.274	16.0
23	2	3	1	1.80230	50.605	4.0
24	2	2	2	1.76850	51.643	7.0
25	0	4	2	1.72530	53.035	5.0
26	3	1	0	1.66840	54.994	3.0
27	2	4	0	1.62360	56.646	4.0
28	3	1	1	1.60800	57.246	13.0
29	1	5	0	1.59810	57.633	3.0
30	2	4	1	1.56760	58.864	13.0
31	1	5	1	1.54470	59.824	11.0
32	0	0	4	1.50720	61.472	3.0
33	2	2	3	1.47820	62.813	6.0
34	3	1	2	1.45960	63.707	4.0
35	3	3	0	1.45510	63.927	9.0
36	2	4	2	1.42930	65.222	6.0

Annex II

Reference mineral file

Fluorite

Reference Pattern: 01-089-4794

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	1	1	3.15378	28.275	100.0
2	2	0	0	2.73125	32.763	0.5
3	2	2	0	1.93129	47.013	97.1
4	3	1	1	1.64701	55.770	28.6
5	2	2	2	1.57689	58.483	0.3
6	4	0	0	1.36563	68.674	9.6
7	3	3	1	1.25318	75.857	8.1
8	4	2	0	1.22145	78.195	0.5
9	4	2	2	1.11503	87.392	14.3

Annex III

Tables to convert °2θ to d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1.541838

Cu $K\bar{\alpha}$ 0–20°

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
0.00		4417.0	2208.5	1472.3	1104.3	883.41	736.17	631.01	552.13	490.78
.20	441.70	401.55	368.09	339.77	315.50	294.47	276.07	259.83	245.39	232.48
.40	220.85	210.34	200.78	192.05	184.04	176.68	169.89	163.59	157.75	152.31
.60	147.24	142.49	138.03	133.85	129.91	126.20	122.70	119.38	116.24	113.26
.80	110.43	107.73	105.17	102.72	100.39	98.158	96.024	93.981	92.023	90.145
1.00	88.342	86.610	84.944	83.342	81.798	80.311	78.877	77.493	76.157	74.866
.20	73.619	72.412	71.244	70.113	69.018	67.956	66.926	65.928	64.958	64.017
.40	63.102	62.213	61.349	60.509	59.691	58.896	58.121	57.366	56.630	55.914
.60	55.215	54.533	53.868	53.219	52.586	51.967	51.363	50.773	50.196	49.632
.80	49.080	48.541	48.013	47.497	46.992	46.497	46.013	45.539	45.074	44.619
2.00	44.173	43.735	43.307	42.886	42.474	42.069	41.673	41.283	40.901	40.526
.20	40.157	39.796	39.440	39.091	38.749	38.412	38.081	37.755	37.435	37.121
.40	36.811	36.507	36.208	35.914	35.624	35.339	35.059	34.783	34.511	34.244
.60	33.980	33.721	33.465	33.214	32.966	32.722	32.481	32.244	32.011	31.780
.80	31.553	31.330	31.109	30.892	30.677	30.466	30.257	30.051	29.848	29.648
3.00	29.450	29.255	29.063	28.873	28.686	28.501	28.318	28.138	27.959	27.784
.20	27.610	27.439	27.269	27.102	26.937	26.774	26.612	26.453	26.296	26.140
.40	25.986	25.834	25.684	25.536	25.389	25.244	25.101	24.959	24.819	24.680
.60	24.543	24.408	24.274	24.141	24.010	23.880	23.752	23.625	23.499	23.375
