

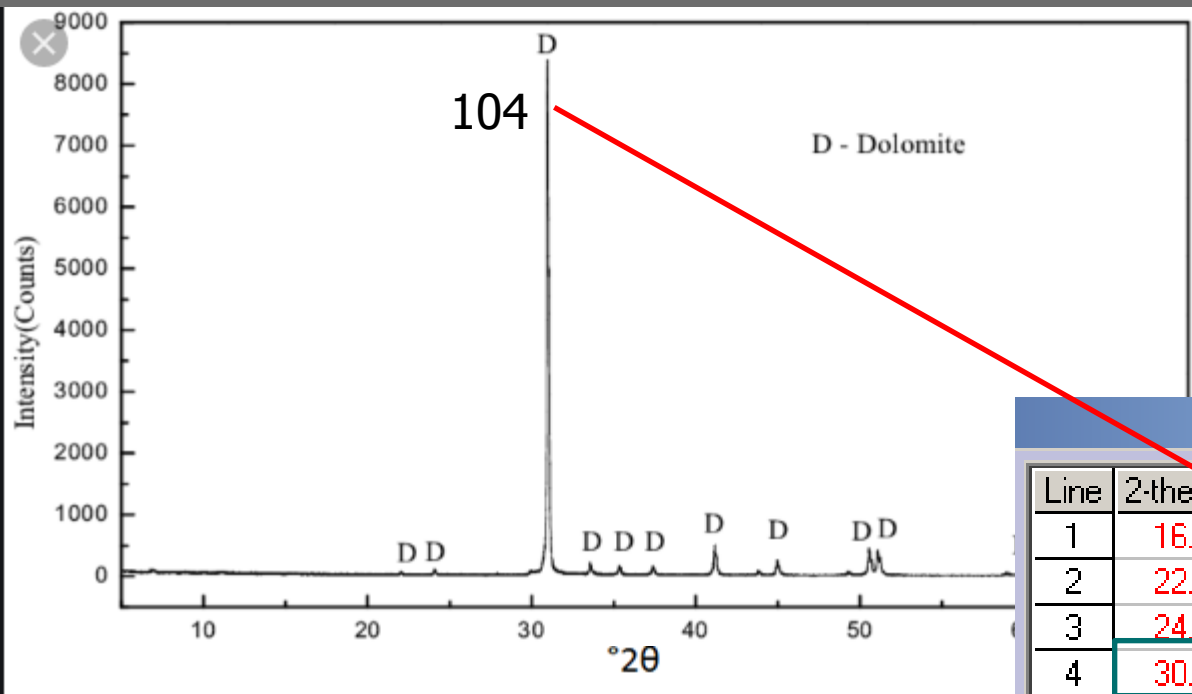
Identificación y cuantificación
manual de fases minerales –
práctica de DRX

Introducción

Este documento muestra paso por paso el proceso de identificación y cuantificación manual de fases minerales utilizando (1) tablas de conversión de $^{\circ}2\theta$ a d_{hkl} , (2) fichas de minerales de referencia y (3) poderes reflectantes experimentales.

La siguiente imagen demuestra la relación entre los planos cristalográficos de un mineral y los picos de un difractograma. En el caso de la dolomita, la radiación X emitida coherentemente (difractada) por los átomos de los planos paralelos a la cara (104) genera el pico más intenso (d_{104}) en el difractograma. La distancia entre plano y plano es 2.88 Å.

La tabla de los poderes reflectantes experimentales se encuentra en el Anexo I. Las fichas de minerales de referencia y las tablas de conversión están incluidos en el Anexo II y III, respectivamente.



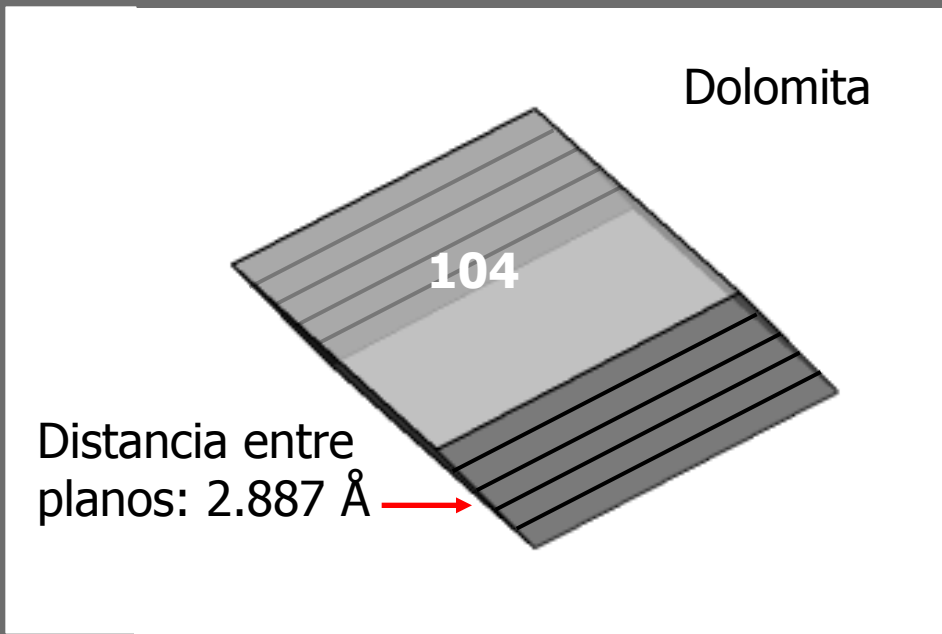
$^{\circ}2\theta$

Espaciado en Ångstrom (Å)

