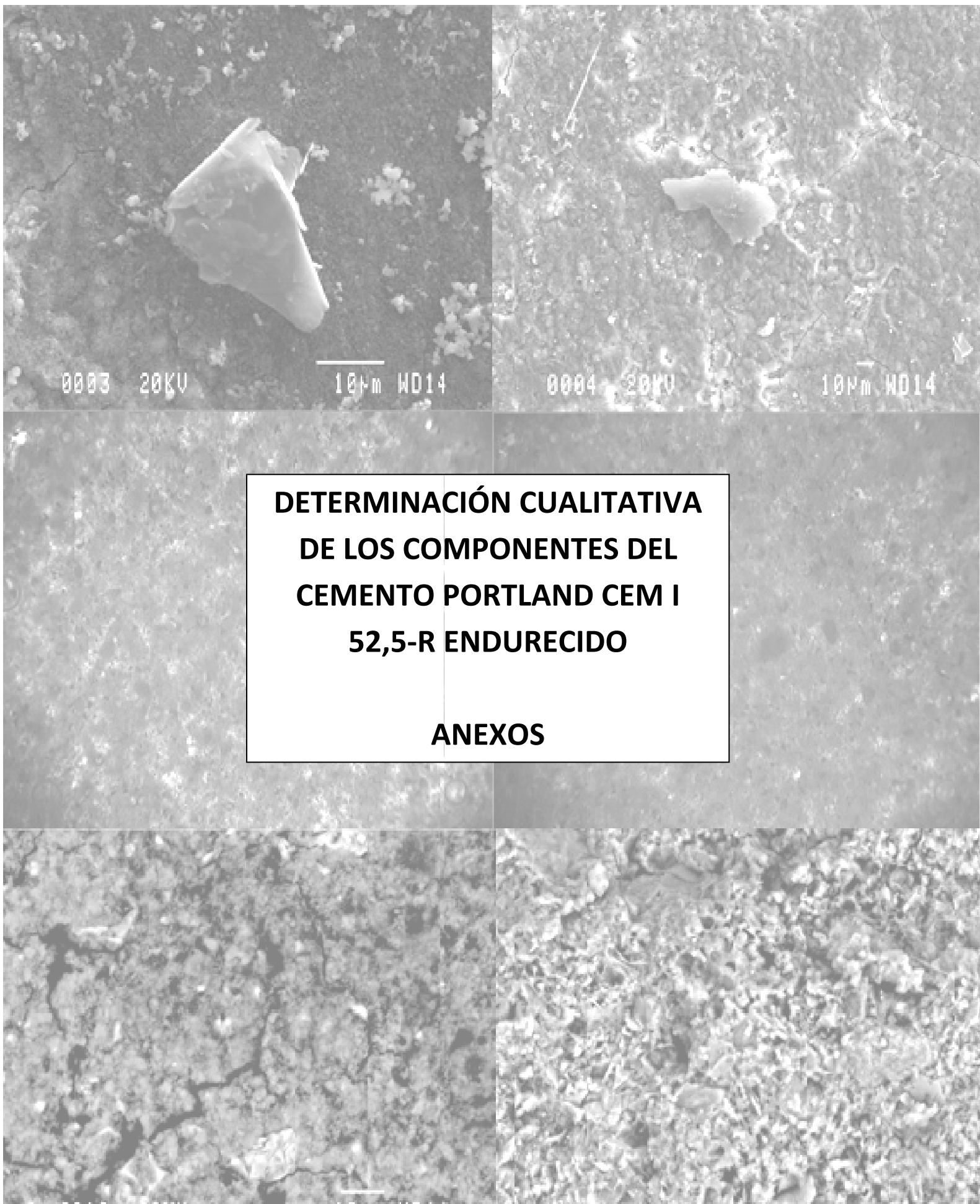




**DETERMINACIÓN CUALITATIVA
DE LOS COMPONENTES DEL
CEMENTO PORTLAND CEM I
52,5-R ENDURECIDO**

ANEXOS

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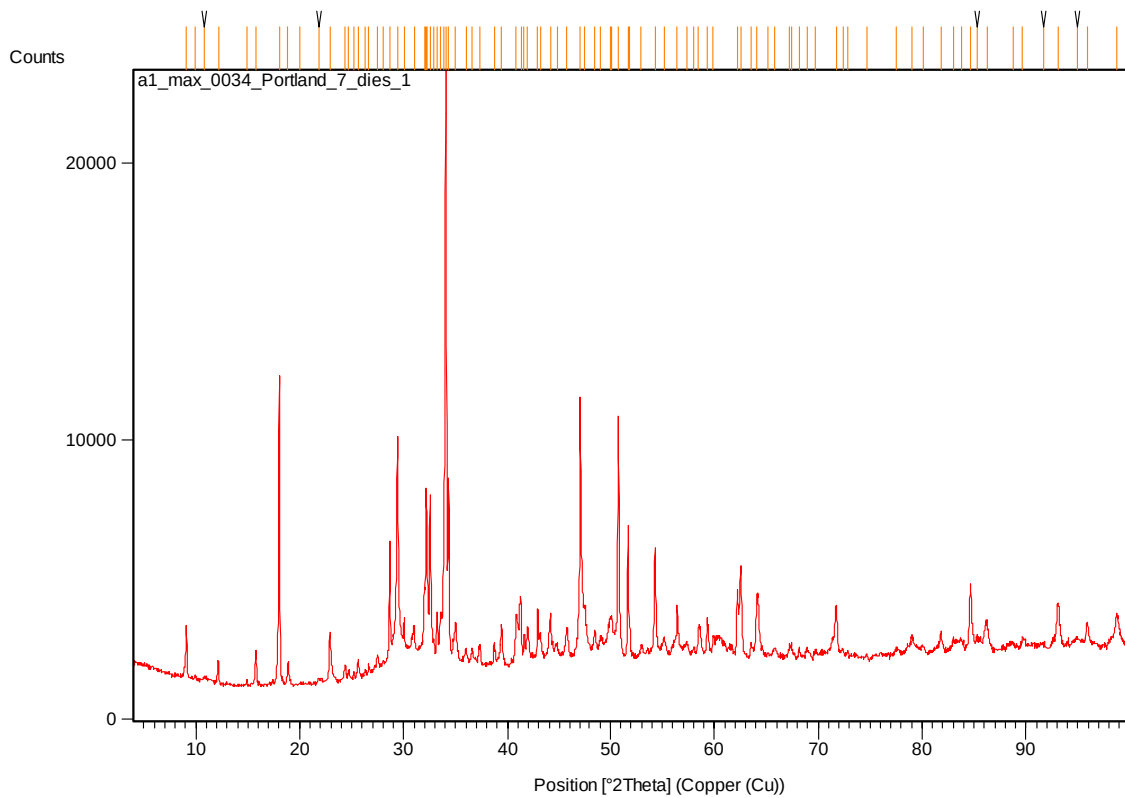
1.-Informe del resultado del estudio del drx de la pasta de cemento portland de 7 días de edad

Measurement Conditions: *(Bookmark 1)*

Dataset Name	a1_max_0034_Portland_7_dies_1
File name	C:\Documents and
Settings\Joan\Escritorio\Francisco\DRX\	a1_max_0034_Portland_7_dies_1.xrdml
Sample Identification	Portland_7_dies
Comment	Configuration=Sample Spinner, Owner=User-1, Creation date=6/30/2004 5:11:04 PM
	Goniometer=PW3050/60 (Theta/2Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001
	Sample stage=Spinner PW3064
	Diffraction system=XPRT-PRO
	Measurement program=max_riet_quan, Owner=User-1, Creation date=6/12/2009 7:06:33 PM
	Fine Calibration Offset for 2Theta = -0.010 deg
	Batch program=17-6-09_gb_max, Owner=User-1, Creation date=6/17/2009 4:58:02 PM
	Laia_Haurie_(max)_Rietveld_quantitativ_juny-2009
Measurement Date / Time	17/06/2009 19:28:07
Operator	Univ. De Barcelona
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	4,0173
End Position [°2Th.]	99,9823
Step Size [°2Th.]	0,0170
Scan Step Time [s]	510,5436
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2,11
Offset [°2Th.]	0,0000
Divergence Slit Type	Automatic
Irradiated Length [mm]	10,00
Specimen Length [mm]	10,00
Measurement Temperature [°C]	25,00
Anode Material	Cu
K-Alpha1 [Å]	1,54060
Generator Settings	40 mA, 45 kV
Diffraction Type	0000000085010818
Diffraction Number	0
Goniometer Radius [mm]	240,00
Dist. Focus-Diverg. Slit [mm]	100,00