.80	23.252	23.130	23.010	22.891	22.773	22.656	22.540	22.426	22.313	22.201
4.00	22.090	21.980	21.871	21.763	21.657	21.551	21.447	21.343	21.240	21.139
.20	21.038	20.939	20.840	20.742	20.645	20.549	20.454	20.360	20.267	20.174
.40	20.082	19.992	19.902	19.812	19.724	19.636	19.549	19.463	19.378	19.294
.60	19.210	19.127	19.044	18.962	18.881	18.801	18.722	18.643	18.564	18.487
.80	18.410	18.333	18.258	18.183	18.108	18.034	17.961	17.888	17.816	17.745
5.00	17.674	17.603	17.534	17.464	17.396	17.327	17.260	17.193	17.126	17.060
.20	16.994	16.929	16.865	16.801	16.737	16.674	16.611	16.549	16.488	16.426
.40	16.365	16.305	16.245	16.186	16.127	16.068	16.010	15.952	15.895	15.838
.60	15.781	15.725	15.670	15.614	15.559	15.505	15.451	15.397	15.343	15.290
.80	15.238	15.185	15.133	15.082	15.031	14.980	14.929	14.879	14.829	14.779
6.00	14.730	14.681	14.633	14.584	14.537	14.489	14.442	14.395	14.348	14.302
.20	14.255	14.210	14.164	14.119	14.074	14.029	13.985	13.941	13.897	13.854
.40	13.810	13.767	13.725	13.682	13.640	13.598	13.557	13.515	13.474	13.433
.60	13.392	13.352	13.312	13.272	13.232	13.193	13.153	13.115	13.076	13.037
.80	12.999	12.961	12.923	12.885	12.848	12.811	12.774	12.737	12.700	12.664
7.00	12.628	12.592	12.556	12.521	12.485	12.450	12.415	12.381	12.346	12.312
.20	12.278	12.244	12.210	12.176	12.143	12.110	12.077	12.044	12.011	11.979
.40	11.946	11.914	11.882	11.850	11.819	11.787	11.756	11.725	11.694	11.663
.60	11.632	11.602	11.572	11.541	11.511	11.481	11.452	11.422	11.393	11.364
.80	11.335	11.306	11.277	11.248	11.220	11.191	11.163	11.135	11.107	11.079
8.00	11.052	11.024	10.997	10.969	10.942	10.915	10.889	10.862	10.835	10.809
.20	10.782	10.756	10.730	10.704	10.678	10.653	10.627	10.602	10.576	10.551
.40	10.526	10.501	10.476	10.452	10.427	10.403	10.378	10.354	10.330	10.306
.60	10.282	10.258	10.234	10.211	10.187	10.164	10.141	10.117	10.094	10.071
.80	10.049	10.026	10.003	9.9807	9.9583	9.9359	9.9137	9.8916	9.8695	9.8476
9.00	9.8258	9.8040	9.7824	9.7608	9.7394	9.7180	9.6967	9.6756	9.6545	9.6335
.20	9.6126	9.5918	9.5711	9.5504	9.5299	9.5095	9.4891	9.4688	9.4486	9.4285
.40	9.4085	9.3886	9.3687	9.3490	9.3293	9.3097	9.2902	9.2707	9.2514	9.2321
.60	9.2129	9.1938	9.1748	9.1559	9.1370	9.1182	9.0995	9.0808	9.0623	9.0438
.80	9.0254	9.0070	8.9888	8.9706	8.9525	8.9344	8.9165	8.8986	8.8807	8.8630