Índices de Miller

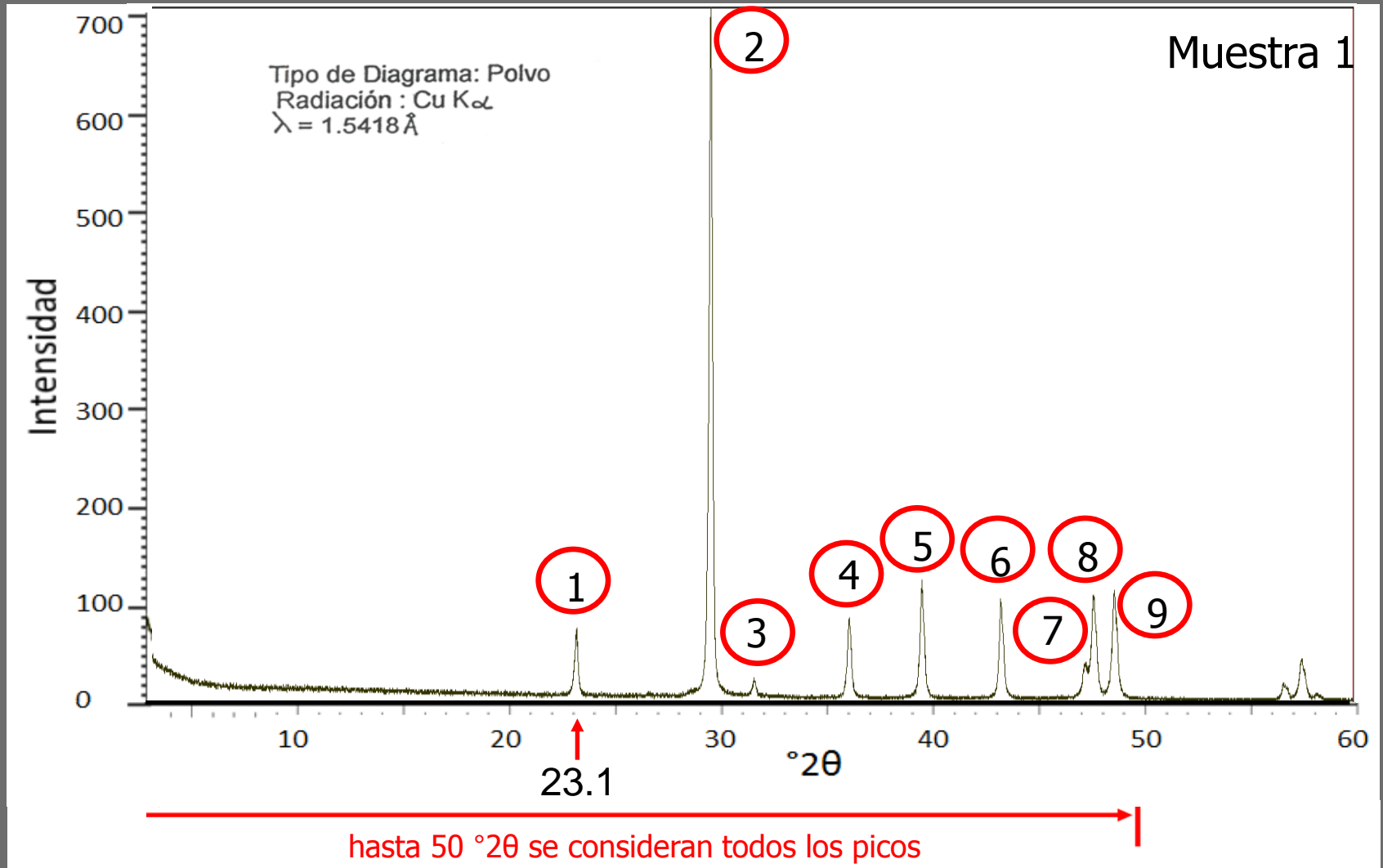
Ficha de la Dolomita

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



Identificación manual

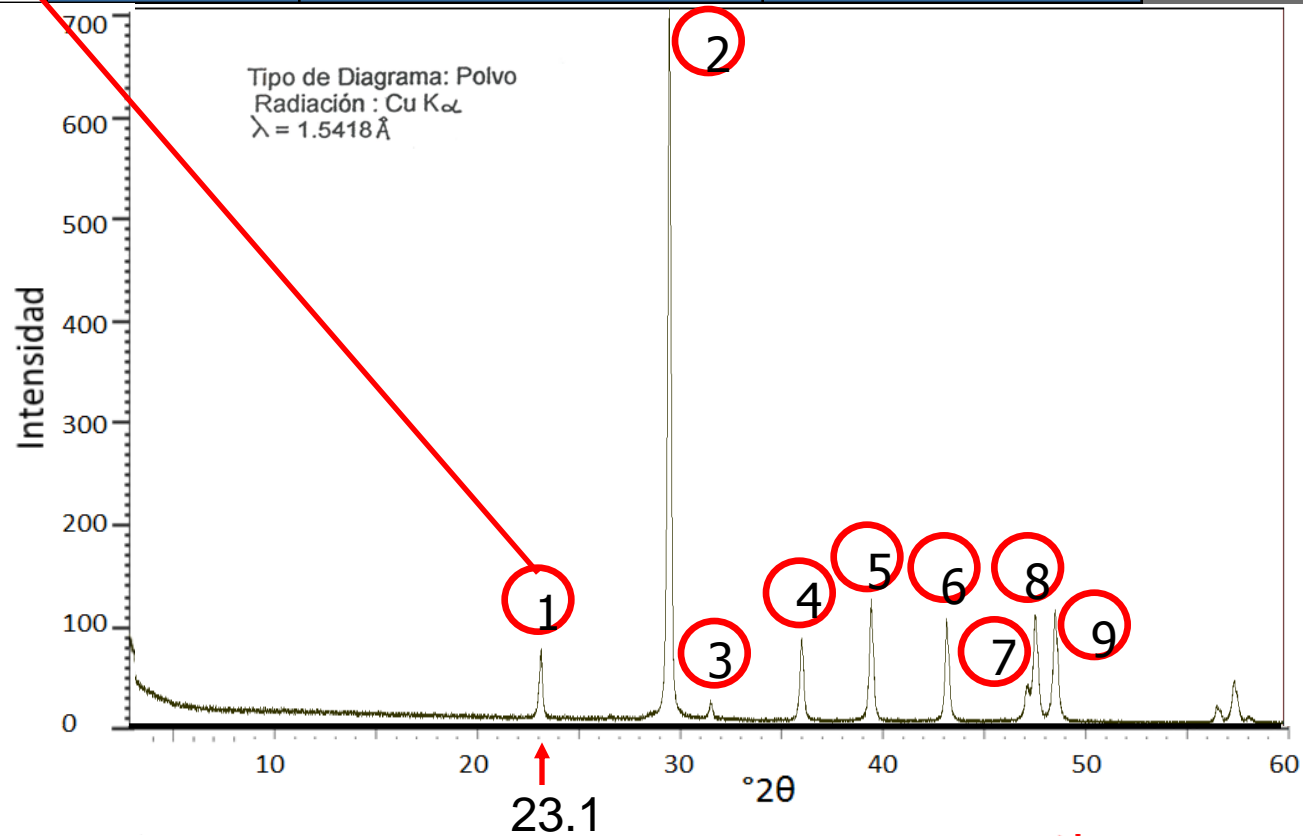
Primero se numeran los picos y se determina el valor $^{\circ}2\theta$ para cada pico.



Identificación manual

Determinación del $^{\circ}2\theta$ de los picos

Pico	$^{\circ}2\theta$	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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			



Identificación manual

Conversión de $^{\circ}2\theta$ a d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1.541838

40.10

2.25 Å

	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	2.0878	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	2.0102	2.0094	2.0086	2.0077	2.0069
.20	2.0061	2.0052	2.0044	2.0035	2.0027	2.0018	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