Incident Beam Monochromator Yes
 Spinning Yes

Main Graphics, Analyze View: (Bookmark 2)



Peak List: (Bookmark 3)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
9,0953	1855,28	0,1020	9,71518	8,35
9,9858	89,16	0,1224	8,85077	0,40
10,8222	164,21	0,2448	8,16852	0,74
12,1552	794,42	0,1224	7,27554	3,58
14,8893	187,43	0,0816	5,94510	0,84
15,7719	1266,00	0,1224	5,61435	5,70
18,0224	11216,46	0,1020	4,91802	50,51

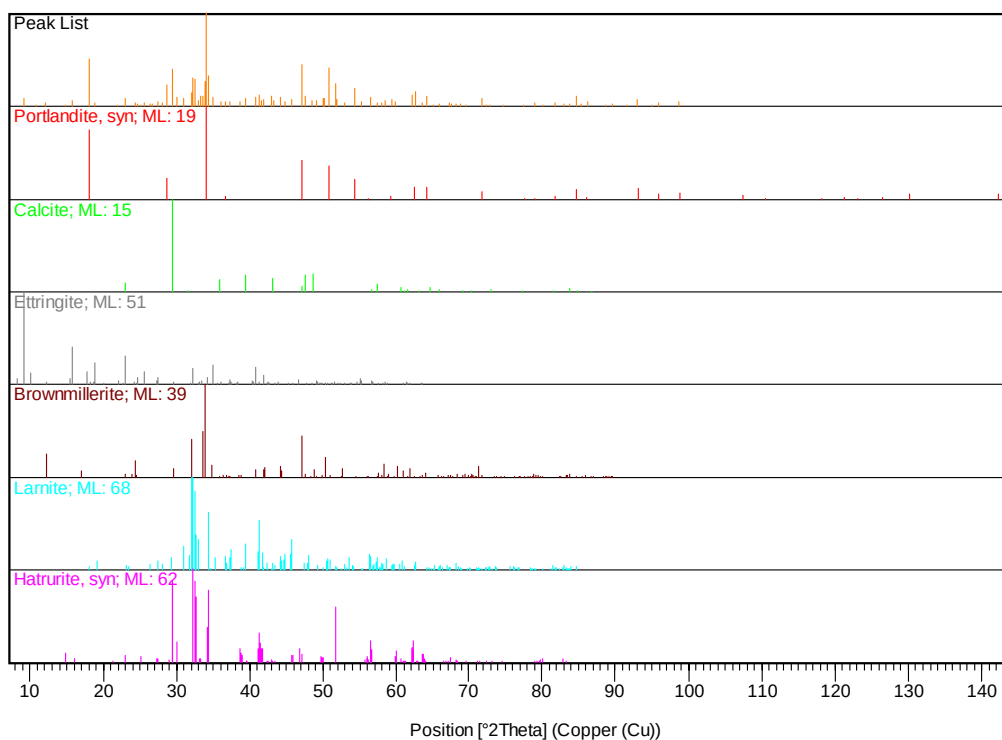
18,8624	733,36	0,1020	4,70086	3,30
20,0088	58,67	0,2448	4,43404	0,26
21,8311	175,91	0,1224	4,06787	0,79
22,9148	1853,04	0,1224	3,87787	8,34
24,3705	674,00	0,1020	3,64943	3,03
24,6965	432,74	0,1632	3,60200	1,95
25,1915	355,39	0,0816	3,53234	1,60
25,6209	798,52	0,1020	3,47410	3,60
26,3227	416,45	0,1224	3,38304	1,88
26,6380	609,00	0,0816	3,34371	2,74
27,4843	925,62	0,1632	3,24265	4,17
28,0198	747,43	0,1224	3,18187	3,37
28,6627	5044,63	0,1020	3,11196	22,72
29,4036	8721,58	0,1428	3,03521	39,27
30,0413	2208,87	0,1020	2,97221	9,95
31,0136	1904,35	0,1020	2,88121	8,58
31,9836	3177,93	0,0816	2,79601	14,31
32,1477	6762,36	0,1020	2,78211	30,45
32,2309	5769,26	0,0408	2,77511	25,98
32,5372	6532,49	0,0816	2,74969	29,42
32,9057	1369,39	0,0816	2,71973	6,17
33,2100	2383,31	0,0816	2,69550	10,73
33,5783	2340,30	0,1836	2,66678	10,54
33,8765	5978,52	0,0612	2,64398	26,92
34,0654	22207,89	0,1020	2,62975	100,00
34,3353	7133,05	0,1020	2,60969	32,12
34,9736	2027,53	0,1428	2,56351	9,13