COPPER K ALPHA(1,2)
LAMBDA=1.541838

Cu $K\bar{\alpha}$ 0–20°

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
10.00	8.8453	8.8277	8.8102	8.7927	8.7753	8.7580	8.7407	8.7235	8.7064	8.6893
.20	8.6723	8.6554	8.6385	8.6217	8.6050	8.5883	8.5717	8.5552	8.5387	8.5223
.40	8.5060	8.4897	8.4735	8.4573	8.4412	8.4252	8.4092	8.3933	8.3775	8.3617
.60	8.3459	8.3303	8.3147	8.2991	8.2836	8.2682	8.2528	8.2375	8.2222	8.2070
.80	8.1918	8.1767	8.1617	8.1467	8.1318	8.1169	8.1021	8.0873	8.0726	8.0579
11.00	8.0433	8.0288	8.0143	7.9998	7.9854	7.9711	7.9568	7.9426	7.9284	7.9142
.20	7.9001	7.8861	7.8721	7.8582	7.8443	7.8305	7.8167	7.8029	7.7892	7.7756
.40	7.7620	7.7484	7.7349	7.7215	7.7081	7.6947	7.6814	7.6681	7.6549	7.6417
.60	7.6286	7.6155	7.6025	7.5895	7.5765	7.5636	7.5508	7.5380	7.5252	7.5125
.80	7.4998	7.4871	7.4745	7.4620	7.4494	7.4370	7.4245	7.4121	7.3998	7.3875
12.00	7.3752	7.3630	7.3508	7.3386	7.3265	7.3145	7.3025	7.2905	7.2786	7.2666
.20	7.2548	7.2429	7.2311	7.2194	7.2077	7.1960	7.1844	7.1728	7.1612	7.1497
.40	7.1382	7.1267	7.1153	7.1039	7.0926	7.0813	7.0700	7.0588	7.0476	7.0365
.60	7.0253	7.0142	7.0032	6.9922	6.9812	6.9702	6.9593	6.9484	6.9376	6.9268
.80	6.9160	6.9053	6.8945	6.8839	6.8732	6.8626	6.8520	6.8415	6.8310	6.8205
13.00	6.8101	6.7996	6.7893	6.7789	6.7686	6.7583	6.7480	6.7378	6.7276	6.7174
.20	6.7073	6.6972	6.6871	6.6771	6.6671	6.6571	6.6472	6.6372	6.6273	6.6175
.40	6.6076	6.5978	6.5881	6.5783	6.5686	6.5589	6.5493	6.5396	6.5300	6.5205
.60	6.5109	6.5014	6.4919	6.4825	6.4730	6.4636	6.4542	6.4449	6.4356	6.4263
.80	6.4170	6.4078	6.3986	6.3894	6.3802	6.3711	6.3620	6.3529	6.3438	6.3348
14.00	6.3258	6.3168	6.3079	6.2989	6.2900	6.2811	6.2723	6.2635	6.2547	6.2459
.20	6.2371	6.2284	6.2197	6.2110	6.2024	6.1937	6.1851	6.1766	6.1680	6.1595
.40	6.1510	6.1425	6.1340	6.1256	6.1172	6.1088	6.1004	6.0920	6.0837	6.0754
.60	6.0671	6.0589	6.0507	6.0424	6.0343	6.0261	6.0180	6.0098	6.0017	5.9937
.80	5.9856	5.9776	5.9696	5.9616	5.9536	5.9457	5.9377	5.9298	5.9219	5.9141