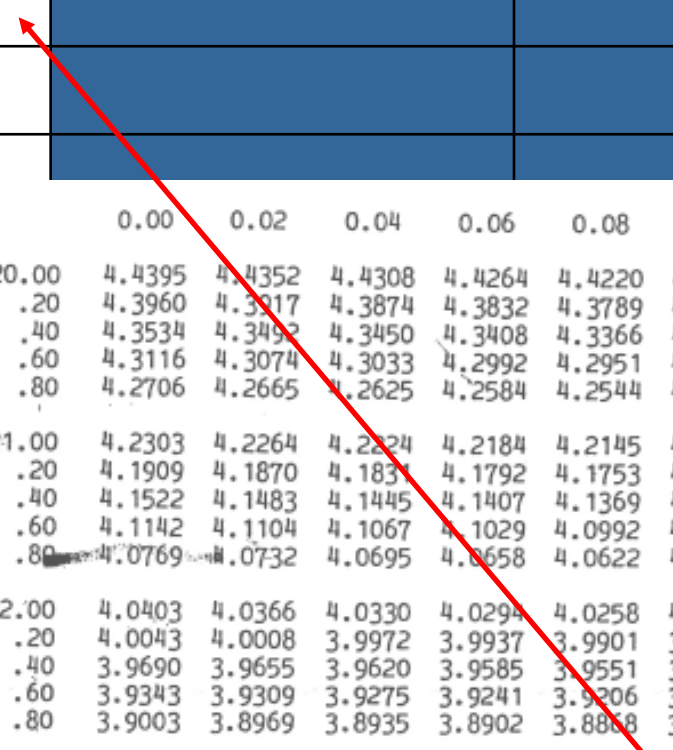
Importante: La longitud de onda de la radiación X de la tabla y del análisis de nuestra muestra tienen que ser idénticas (generalmente Cu K α).

Identificación manual

Conversión de $^{\circ}2\theta$ a d_{hkl}

Pico	$^{\circ}2\theta$	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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



Identificación manual

Conversión de $^{\circ}2\theta$ a d_{hkl} usando la fórmula de Bragg

Fórmula de Bragg:

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

Fórmula de Bragg reorganizada
para despejar d_{hkl} , considerando
una longitud de onda
de Cu K α = 1.5418 Å:

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

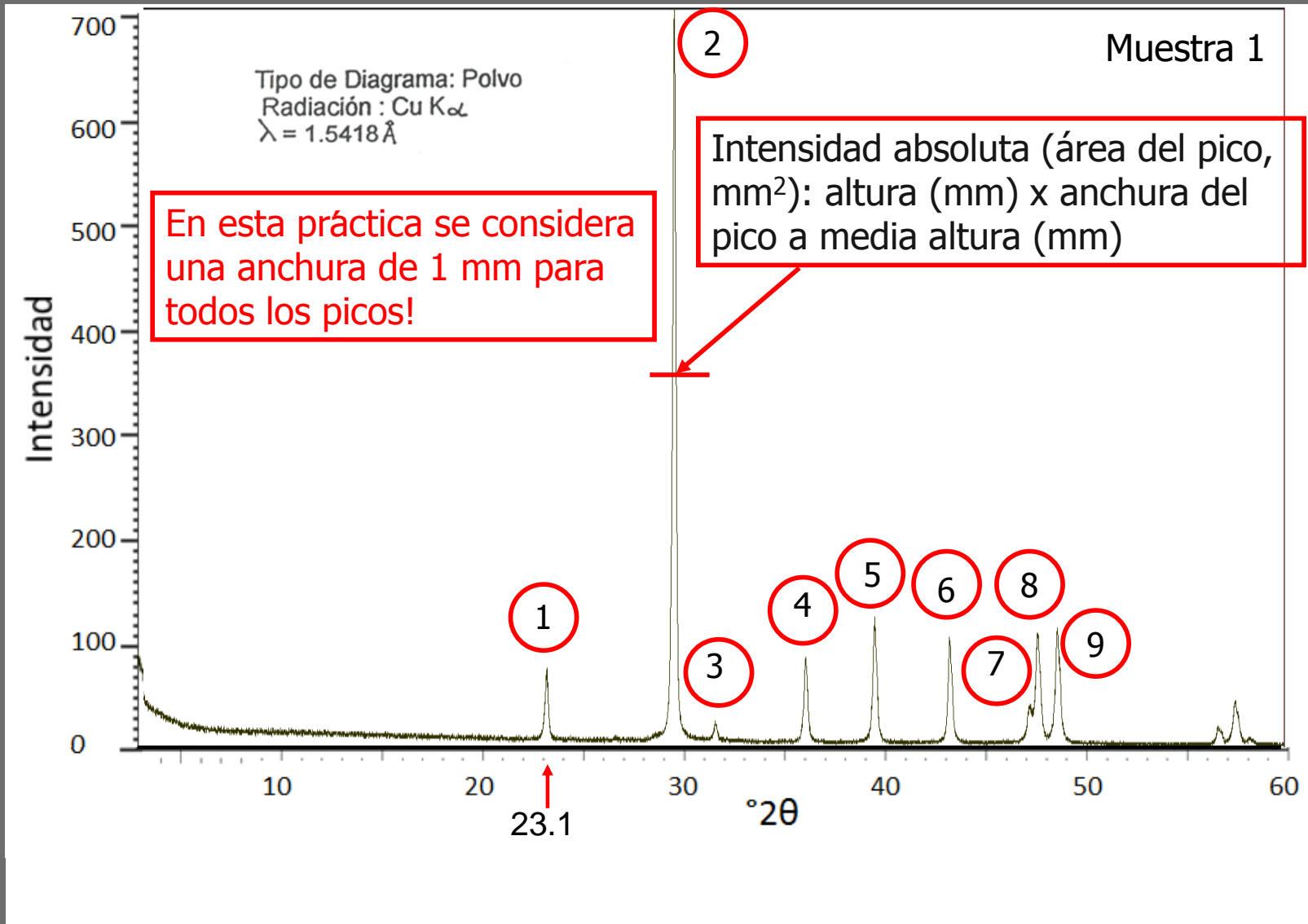
Identificación manual

Conversión de $^{\circ}2\theta$ a d_{hkl}

Pico	$^{\circ}2\theta$	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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		