36,0126	1057,85	0,1632	2,49190	4,76
36,6177	956,97	0,2040	2,45210	4,31
37,3229	1101,22	0,2448	2,40737	4,96
38,6980	1180,56	0,1020	2,32493	5,32
39,4273	1762,61	0,1836	2,28359	7,94
40,8291	2057,44	0,1020	2,20836	9,26
41,2943	2574,33	0,1224	2,18455	11,59
41,5953	1437,06	0,0816	2,16944	6,47
41,9267	1709,51	0,1020	2,15305	7,70
42,8954	2338,39	0,0816	2,10665	10,53
43,1774	1411,33	0,1224	2,09354	6,36
44,1398	2132,30	0,1020	2,05010	9,60
44,8018	990,48	0,1224	2,02133	4,46
45,7160	1589,55	0,1632	1,98301	7,16
47,0656	9888,13	0,2040	1,92925	44,53
47,5511	2304,09	0,1632	1,91068	10,38
48,5248	1420,44	0,1224	1,87459	6,40
49,0651	1209,36	0,1632	1,85520	5,45
49,9545	1847,27	0,2040	1,82424	8,32
50,1465	1828,40	0,1632	1,81770	8,23
50,7663	9093,39	0,1224	1,79695	40,95
51,7115	5244,66	0,1020	1,76631	23,62
51,8953	1492,97	0,0816	1,76048	6,72
52,9346	855,60	0,1632	1,72834	3,85
54,3010	4326,86	0,1428	1,68803	19,48
55,1689	1069,79	0,1428	1,66351	4,82
56,4118	2221,79	0,1020	1,62977	10,00

57,3299	911,02	0,1224	1,60584	4,10
58,0362	680,47	0,1632	1,58796	3,06
58,4713	1305,60	0,1428	1,57718	5,88
59,3247	1682,35	0,1020	1,55651	7,58
59,8479	985,54	0,1020	1,54415	4,44
62,2110	2608,33	0,1428	1,49105	11,75
62,5639	3539,27	0,1428	1,48348	15,94
63,5451	745,76	0,1632	1,46292	3,36
64,1093	2488,82	0,1020	1,45140	11,21
65,1257	358,60	0,2448	1,43118	1,61
65,8028	517,40	0,3264	1,41809	2,33
67,2521	650,74	0,0816	1,39101	2,93
67,4366	601,90	0,1224	1,38765	2,71
68,1712	493,92	0,1632	1,37448	2,22
68,9138	425,49	0,3264	1,36147	1,92
69,7222	334,34	0,2448	1,34765	1,51
71,7359	1955,16	0,1428	1,31469	8,80
72,4385	339,98	0,1428	1,30365	1,53
72,8660	297,60	0,1224	1,29706	1,34
74,6801	145,15	0,1224	1,26998	0,65
77,5516	328,25	0,3264	1,22997	1,48
79,0134	685,55	0,2856	1,21084	3,09
80,0983	332,54	0,4080	1,19715	1,50
81,8052	841,94	0,1428	1,17643	3,79
83,0056	486,12	0,2448	1,16244	2,19
83,7558	508,58	0,2448	1,15393	2,29
84,6638	2490,00	0,2040	1,14385	11,21