15.00	5.9062	5.8984	5.8906	5.8828	5.8751	5.8674	5.8596	5.8519	5.8443	5.8366
.20	5.8290	5.8214	5.8138	5.8062	5.7986	5.7911	5.7836	5.7761	5.7686	5.7612
.40	5.7537	5.7463	5.7389	5.7315	5.7242	5.7168	5.7095	5.7022	5.6949	5.6877
.60	5.6804	5.6732	5.6660	5.6588	5.6516	5.6444	5.6373	5.6302	5.6231	5.6160
.80	5.6089	5.6019	5.5949	5.5879	5.5809	5.5739	5.5669	5.5600	5.5531	5.5462
16.00	5.5393	5.5324	5.5256	5.5187	5.5119	5.5051	5.4983	5.4915	5.4848	5.4781
.20	5.4713	5.4646	5.4580	5.4513	5.4446	5.4380	5.4314	5.4248	5.4182	5.4116
.40	5.4051	5.3985	5.3920	5.3855	5.3790	5.3725	5.3661	5.3596	5.3532	5.3468
.60	5.3404	5.3340	5.3277	5.3213	5.3150	5.3086	5.3023	5.2961	5.2898	5.2835
.80	5.2773	5.2710	5.2648	5.2586	5.2524	5.2463	5.2401	5.2340	5.2278	5.2217
17.00	5.2156	5.2096	5.2035	5.1974	5.1914	5.1854	5.1793	5.1733	5.1674	5.1614
.20	5.1554	5.1495	5.1436	5.1376	5.1317	5.1259	5.1200	5.1141	5.1083	5.1024
.40	5.0966	5.0908	5.0850	5.0792	5.0735	5.0677	5.0620	5.0563	5.0505	5.0448
.60	5.0392	5.0335	5.0278	5.0222	5.0165	5.0109	5.0053	4.9997	4.9941	4.9885
.80	4.9830	4.9774	4.9719	4.9664	4.9609	4.9554	4.9499	4.9444	4.9390	4.9335
18.00	4.9281	4.9226	4.9172	4.9118	4.9064	4.9011	4.8957	4.8903	4.8850	4.8797
.20	4.8744	4.8691	4.8638	4.8585	4.8532	4.8480	4.8427	4.8375	4.8322	4.8270
.40	4.8218	4.8166	4.8115	4.8063	4.8011	4.7960	4.7909	4.7857	4.7806	4.7755
.60	4.7704	4.7654	4.7603	4.7552	4.7502	4.7451	4.7401	4.7351	4.7301	4.7251
.80	4.7201	4.7152	4.7102	4.7052	4.7003	4.6954	4.6905	4.6856	4.6807	4.6758
19.00	4.6709	4.6660	4.6612	4.6563	4.6515	4.6467	4.6418	4.6370	4.6322	4.6275
.20	4.6227	4.6179	4.6132	4.6084	4.6037	4.5990	4.5942	4.5895	4.5848	4.5802
.40	4.5755	4.5708	4.5662	4.5615	4.5569	4.5522	4.5476	4.5430	4.5384	4.5338
.60	4.5292	4.5247	4.5201	4.5156	4.5110	4.5065	4.5019	4.4974	4.4929	4.4884
.80	4.4839	4.4795	4.4750	4.4705	4.4661	4.4616	4.4572	4.4528	4.4484	4.4439

Annex III

Tables to convert °2θ to d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1.541838