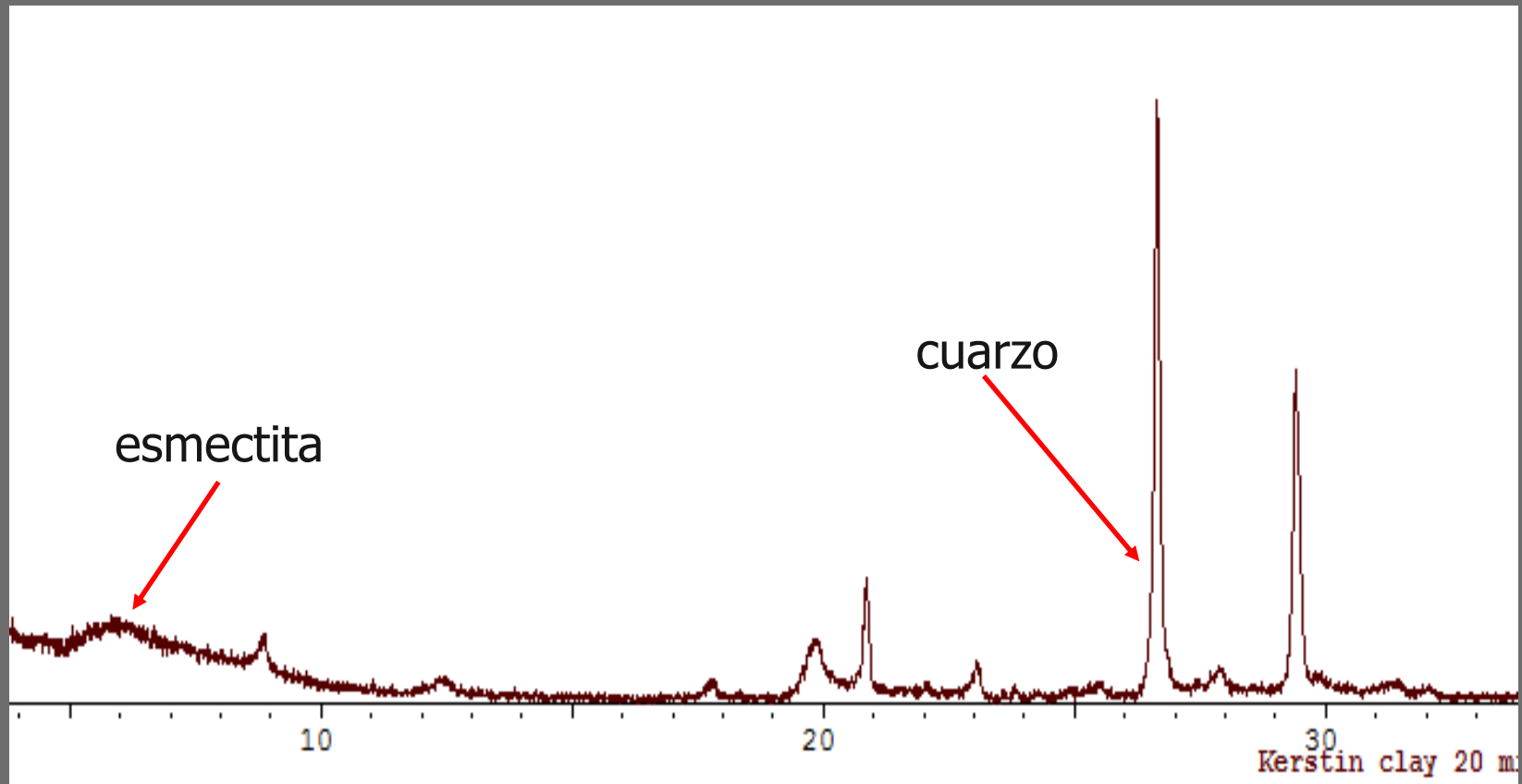
Identificación manual

Determinación de la intensidad absoluta



Identificación manual

La anchura de los picos generalmente depende de la cristalinidad del mineral. Fases poco cristalinas como la esmectita tienen picos muy anchos, mientras el cuarzo es bastante más cristalino y suele tener picos estrechos.



Identificación manual

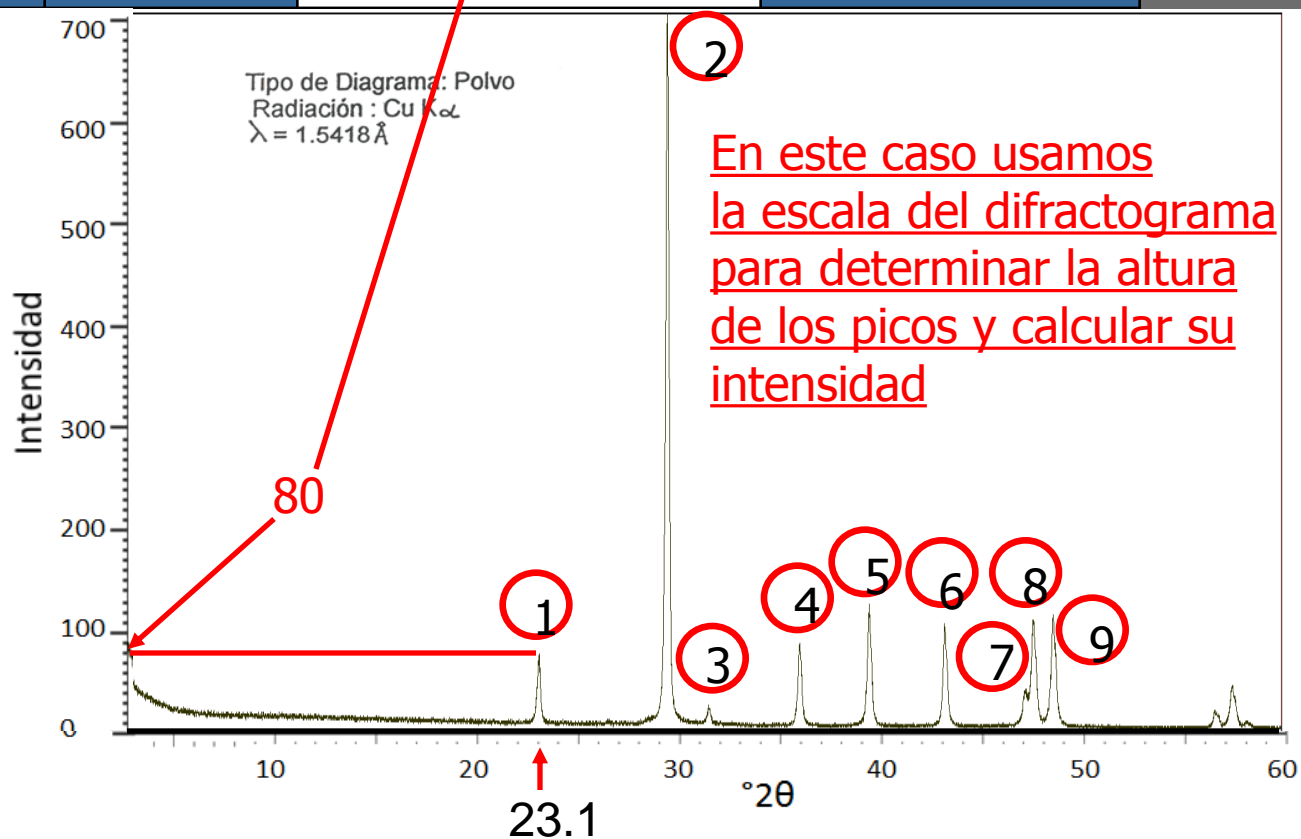
Substracción del fondo



Identificación manual

Determinación de la intensidad absoluta de los picos

Pico	2θ	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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			



Identificación manual

Determinación de la intensidad absoluta de los picos

Pico	2θ	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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	