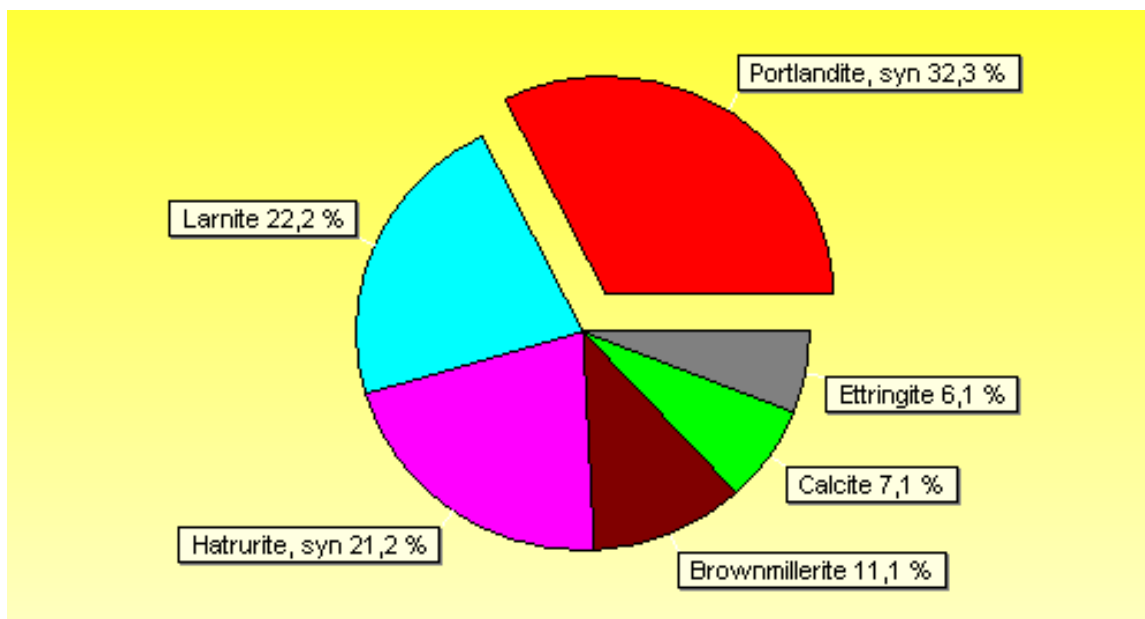
85,2794	546,47	0,1224	1,13716	2,46
86,2737	1117,47	0,4896	1,12659	5,03
88,7235	309,11	0,3264	1,10171	1,39
89,6693	471,67	0,1632	1,09253	2,12
91,6651	189,52	0,4080	1,07388	0,85
93,0751	1595,18	0,1020	1,06127	7,18
94,9800	294,81	0,4896	1,04496	1,33
95,8920	885,46	0,1020	1,03742	3,99
98,6886	989,54	0,2856	1,01537	4,46

Document History: (Bookmark 5)



Visible	Ref. Code	Score	Compound Name	Displacement [°2Th.]	Scale Factor	Chemical Formula	Matched Lines	SemiQuant [%]
*	00-004-0733	49	Portlandite, syn	-0,035	0,814	Ca (OH)_2	19	32
*	01-072-1652	30	Calcite	-0,020	0,403	CaCO_3	15	7
*	01-072-0646	21	Ettringite	0,060	0,177	$\text{Ca}_6 (\text{Al (OH)}_6)_2 (\text{SO}_4)_3 (\text{H}_2\text{O})_{25.7}$	51	6
*	01-074-1346	17	Brownmillerite	0,007	0,381	$\text{Fe Al O}_3 (\text{CaO})_2$	39	11
*	01-077-0388	30	Larnite	-0,011	0,286	Ca_2SiO_4	68	22
*	01-086-0402	37	Hatrumite, syn	-0,001	0,353	Ca_3SiO_5	62	21

More items... (Bookmark 8)