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
20.00	4.4395	4.4352	4.4308	4.4264	4.4220	4.4177	4.4133	4.4090	4.4047	4.4004
.20	4.3960	4.3917	4.3874	4.3832	4.3789	4.3746	4.3704	4.3661	4.3619	4.3576
.40	4.3534	4.3492	4.3450	4.3408	4.3366	4.3324	4.3282	4.3240	4.3199	4.3157
.60	4.3116	4.3074	4.3033	4.2992	4.2951	4.2910	4.2869	4.2828	4.2787	4.2746
.80	4.2706	4.2665	4.2625	4.2584	4.2544	4.2504	4.2463	4.2423	4.2383	4.2343
21.00	4.2303	4.2264	4.2224	4.2184	4.2145	4.2105	4.2066	4.2026	4.1987	4.1948
.20	4.1909	4.1870	4.1831	4.1792	4.1753	4.1714	4.1676	4.1637	4.1599	4.1560
.40	4.1522	4.1483	4.1445	4.1407	4.1369	4.1331	4.1293	4.1255	4.1217	4.1179
.60	4.1142	4.1104	4.1067	4.1029	4.0992	4.0954	4.0917	4.0880	4.0843	4.0806
.80	4.0769	4.0732	4.0695	4.0658	4.0622	4.0585	4.0548	4.0512	4.0475	4.0439
22.00	4.0403	4.0366	4.0330	4.0294	4.0258	4.0222	4.0186	4.0150	4.0115	4.0079
.20	4.0043	4.0008	3.9972	3.9937	3.9901	3.9866	3.9831	3.9795	3.9760	3.9725
.40	3.9690	3.9655	3.9620	3.9585	3.9551	3.9516	3.9481	3.9447	3.9412	3.9378
.60	3.9343	3.9309	3.9275	3.9241	3.9206	3.9172	3.9138	3.9104	3.9070	3.9037
.80	3.9003	3.8969	3.8935	3.8902	3.8868	3.8835	3.8801	3.8768	3.8735	3.8701
23.00	3.8668	3.8635	3.8602	3.8569	3.8536	3.8503	3.8470	3.8437	3.8405	3.8372
.20	3.8339	3.8307	3.8274	3.8242	3.8209	3.8177	3.8145	3.8113	3.8080	3.8048
.40	3.8016	3.7984	3.7952	3.7920	3.7888	3.7857	3.7825	3.7793	3.7762	3.7730
.60	3.7698	3.7667	3.7636	3.7604	3.7573	3.7542	3.7510	3.7479	3.7448	3.7417
.80	3.7386	3.7355	3.7324	3.7294	3.7263	3.7232	3.7201	3.7171	3.7140	3.7110
24.00	3.7079	3.7049	3.7018	3.6988	3.6958	3.6928	3.6897	3.6867	3.6837	3.6807
.20	3.6777	3.6747	3.6717	3.6688	3.6658	3.6628	3.6598	3.6569	3.6539	3.6510
.40	3.6480	3.6451	3.6422	3.6392	3.6363	3.6334	3.6304	3.6275	3.6246	3.6217
.60	3.6188	3.6159	3.6130	3.6102	3.6073	3.6044	3.6015	3.5987	3.5958	3.5929
.80	3.5901	3.5872	3.5844	3.5816	3.5787	3.5759	3.5731	3.5703	3.5674	3.5646
25.00	3.5618	3.5590	3.5562	3.5534	3.5506	3.5479	3.5451	3.5423	3.5395	3.5368
.20	3.5340	3.5312	3.5285	3.5257	3.5230	3.5203	3.5175	3.5148	3.5121	3.5093
.40	3.5066	3.5039	3.5012	3.4985	3.4958	3.4931	3.4904	3.4877	3.4850	3.4824
.60	3.4797	3.4770	3.4743	3.4717	3.4690	3.4664	3.4637	3.4611	3.4584	3.4558
.80	3.4532	3.4505	3.4479	3.4453	3.4427	3.4401	3.4375	3.4348	3.4322	3.4296
26.00	3.4271	3.4245	3.4219	3.4193	3.4167	3.4141	3.4116	3.4090	3.4065	3.4039
.20	3.4013	3.3988	3.3963	3.3937	3.3912	3.3886	3.3861	3.3836	3.3811	3.3785
.40	3.3760	3.3735	3.3710	3.3685	3.3660	3.3635	3.3610	3.3585	3.3561	3.3536
.60	3.3511	3.3486	3.3462	3.3437	3.3412	3.3388	3.3363	3.3339	3.3314	3.3290
.80	3.3265	3.3241	3.3217	3.3192	3.3168	3.3144	3.3120	3.3096	3.3072	3.3048
27.00	3.3024	3.3000	3.2976	3.2952	3.2928	3.2904	3.2880	3.2856	3.2833	3.2809
.20	3.2785	3.2762	3.2738	3.2714	3.2691	3.2667	3.2644	3.2621	3.2597	3.2574
.40	3.2550	3.2527	3.2504	3.2481	3.2458	3.2434	3.2411	3.2388	3.2365	3.2342
.60	3.2319	3.2296	3.2273	3.2250	3.2228	3.2205	3.2182	3.2159	3.2136	3.2114
.80	3.2091	3.2069	3.2046	3.2023	3.2001	3.1978	3.1956	3.1934	3.1911	3.1889
28.00	3.1866	3.1844	3.1822	3.1800	3.1777	3.1755	3.1733	3.1711	3.1689	3.1667
.20	3.1645	3.1623	3.1601	3.1579	3.1557	3.1535	3.1514	3.1492	3.1470	3.1448
.40	3.1427	3.1405	3.1383	3.1362	3.1340	3.1319	3.1297	3.1276	3.1254	3.1233
.60	3.1211	3.1190	3.1169	3.1147	3.1126	3.1105	3.1084	3.1063	3.1041	3.1020
.80	3.0999	3.0978	3.0957	3.0936	3.0915	3.0894	3.0873	3.0852	3.0832	3.0811
29.00	3.0790	3.0769	3.0748	3.0728	3.0707	3.0686	3.0666	3.0645	3.0625	3.0604
.20	3.0584	3.0563	3.0543	3.0522	3.0502	3.0482	3.0461	3.0441	3.0421	3.0400
.40	3.0380	3.0360	3.0340	3.0320	3.0299	3.0279	3.0259	3.0239	3.0219	3.0199
.60	3.0179	3.0159	3.0140	3.0120	3.0100	3.0080	3.0060	3.0040	3.0021	3.0001
.80	2.9981	2.9962	2.9942	2.9922	2.9903	2.9883	2.9864	2.9844	2.9825	2.9805