Identificación manual

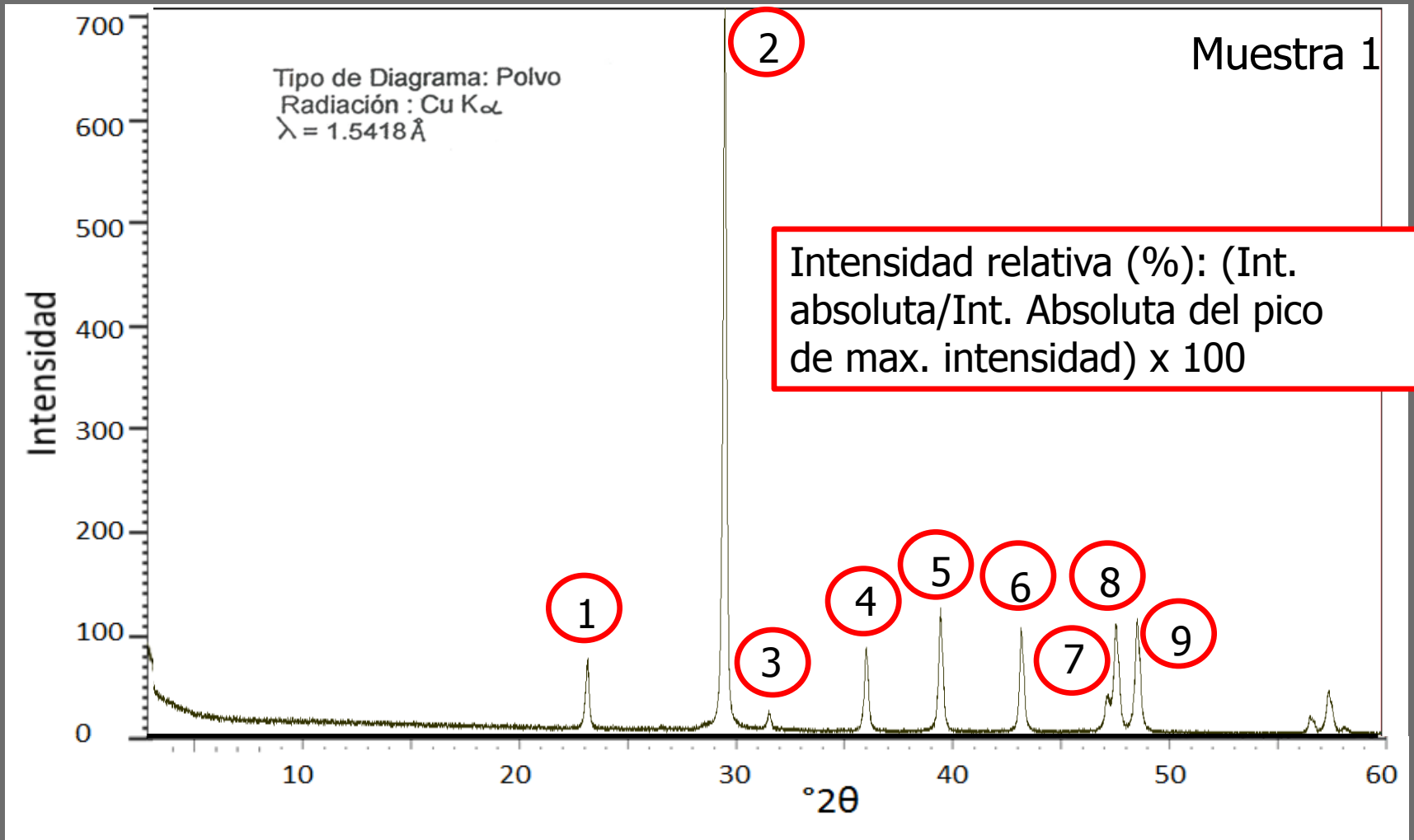
Para poder usar los datos de las fichas de los minerales de referencia, comparando los d_{hkl} y las intensidades de sus picos, con los picos del difractograma de nuestra muestra, tenemos que calcular la intensidad relativa (%).



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

Identificación manual


Determinación de la intensidad relativa de los picos



Identificación manual

Determinación de la intensidad relativa de los picos

Pico	2θ	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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	


$$(80/700)*100 = 11$$

Identificación manual

Identificación del mineral considerando el pico de max. intensidad (100%) y comprobación por la posición (espaciado d_{hkl}) e intensidad de los demás picos.

Pico	2θ	d_{hkl} (Å)	Intensidad absoluta (mm ²)	Intensidad relativa (%)
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

Calcita

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

Identificación y cuantificación manual

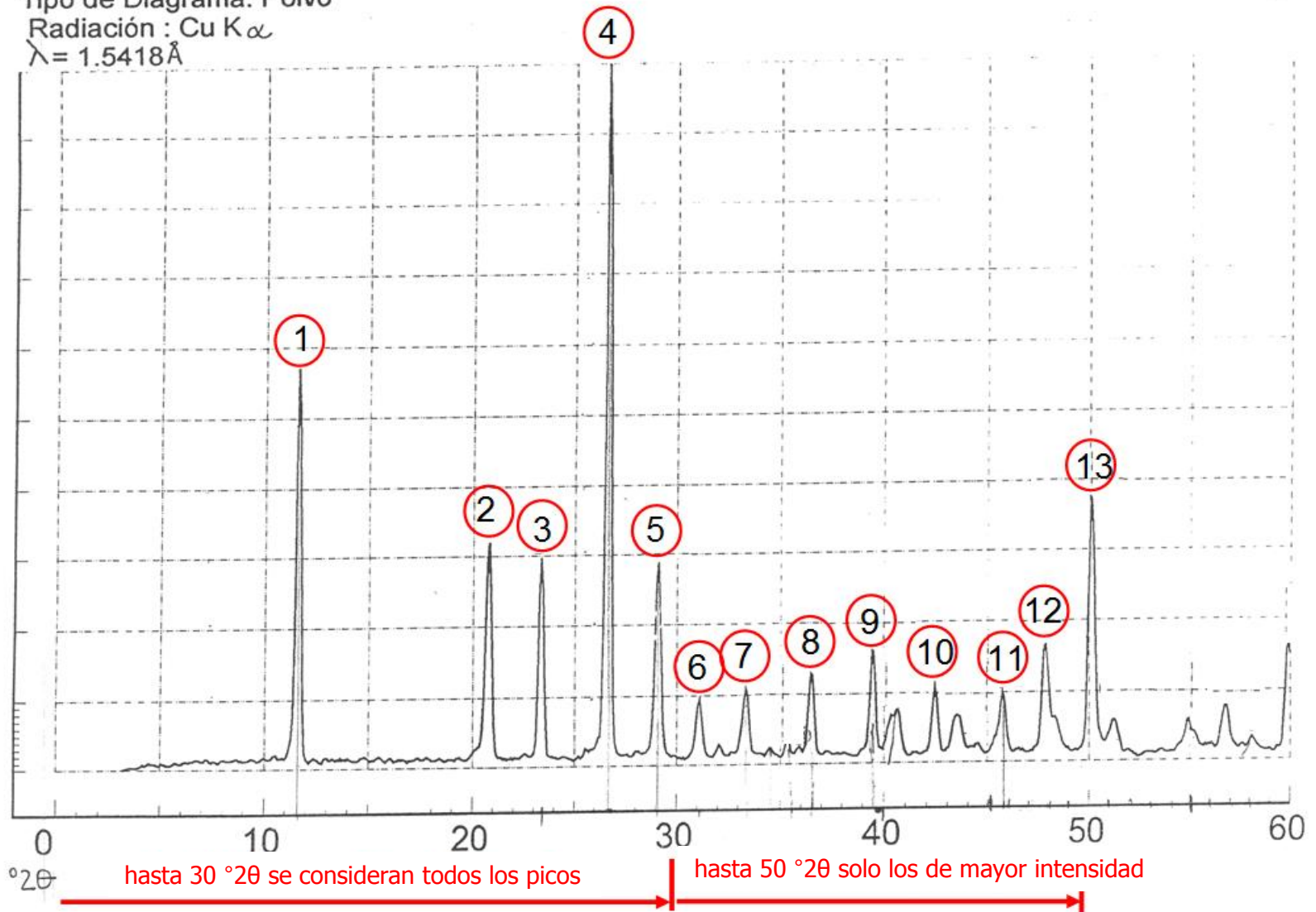
Identificación y cuantificación de una mezcla de minerales