Phase Portlandite, syn

Weight fraction/ % 32,0

Phase Calcite

Weight fraction/ % 7,0

Phase Ettringite

Weight fraction/ % 6,0

Phase Brownmillerite

Weight fraction/ % 11,0

Phase Larnite

Weight fraction/ % 22,0

Phase Hatrurite, syn

Weight fraction/ % 21,0

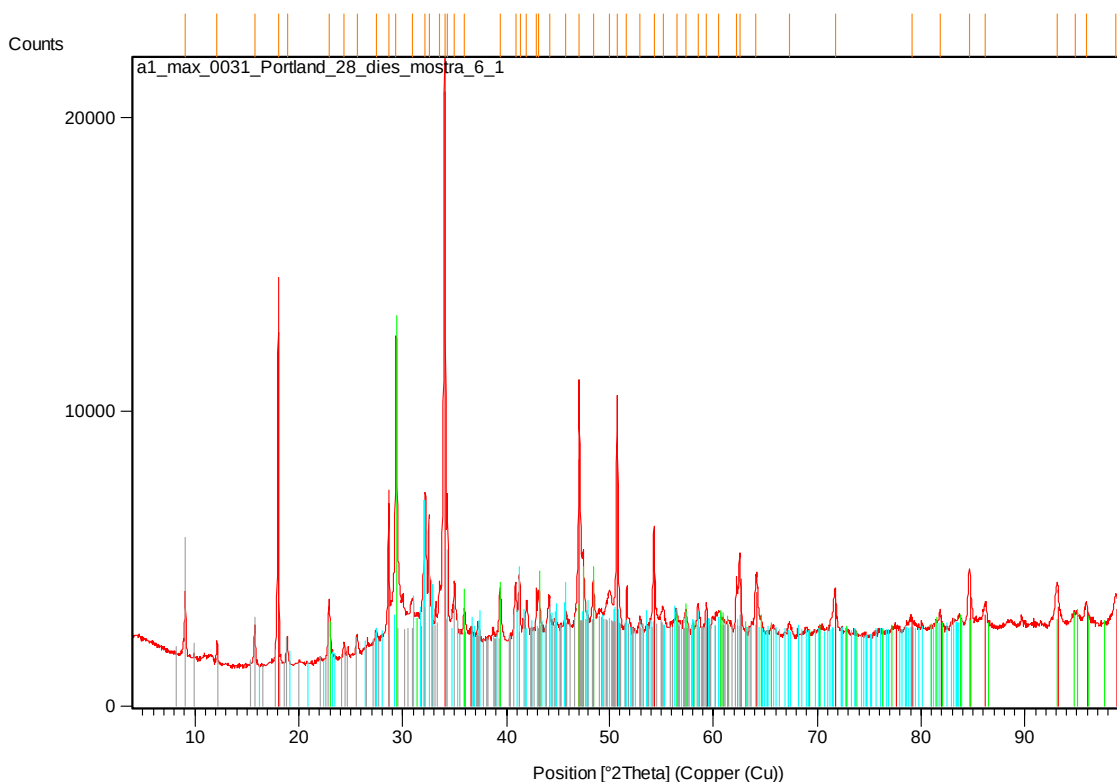
2.- Informe del resultado del estudio del drx de la pasta de cemento portland de 28 días de edad

Measurement Conditions: (Bookmark 1)

Dataset Name	a1_max_0031_Portland_28_dies_mostra_6_1
File name	F:\tfc\DRX\ a1_max_0031_Portland_28_dies_mostra_6_1.xrd
ml	
Sample Identification	Portland_28_dies_mostra_6
Comment	Configuration=Sample Spinner, Owner=User-1, Creation date=6/30/2004 5:11:04 PM
	Goniometer=PW3050/60 (Theta/2Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001
	Sample stage=Spinner PW3064
	Diffraction system=XPRT-PRO
	Measurement program=max_riet_quan, Owner=User-1, Creation date=6/12/2009 7:06:33 PM
	Fine Calibration Offset for 2Theta = -0.010 deg
	Batch program=12-6-09_gb_max, Owner=User-1, Creation date=6/12/2009 7:11:08 PM
	Laia_Haurie_(max)_Rietveld_quantitativ_juny-2009
Measurement Date / Time	12/06/2009 19:14:57
Operator	Univ. De Barcelona
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	4,0173
End Position [°2Th.]	99,9823
Step Size [°2Th.]	0,0170
Scan Step Time [s]	510,5436
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2,11
Offset [°2Th.]	0,0000
Divergence Slit Type	Automatic
Irradiated Length [mm]	10,00
Specimen Length [mm]	10,00
Measurement Temperature [°C]	25,00
Anode Material	Cu
K-Alpha1 [Å]	1,54060
Generator Settings	40 mA, 45 kV
Diffraction Type	0000000085010818
Diffraction Number	0
Goniometer Radius [mm]	240,00