COPPER K ALPHA(1,2)
LAMBDA=1.541838

Cu $K\bar{\alpha}$
20–40°

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
30.00	2.9786	2.9767	2.9747	2.9728	2.9709	2.9689	2.9670	2.9651	2.9632	2.9612
.20	2.9593	2.9574	2.9555	2.9536	2.9517	2.9498	2.9479	2.9460	2.9441	2.9422
.40	2.9403	2.9384	2.9365	2.9347	2.9328	2.9309	2.9290	2.9272	2.9253	2.9234
.60	2.9216	2.9197	2.9178	2.9160	2.9141	2.9123	2.9104	2.9086	2.9067	2.9049
.80	2.9030	2.9012	2.8994	2.8975	2.8957	2.8939	2.8920	2.8902	2.8884	2.8866
31.00	2.8848	2.8829	2.8811	2.8793	2.8775	2.8757	2.8739	2.8721	2.8703	2.8685
.20	2.8667	2.8649	2.8631	2.8614	2.8596	2.8578	2.8560	2.8542	2.8525	2.8507
.40	2.8489	2.8472	2.8454	2.8436	2.8419	2.8401	2.8383	2.8366	2.8348	2.8331
.60	2.8313	2.8296	2.8279	2.8261	2.8244	2.8226	2.8209	2.8192	2.8174	2.8157
.80	2.8140	2.8123	2.8105	2.8088	2.8071	2.8054	2.8037	2.8020	2.8003	2.7986
32.00	2.7969	2.7952	2.7935	2.7918	2.7901	2.7884	2.7867	2.7850	2.7833	2.7816
.20	2.7799	2.7783	2.7766	2.7749	2.7732	2.7716	2.7699	2.7682	2.7666	2.7649
.40	2.7632	2.7616	2.7599	2.7583	2.7566	2.7550	2.7533	2.7517	2.7500	2.7484
.60	2.7467	2.7451	2.7435	2.7418	2.7402	2.7386	2.7369	2.7353	2.7337	2.7321
.80	2.7305	2.7288	2.7272	2.7256	2.7240	2.7224	2.7208	2.7192	2.7176	2.7160
33.00	2.7144	2.7128	2.7112	2.7096	2.7080	2.7064	2.7048	2.7032	2.7016	2.7000
.20	2.6985	2.6969	2.6953	2.6937	2.6922	2.6906	2.6890	2.6874	2.6859	2.6843
.40	2.6828	2.6812	2.6796	2.6781	2.6765	2.6750	2.6734	2.6719	2.6703	2.6688
.60	2.6672	2.6657	2.6642	2.6626	2.6611	2.6596	2.6580	2.6565	2.6550	2.6534
.80	2.6519	2.6504	2.6489	2.6474	2.6458	2.6443	2.6428	2.6413	2.6398	2.6383
34.00	2.6368	2.6353	2.6338	2.6323	2.6308	2.6293	2.6278	2.6263	2.6248	2.6233
.20	2.6218	2.6203	2.6188	2.6174	2.6159	2.6144	2.6129	2.6114	2.6100	2.6085
.40	2.6070	2.6056	2.6041	2.6026	2.6012	2.5997	2.5982	2.5968	2.5953	2.5939
.60	2.5924	2.5910	2.5895	2.5881	2.5866	2.5852	2.5837	2.5823	2.5808	2.5794
.80	2.5780	2.5765	2.5751	2.5737	2.5722	2.5708	2.5694	2.5680	2.5665	2.5651
35.00	2.5637	2.5623	2.5609	2.5594	2.5580	2.5566	2.5552	2.5538	2.5524	2.5510
.20	2.5496	2.5482	2.5468	2.5454	2.5440	2.5426	2.5412	2.5398	2.5384	2.5370
.40	2.5356	2.5343	2.5329	2.5315	2.5301	2.5287	2.5274	2.5260	2.5246	2.5232
.60	2.5219	2.5205	2.5191	2.5178	2.5164	2.5150	2.5137	2.5123	2.5109	2.5096
.80	2.5082	2.5069	2.5055	2.5042	2.5028	2.5015	2.5001	2.4988	2.4974	2.4961
36.00	2.4947	2.4934	2.4921	2.4907	2.4894	2.4881	2.4867	2.4854	2.4841	2.4827
.20	2.4814	2.4801	2.4788	2.4775	2.4761	2.4748	2.4735	2.4722	2.4709	2.4696
.40	2.4682	2.4669	2.4656	2.4643	2.4630	2.4617	2.4604	2.4591	2.4578	2.4565
.60	2.4552	2.4539	2.4526	2.4513	2.4500	2.4488	2.4475	2.4462	2.4449	2.4436
.80	2.4423	2.4410	2.4398	2.4385	2.4372	2.4359	2.4347	2.4334	2.4321	2.4309
37.00	2.4296	2.4283	2.4271	2.4258	2.4245	2.4233	2.4220	2.4207	2.4195	2.4182
.20	2.4170	2.4157	2.4145	2.4132	2.4120	2.4107	2.4095	2.4082	2.4070	2.4058
.40	2.4045	2.4033	2.4020	2.4008	2.3996	2.3983	2.3971	2.3959	2.3946	2.3934
.60	2.3922	2.3910	2.3897	2.3885	2.3873	2.3861	2.3849	2.3836	2.3824	2.3812
.80	2.3800	2.3788	2.3776	2.3764	2.3751	2.3739	2.3727	2.3715	2.3703	2.3691
38.00	2.3679	2.3667	2.3655	2.3643	2.3631	2.3619	2.3607	2.3595	2.3584	2.3572
.20	2.3560	2.3548	2.3536	2.3524	2.3512	2.3501	2.3489	2.3477	2.3465	2.3453
.40	2.3442	2.3430	2.3418	2.3407	2.3395	2.3383	2.3371	2.3360	2.3348	2.3336
.60	2.3325	2.3313	2.3302	2.3290	2.3278	2.3267	2.3255	2.3244	2.3232	2.3221
.80	2.3209	2.3198	2.3186	2.3175	2.3163	2.3152	2.3140	2.3129	2.3118	2.3106
39.00	2.3095	2.3083	2.3072	2.3061	2.3049	2.3038	2.3027	2.3015	2.3004	2.2993
.20	2.2982	2.2970	2.2959	2.2948	2.2937	2.2925	2.2914	2.2903	2.2892	2.2881
.40	2.2869	2.2858	2.2847	2.2836	2.2825	2.2814	2.2803	2.2792	2.2781	2.2770
.60	2.2759	2.2748	2.2737	2.2726	2.2715	2.2704	2.2693	2.2682	2.2671	2.2660
.80	2.2649	2.2638	2.2627	2.2616	2.2605	2.2594	2.2583	2.2573	2.2562	2.2551