5

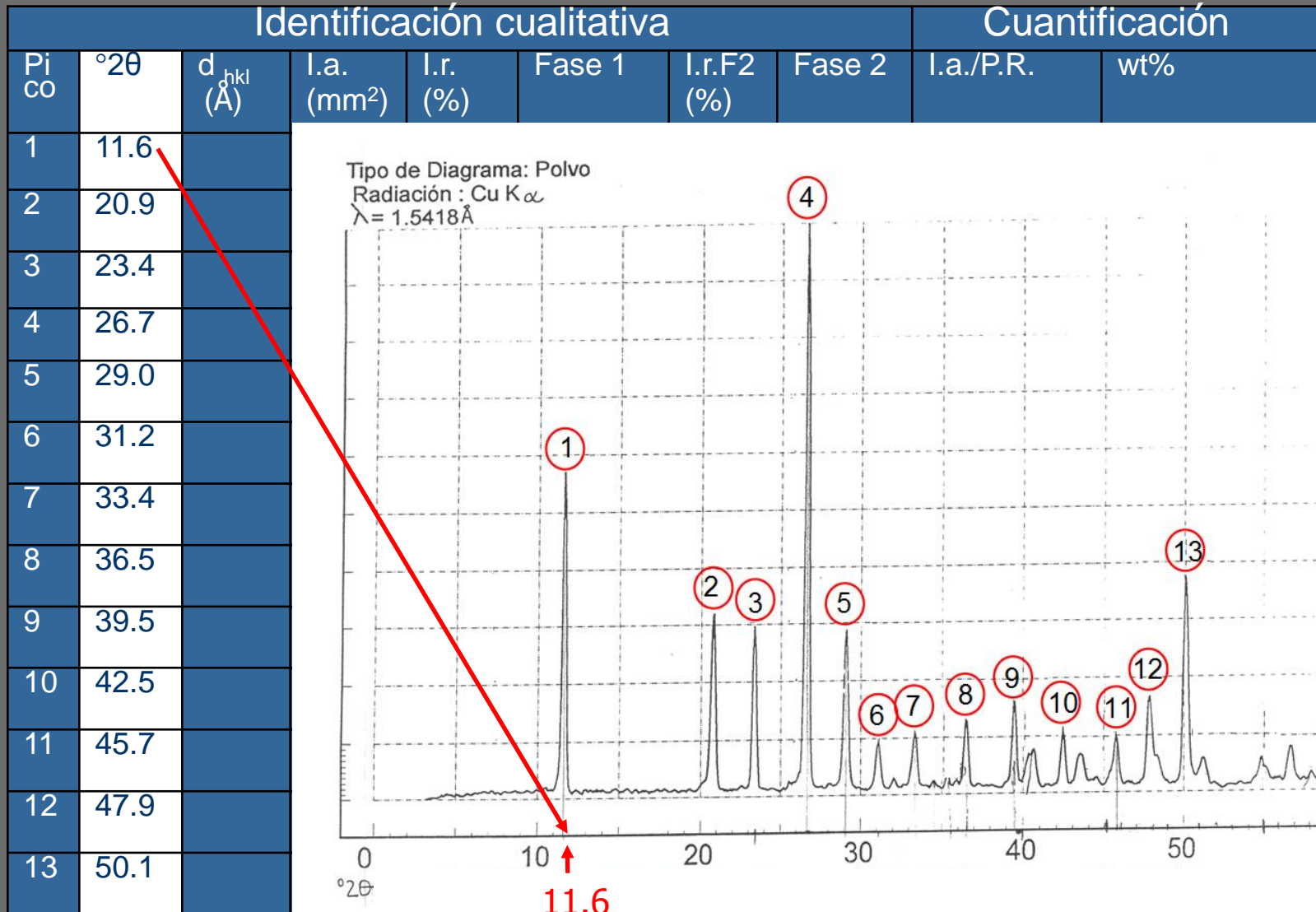
Tipo de Diagrama: Polvo

Radiación : Cu K α

$\lambda = 1.5418 \text{ \AA}$



Determinación del 2θ de los picos



d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

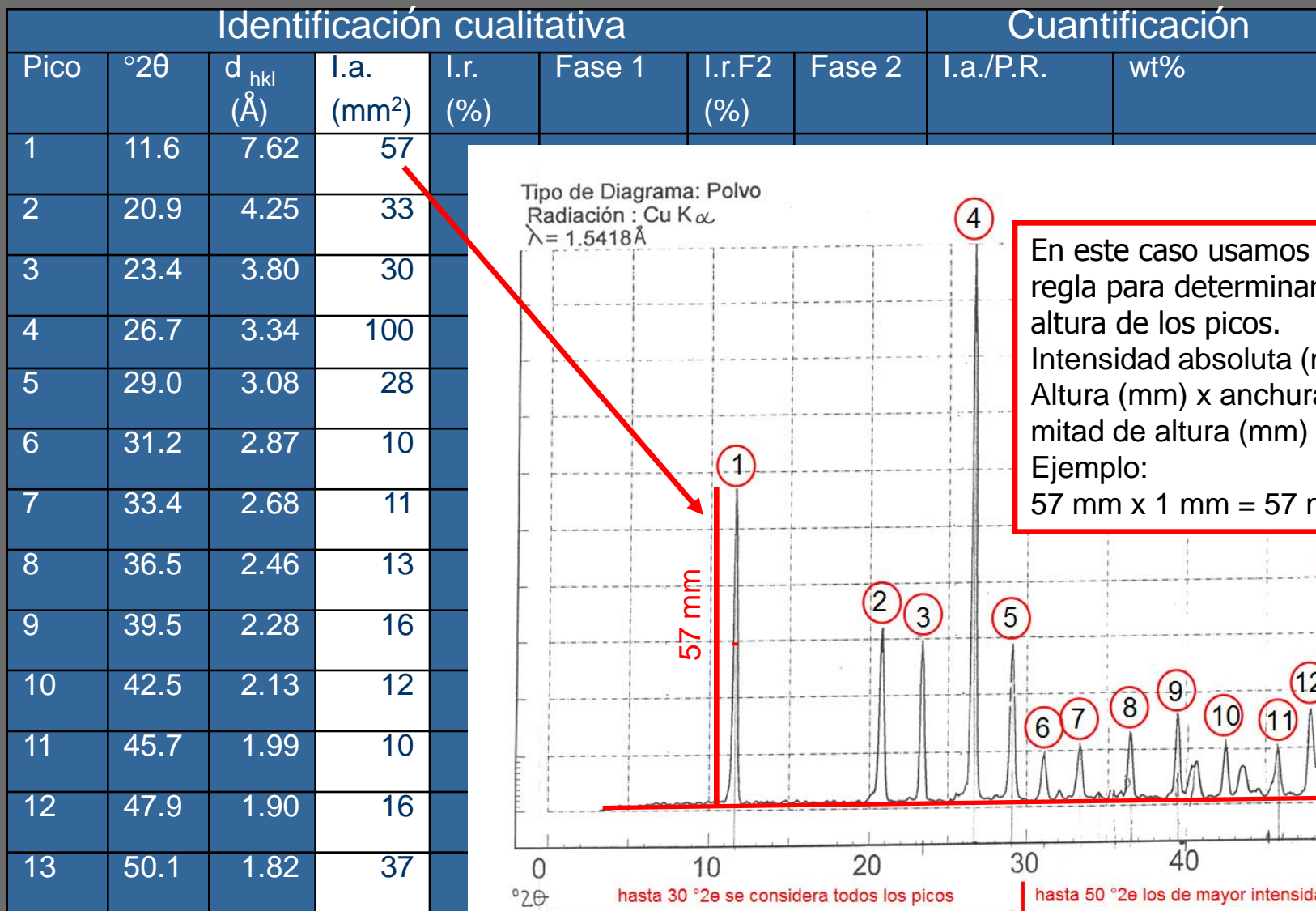
Conversión de $^{\circ}2\theta$ a d_{hkl}