Dist. Focus-Diverg. Slit [mm] 100,00
Incident Beam Monochromator Yes
Spinning Yes

Main Graphics, Analyze View: (Bookmark 2)



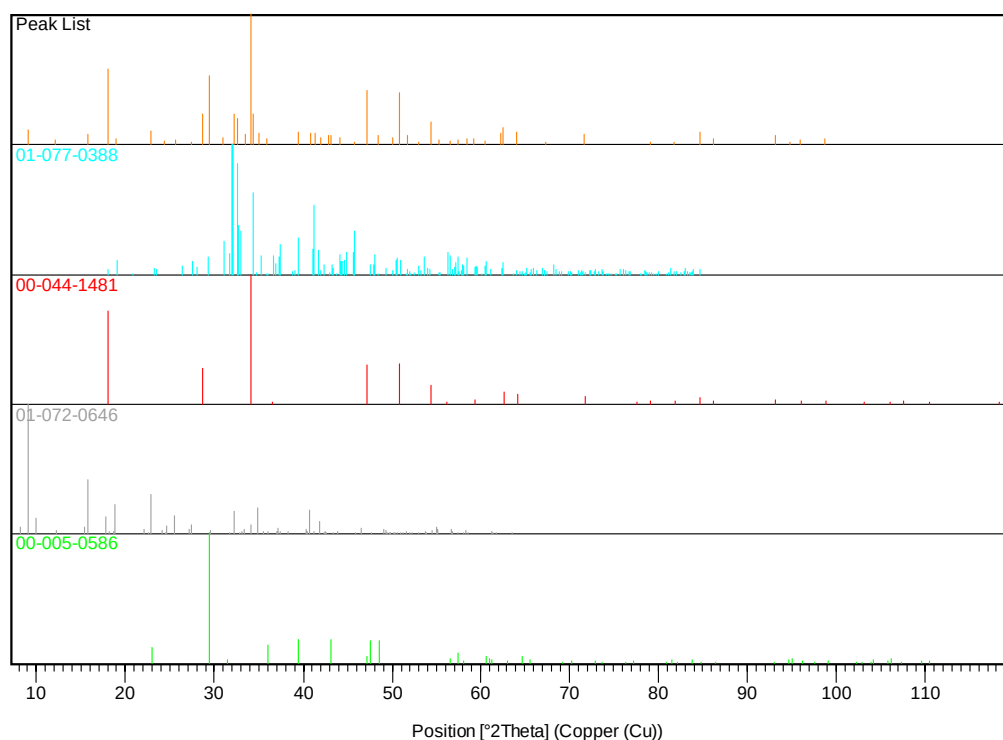
Peak List: (Bookmark 3)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
9,0849	2192,67	0,1224	9,72633	11,29
12,1289	743,49	0,1020	7,29123	3,83
15,7737	1430,84	0,1020	5,61371	7,37
18,0095	11250,28	0,1224	4,92154	57,92
18,8809	894,39	0,1632	4,69630	4,61
22,9093	1981,19	0,1224	3,87880	10,20

24,3273	455,42	0,2448	3,65582	2,34
25,5949	663,79	0,2040	3,47757	3,42
27,4382	322,15	0,4896	3,24798	1,66
28,6476	4487,94	0,1020	3,11356	23,11
29,3706	10161,69	0,1224	3,03854	52,32
30,9098	997,24	0,2448	2,89065	5,13
32,1681	4472,00	0,1428	2,78039	23,03
32,5318	3867,65	0,1020	2,75013	19,91
33,5351	1511,43	0,1632	2,67011	7,78
34,0525	19422,19	0,1224	2,63071	100,00
34,3247	4503,76	0,0816	2,61048	23,19
34,9912	1639,69	0,1632	2,56226	8,44
35,9338	891,24	0,2040	2,49718	4,59
39,3772	1772,09	0,2040	2,28638	9,12
40,8731	1742,84	0,2040	2,20609	8,97
41,2966	1663,15	0,1632	2,18444	8,56
41,9167	1062,07	0,2448	2,15354	5,47
42,8857	1409,89	0,0816	2,10710	7,26
43,0987	1267,98	0,1632	2,09718	6,53
44,1073	1020,01	0,2040	2,05154	5,25
45,7097	356,24	0,4896	1,98327	1,83
47,0809	8129,16	0,2244	1,92866	41,86
48,4516	1354,67	0,2040	1,87725	6,97
50,0416	1067,75	0,4896	1,82127	5,50
50,7514	7781,78	0,1224	1,79744	40,07
51,6813	1373,14	0,1020	1,76727	7,07
52,9622	265,04	0,3264	1,72751	1,36