Annex III

Tables to convert °2θ to d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1.541838

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
40.00	2.2540	2.2529	2.2519	2.2508	2.2497	2.2486	2.2476	2.2465	2.2454	2.2443
.20	2.2433	2.2422	2.2411	2.2401	2.2390	2.2379	2.2369	2.2358	2.2347	2.2337
.40	2.2326	2.2316	2.2305	2.2294	2.2284	2.2273	2.2263	2.2252	2.2242	2.2231
.60	2.2221	2.2210	2.2200	2.2189	2.2179	2.2169	2.2158	2.2148	2.2137	2.2127
.80	2.2116	2.2106	2.2096	2.2085	2.2075	2.2065	2.2054	2.2044	2.2034	2.2023
41.00	2.2013	2.2003	2.1993	2.1982	2.1972	2.1962	2.1952	2.1942	2.1931	2.1921
.20	2.1911	2.1901	2.1891	2.1880	2.1870	2.1860	2.1850	2.1840	2.1830	2.1820
.40	2.1810	2.1800	2.1790	2.1780	2.1770	2.1760	2.1749	2.1739	2.1729	2.1719
.60	2.1709	2.1700	2.1690	2.1680	2.1670	2.1660	2.1650	2.1640	2.1630	2.1620
.80	2.1610	2.1600	2.1591	2.1581	2.1571	2.1561	2.1551	2.1541	2.1532	2.1522
42.00	2.1512	2.1502	2.1492	2.1483	2.1473	2.1463	2.1453	2.1444	2.1434	2.1424
.20	2.1415	2.1405	2.1395	2.1386	2.1376	2.1366	2.1357	2.1347	2.1337	2.1328
.40	2.1318	2.1309	2.1299	2.1289	2.1280	2.1270	2.1261	2.1251	2.1242	2.1232
.60	2.1223	2.1213	2.1204	2.1194	2.1185	2.1175	2.1166	2.1156	2.1147	2.1138
.80	2.1128	2.1119	2.1109	2.1100	2.1091	2.1081	2.1072	2.1063	2.1053	2.1044
43.00	2.1035	2.1025	2.1016	2.1007	2.0997	2.0988	2.0979	2.0970	2.0960	2.0951
.20	2.0942	2.0933	2.0923	2.0914	2.0905	2.0896	2.0887	2.0877	2.0868	2.0859
.40	2.0850	2.0841	2.0832	2.0823	2.0813	2.0804	2.0795	2.0786	2.0777	2.0768
.60	2.0759	2.0750	2.0741	2.0732	2.0723	2.0714	2.0705	2.0696	2.0687	2.0678
.80	2.0669	2.0660	2.0651	2.0642	2.0633	2.0624	2.0615	2.0606	2.0597	2.0588
44.00	2.0579	2.0571	2.0562	2.0553	2.0544	2.0535	2.0526	2.0517	2.0509	2.0500
.20	2.0491	2.0482	2.0473	2.0465	2.0456	2.0447	2.0438	2.0429	2.0421	2.0412
.40	2.0403	2.0395	2.0386	2.0377	2.0368	2.0360	2.0351	2.0342	2.0334	2.0325
.60	2.0316	2.0308	2.0299	2.0291	2.0282	2.0273	2.0265	2.0256	2.0248	2.0239
.80	2.0230	2.0222	2.0213	2.0205	2.0196	2.0188	2.0179	2.0171	2.0162	2.0154
45.00	2.0145	2.0137	2.0128	2.0120	2.0111	2.0103	2.0094	2.0086	2.0077	2.0069
.20	2.0061	2.0052	2.0044	2.0035	2.0027	2.0019	2.0010	2.0002	1.9994	1.9985
.40	1.9977	1.9969	1.9960	1.9952	1.9944	1.9935	1.9927	1.9919	1.9910	1.9902
.60	1.9894	1.9886	1.9877	1.9869	1.9861	1.9853	1.9844	1.9836	1.9828	1.9820
.80	1.9812	1.9803	1.9795	1.9787	1.9779	1.9771	1.9763	1.9755	1.9746	1.9738
46.00	1.9730	1.9722	1.9714	1.9706	1.9698	1.9690	1.9682	1.9674	1.9666	1.9657
.20	1.9649	1.9641	1.9633	1.9625	1.9617	1.9609	1.9601	1.9593	1.9585	1.9577
.40	1.9569	1.9561	1.9553	1.9545	1.9538	1.9530	1.9522	1.9514	1.9506	1.9498
.60	1.9490	1.9482	1.9474	1.9466	1.9458	1.9451	1.9443	1.9435	1.9427	1.9419
.80	1.9411	1.9404	1.9396	1.9388	1.9380	1.9372	1.9365	1.9357	1.9349	1.9341
47.00	1.9333	1.9326	1.9318	1.9310	1.9302	1.9295	1.9287	1.9279	1.9272	1.9264
.20	1.9256	1.9248	1.9241	1.9233	1.9225	1.9218	1.9210	1.9202	1.9195	1.9187
.40	1.9180	1.9172	1.9164	1.9157	1.9149	1.9142	1.9134	1.9126	1.9119	1.9111
.60	1.9104	1.9096	1.9089	1.9081	1.9073	1.9066	1.9058	1.9051	1.9043	1.9036
.80	1.9028	1.9021	1.9013	1.9006	1.8998	1.8991	1.8984	1.8976	1.8969	1.8961
48.00	1.8954	1.8946	1.8939	1.8932	1.8924	1.8917	1.8909	1.8902	1.8895	1.8887
.20	1.8880	1.8872	1.8865	1.8858	1.8850	1.8843	1.8836	1.8828	1.8821	1.8814
.40	1.8806	1.8799	1.8792	1.8785	1.8777	1.8770	1.8763	1.8755	1.8748	1.8741
.60	1.8734	1.8726	1.8719	1.8712	1.8705	1.8698	1.8690	1.8683	1.8676	1.8669
.80	1.8662	1.8654	1.8647	1.8640	1.8633	1.8626	1.8619	1.8611	1.8604	1.8597
49.00	1.8590	1.8583	1.8576	1.8569	1.8562	1.8555	1.8547	1.8540	1.8533	1.8526
.20	1.8519	1.8512	1.8505	1.8498	1.8491	1.8484	1.8477	1.8470	1.8463	1.8456
.40	1.8449	1.8442	1.8435	1.8428	1.8421	1.8414	1.8407	1.8400	1.8393	1.8386
.60	1.8379	1.8372	1.8365	1.8358	1.8351	1.8345	1.8338	1.8331	1.8324	1.8317
.80	1.8310	1.8303	1.8296	1.8289	1.8283	1.8276	1.8269	1.8262	1.8255	1.8248