Identificación cualitativa							Cuantificación		
Pico	$^{\circ}2\theta$	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase 1	I.r.F2 (%)	Fase 2	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							

	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	8.6729	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	7.7620	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	7.4998	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} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Determinación de la intensidad absoluta de los picos



d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Determinación de la intensidad relativa de los picos

Identificación cualitativa					Cuantificación				
Pico	°2θ	d _{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase 1	I.r. (%)	Fase 2	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					

Para poder usar los datos de los ficheros para la identificación de las fases minerales tenemos que calcular la intensidad relativa (%)

Intensidad relativa (%) = (Intensidad absoluta (mm²) / Intensidad absoluta del pico de max. intensidad (mm²)) x 100

Ejemplo:
(57 mm² / 100 mm²) x 100% = 57%

En nuestro ejemplo ambos tienen el mismo valor porque la intensidad absoluta del pico de max. intensidad = 100 mm²

d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Identificación de la primera fase considerando el pico de max. intensidad (100%) y comprobación por la posición e intensidad de los demás picos.

Identificación cualitativa						Cuantificación				
Pico	$^{\circ}2\theta$	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase	Quartz				
						Line	2-theta angle	d-spacing	Intensity	H K L
1	11.6	7.62	57	57		1	20.83469	4.260	35	1 0 0
2	20.9	4.25	33	33	Cuarzo	2	26.64311	3.343	100	1 0 1
3	23.4	3.80	30	30		3	36.52569	2.458	12	1 1 0
4	26.7	3.34	100	100	Cuarzo	4	39.45487	2.282	12	1 0 2
5	29.0	3.08	28	28		5	40.28256	2.237	6	1 1 1
6	31.2	2.87	10	10		6	42.44291	2.128	9	2 0 0
7	33.4	2.68	11	11		7	45.79835	1.980	6	2 0 1
8	36.5	2.46	13	13	Cuarzo	8	50.16585	1.817	17	1 1 2
9	39.5	2.28	16	16	Cuarzo	9	50.64283	1.801	1	0 0 3
10	42.5	2.13	12	12	Cuarzo	10	54.86377	1.672	7	2 0 2
11	45.7	1.99	10	10	Cuarzo	11	55.33035	1.659	3	1 0 3
12	47.9	1.90	16	16		12	57.24412	1.608	1	2 1 0
13	50.1	1.82	37	37	Cuarzo	13	59.98111	1.541	15	2 1 1

d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Determinación de la intensidad relativa de las picos restantes

Identificación cualitativa							Cuantificación		
Pico	2θ	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase 1	I.r.F2 (%)	Fase 2	I.a./P.R.	wt%
1	11.6	7.62	57	57		100			
2	20.9	4.25	33	33	Cuarzo				
3	23.4	3.80	30	30		53			
4	26.7	3.34	100	100	Cuarzo				
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	Cuarzo				
9	39.5	2.28	16	16	Cuarzo				
10	42.5	2.13	12	12	Cuarzo	21			
11	45.7	1.99	10	10	Cuarzo	18			
12	47.9	1.90	16	16		28			
13	50.1	1.82	37	37	Cuarzo	65			

Para poder identificar las demás fases minerales tenemos que calcular la intensidad relativa de los picos restantes que no coinciden con los del cuarzo. La intensidad del pico de max. intensidad de los restantes es igual a 100%. La de los picos restantes se multiplica por un factor obtenido al dividir 100% por la intensidad relativa de ese pico:
Ejemplo: $100\%/57\% = 1.75$

$$30\% \times 1.75 = 53\%$$

d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Identificación de la segunda fase considerando el pico de max. intensidad (100%) y comprobación por la posición e intensidad de los demás picos.

Identificación cualitativa							Cuantificación				
Pico	°2θ	d _{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase1	I.r.F2 (%)	Fase 2	Gypsum			
								Line	2-theta angle	d-spacing	Intensity
1	11.6	7.62	57	57		100	Yeso	1	11.6959	7.560	100
2	20.9	4.25	33	33	Cuarzo			2	20.78535	4.270	50
3	23.4	3.80	30	30		53	Yeso	3	23.45299	3.790	20
4	26.7	3.34	100	100	Cuarzo			4	28.18975	3.163	4
5	29.0	3.08	28	28		49	Yeso	5	29.16983	3.059	55
6	31.2	2.87	10	10		18	Yeso	6	31.1704	2.867	25
7	33.4	2.68	11	11		19	Yeso	7	32.10075	2.786	6
8	36.5	2.46	13	13	Cuarzo			8	33.4197	2.679	28
9	39.5	2.28	16	16	Cuarzo			9	34.58989	2.591	4
10	42.5	2.13	12	12	Cuarzo	21	Yeso	10	35.45118	2.530	1
11	45.7	1.99	10	10	Cuarzo	18	Yeso	11	35.96536	2.495	6
12	47.9	1.90	16	16		28	Yeso	12	36.64919	2.450	4
13	50.1	1.82	37	37	Cuarzo	65	Yeso	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} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder relectante

Identificación de la segunda fase considerando el pico de max. intensidad (100%) y comprobación por la posición e intensidad de los demás picos.