COPPER K ALPHA(1,2)
LAMBDA=1.541838

Cu K
40–60

	0.00	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16	0.18
50.00	1.8241	1.8235	1.8228	1.8221	1.8214	1.8207	1.8201	1.8194	1.8187	1.8180
.20	1.8174	1.8167	1.8160	1.8153	1.8146	1.8140	1.8133	1.8126	1.8120	1.8113
.40	1.8106	1.8099	1.8093	1.8086	1.8079	1.8073	1.8066	1.8059	1.8053	1.8046
.60	1.8039	1.8033	1.8026	1.8019	1.8013	1.8006	1.7999	1.7993	1.7986	1.7979
.80	1.7973	1.7966	1.7960	1.7953	1.7946	1.7940	1.7933	1.7927	1.7920	1.7914
51.00	1.7907	1.7901	1.7894	1.7887	1.7881	1.7874	1.7868	1.7861	1.7855	1.7848
.20	1.7842	1.7835	1.7829	1.7822	1.7816	1.7809	1.7803	1.7796	1.7790	1.7784
.40	1.7777	1.7771	1.7764	1.7758	1.7751	1.7745	1.7738	1.7732	1.7726	1.7719
.60	1.7713	1.7706	1.7700	1.7694	1.7687	1.7681	1.7675	1.7668	1.7662	1.7656
.80	1.7649	1.7643	1.7636	1.7630	1.7624	1.7618	1.7611	1.7605	1.7599	1.7592
52.00	1.7586	1.7580	1.7573	1.7567	1.7561	1.7555	1.7548	1.7542	1.7536	1.7530
.20	1.7523	1.7517	1.7511	1.7505	1.7498	1.7492	1.7486	1.7480	1.7474	1.7467
.40	1.7461	1.7455	1.7449	1.7443	1.7436	1.7430	1.7424	1.7418	1.7412	1.7406
.60	1.7399	1.7393	1.7387	1.7381	1.7375	1.7369	1.7363	1.7357	1.7350	1.7344
.80	1.7338	1.7332	1.7326	1.7320	1.7314	1.7308	1.7302	1.7296	1.7290	1.7284
53.00	1.7278	1.7271	1.7265	1.7259	1.7253	1.7247	1.7241	1.7235	1.7229	1.7223
.20	1.7217	1.7211	1.7205	1.7199	1.7193	1.7187	1.7181	1.7175	1.7169	1.7163
.40	1.7157	1.7152	1.7146	1.7140	1.7134	1.7128	1.7122	1.7116	1.7110	1.7104
.60	1.7098	1.7092	1.7086	1.7080	1.7075	1.7069	1.7063	1.7057	1.7051	1.7045
.80	1.7039	1.7033	1.7028	1.7022	1.7016	1.7010	1.7004	1.6998	1.6993	1.6987
54.00	1.6981	1.6975	1.6969	1.6964	1.6958	1.6952	1.6946	1.6940	1.6935	1.6929
.20	1.6923	1.6917	1.6911	1.6906	1.6900	1.6894	1.6888	1.6883	1.6877	1.6871
.40	1.6866	1.6860	1.6854	1.6848	1.6843	1.6837	1.6831	1.6826	1.6820	1.6814
.60	1.6808	1.6803	1.6797	1.6791	1.6786	1.6780	1.6774	1.6769	1.6763	1.6757
.80	1.6752	1.6746	1.6741	1.6735	1.6729	1.6724	1.6718	1.6712	1.6707	1.6701
55.00	1.6696	1.6690	1.6684	1.6679	1.6673	1.6668	1.6662	1.6657	1.6651	1.6645
.20	1.6640	1.6634	1.6629	1.6623	1.6618	1.6612	1.6607	1.6601	1.6596	1.6590
.40	1.6585	1.6579	1.6574	1.6568	1.6563	1.6557	1.6552	1.6546	1.6541	1.6535
.60	1.6530	1.6524	1.6519	1.6513	1.6508	1.6502	1.6497	1.6491	1.6486	1.6481
.80	1.6475	1.6470	1.6464	1.6459	1.6453	1.6448	1.6443	1.6437	1.6432	1.6426
56.00	1.6421	1.6416	1.6410	1.6405	1.6399	1.6394	1.6389	1.6383	1.6378	1.6373
.20	1.6367	1.6362	1.6357	1.6351	1.6346	1.6341	1.6335	1.6330	1.6325	1.6319
.40	1.6314	1.6309	1.6303	1.6298	1.6293	1.6287	1.6282	1.6277	1.6272	1.6266
.60	1.6261	1.6256	1.6251	1.6245	1.6240	1.6235	1.6230	1.6224	1.6219	1.6214
.80	1.6209	1.6203	1.6198	1.6193	1.6188	1.6182	1.6177	1.6172	1.6167	1.6162
57.00	1.6156	1.6151	1.6146	1.6141	1.6136	1.6131	1.6125	1.6120	1.6115	1.6110
.20	1.6105	1.6100	1.6094	1.6089	1.6084	1.6079	1.6074	1.6069	1.6064	1.6058
.40	1.6053	1.6048	1.6043	1.6038	1.6033	1.6028	1.6023	1.6018	1.6013	1.6007
.60	1.6002	1.5997	1.5992	1.5987	1.5982	1.5977	1.5972	1.5967	1.5962	1.5957
.80	1.5952	1.5947	1.5942	1.5937	1.5932	1.5927	1.5922	1.5917	1.5912	1.5906
58.00	1.5901	1.5896	1.5891	1.5886	1.5881	1.5876	1.5871	1.5867	1.5862	1.5857
.20	1.5852	1.5847	1.5842	1.5837	1.5832	1.5827	1.5822	1.5817	1.5812	1.5807
.40	1.5802	1.5797	1.5792	1.5787	1.5782	1.5777	1.5773	1.5768	1.5763	1.5758
.60	1.5753	1.5748	1.5743	1.5738	1.5733	1.5728	1.5724	1.5719	1.5714	1.5709
.80	1.5704	1.5699	1.5694	1.5689	1.5685	1.5680	1.5675	1.5670	1.5665	1.5660
59.00	1.5656	1.5651	1.5646	1.5641	1.5636	1.5632	1.5627	1.5622	1.5617	1.5612
.20	1.5607	1.5603	1.5598	1.5593	1.5588	1.5584	1.5579	1.5574	1.5569	1.5564
.40	1.5560	1.5555	1.5550	1.5545	1.5541	1.5536	1.5531	1.5526	1.5522	1.5517
.60	1.5512	1.5508	1.5503	1.5498	1.5493	1.5489	1.5484	1.5479	1.5475	1.5470
.80	1.5465	1.5460	1.5456	1.5451	1.5446	1.5442	1.5437	1.5432	1.5428	1.5423