Identificación cualitativa							Cuantificación				
Pico	2θ	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase1	I.r.F2 (%)	Fase 2	Gypsum			
								Line	2-theta angle	d-spacing	Intensity
1	11.6	7.62	57	57		100	Yeso	1	11.6959	7.560	100
2	20.9	4.25	33	33	Cuarzo			2	20.78535	4.270	50
3	23.4	3.80	30	30		53	Yeso	3	23.45299	3.790	20
4	26.6							4	28.18975	3.163	4
5	29.1						Yeso	5	29.16903	3.059	55
6	31.1						Yeso	6	31.1704	2.867	25
7	33.3						Yeso	7	32.10075	2.786	6
8	36.0						Yeso	8	33.4197	2.679	28
9	39.0							9	34.58989	2.591	4
10	42.0						Yeso	10	35.45118	2.530	1
11	45.7	1.99	10	10	Cuarzo	18	Yeso	11	35.96536	2.495	6
12	47.9	1.90	16	16		28	Yeso	12	36.64919	2.450	4
13	50.1	1.82	37	37	Cuarzo	65	Yeso	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

En algunos casos el valor de d_{hkl} puede mostrar pequeñas variaciones en la segunda decimal debido a errores experimentales o cambios en los parámetros de la red (por ejemplo, sustituciones isomórficas). Variaciones significativas en la intensidad son posibles debido a la orientación preferencial de la muestra cristalina.

d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder relectante

Identificación de la segunda fase considerando el pico de max. intensidad (100%) y comprobación por la posición e intensidad de los demás picos.

Identificación cualitativa								Cuantificación	
Pico	2θ	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase1	I.r.F2 (%)	Fase 2	I.a./P.R.	wt%
1	11.6	7.62	57	57		100	Yeso		
2	20.9	4.25	33	33	Cuarzo				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Cuarzo				
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	Cuarzo				
9	39.5	2.28	16	16	Cuarzo				
10	42.5	2.13	12	12	Cuarzo	21	Yeso		
11	45.7	1.99	10	10	Cuarzo	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Cuarzo	65	Yeso		

Algunos de los picos tienen la contribución de ambas fases minerales.
Por tanto su intensidad es mas alta que la reflejada en las fichas correspondientes.

d_{hkl} = espaciado; I.a. = intensidad absoluta; I.r. = intensidad relativa; I.r.F2 = intensidad relativa de la fase 2, I.a./P.R. = intensidad absoluta dividida por el poder reflectante

Cuantificación manual

Para la cuantificación dividimos el valor de la max. intensidad absoluta de cada fase (correspondiente al pico con el espaciado d_{hkl} indicado en la tabla) por el poder reflectante (P.R.) correspondiente. En nuestro caso sería el P.R. de cuarzo y yeso.

Nota: Los nombres de los minerales están incluidos en Inglés porque los programas de identificación usan los nombres en dicho idioma.

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
Fluorite	2.00	3.16
Galena	1.50	2.96
Clays/Arcillas (mica, illite, kaolinite, smectite)	0.09	~4.50

Quantificación manual

Identificación cualitativa								Cuantificación	
Pico	2θ	d_{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase 1	I.r.F2 (%)	Fase 2	I.a./P.R.	wt%
1	11.6	7.62	57	57		100	Yeso	$57/0.7 = 81.4$	
2	20.9	4.25	33	33	Cuarzo				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Cuarzo			$100/1.43 = 69.9$	
5	29.0	3.08	28	28		49	Yeso		
6	31.2	2.87	10	10		18	Yeso		
7									
8									
9									
10	42.5	2.13	12	12	Cuarzo	21	Yeso		
11	45.7	1.99	10	10	Cuarzo	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Cuarzo	65	Yeso		
								sum.:151.4	

Para la cuantificación dividimos el valor de la max. intensidad absoluta de ambas fases por el poder reflectante correspondiente. Se suman ambos resultados.

Cuantificación manual

Identificación cualitativa							Cuantificación		
Pico	°2θ	d _{hkl} (Å)	I.a. (mm ²)	I.r.T (%)	Fase 1	I.r.F2 (%)	Fase 2	I.a./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	Cuarzo				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Cuarzo			100/1.43 = 69.9	(69.9/151.4) x 100 wt% = 46 wt%
5	29.0	3.08	28	28		49	Yeso		
6	30.5	2.90	15	15	Cuarzo				
7	30.5	2.90	15	15	Cuarzo				
8	36.5	2.46	15	15	Cuarzo				
9	39.5	2.28	16	16	Cuarzo				
10	42.5	2.13	12	12	Cuarzo	21	Yeso		
11	45.7	1.99	10	10	Cuarzo	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Cuarzo	65	Yeso		
								sum.:151.4	

Se dividen ambos resultados por la suma de los mismos y se multiplica por 100 para obtener una cuantificación en porcentaje (wt%).

Cuantificación manual

Identificación cualitativa							Cuantificación		
Pico	°2θ	d _{hkl} (Å)	I.a. (mm ²)	I.r. (%)	Fase 1	I.r.F2 (%)	Fase 2	I.r./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	Cuarzo				
3	23.4	3.80	30	30		53	Yeso		
4	26.7	3.34	100	100	Cuarzo			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	Cuarzo				
9	39.5	2.28	16	16	Cuarzo				
10	42.5	2.13	12	12	Cuarzo	21	Yeso		
11	45.7	1.99	10	10	Cuarzo	18	Yeso		
12	47.9	1.90	16	16		28	Yeso		
13	50.1	1.82	37	37	Cuarzo	65	Yeso		
								sum.:151.4	

Anexo I

Poder reflectante (P.R.) de varias fases minerales y d_{hkl} de los picos mas intensos

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
Fluorite	2.00	3.16
Galena	1.50	2.96
Clays/Arcillas (mica, illite, kaolinite, smectite)	0.09	~4.50

Anexo II

Fichas de minerales de referencia

Calcite

Reference Pattern: 01-086-2334

No.	h	k	l	d [Å]	2 θ [°]	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

Anexo II

Fichas de minerales de referencia

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
33	2	1	4	1.03160	96.888	2.0

Anexo II

Fichas de minerales de referencia 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

Anexo II

Fichas de minerales de referencia

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

Anexo II

Fichas de minerales de referencia

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

Anexo II

Fichas de minerales de referencia Strontianite

Reference Pattern: 00-005-0418

No.	h	k	l	d [Å]	2 θ [°]	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

Anexo II

Fichas de minerales de referencia

Fluorite

Reference Pattern: 00-004-0864

No.	h	k	l	d [Å]	2 θ [°]	I [%]
1	1	1	1	3.15300	28.282	94.0
2	2	2	0	1.93100	47.020	100.0
3	3	1	1	1.64700	55.770	35.0
4	4	0	0	1.36600	68.653	12.0
5	3	3	1	1.25300	75.870	10.0
6	4	2	2	1.11500	87.395	16.0
7	5	1	1	1.05120	94.240	7.0
8	4	4	0	0.96570	105.814	5.0
9	5	3	1	0.92330	113.084	7.0
10	6	0	0	0.91050	115.562	1.0
11	6	2	0	0.86370	126.216	9.0
12	5	3	3	0.83300	135.255	3.0

Anexo III

Tablas de conversión °2 θ a d_{hkl}

COPPER K ALPHA(1,2)
LAMBDA=1,541838

Cu K α
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	13.113	13.073	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	9.4095	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	8.8988	8.8807	8.8630

COPPER K ALPHA(1,2)
LAMBDA=1,541838

Cu K α
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	7.2785	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	6.1765	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	5.9774	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	4.9500	4.9444	4.9389	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	4.64			

Anexo III

Tablas de conversión °2θ a 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	3.7635	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

	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	2.29				

Anexo III

Tablas de conversión °2θ a 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	2.1750	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	2.0359	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

	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	1.7151	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	1.55				