54,3098	3346,72	0,1632	1,68778	17,23
55,1812	681,63	0,3264	1,66317	3,51
56,4499	583,58	0,3264	1,62876	3,00
57,3454	632,35	0,3264	1,60544	3,26
58,5318	788,59	0,2040	1,57569	4,06
59,3254	804,26	0,2040	1,55649	4,14
60,5251	437,44	0,8160	1,52848	2,25
62,2641	1715,04	0,1428	1,48990	8,83
62,5451	2448,74	0,1428	1,48389	12,61
64,1370	1895,88	0,2856	1,45084	9,76
67,3080	404,63	0,3264	1,38999	2,08
71,7260	1466,79	0,2856	1,31484	7,55
79,0883	396,68	0,8160	1,20988	2,04
81,8040	417,04	0,4896	1,17645	2,15
84,6816	1864,19	0,2448	1,14366	9,60
86,2024	773,86	0,3264	1,12734	3,98
93,1112	1377,79	0,3264	1,06096	7,09
94,8328	346,81	0,6528	1,04619	1,79
95,8953	673,04	0,3264	1,03739	3,47
98,7372	904,34	0,4896	1,01500	4,66

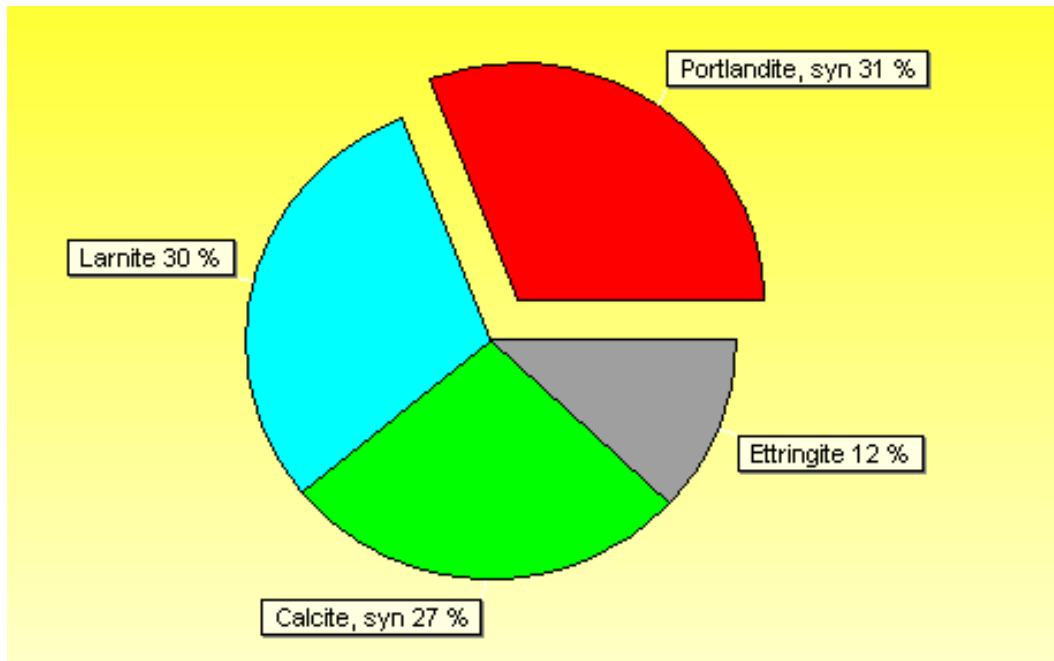
Document History: *(Bookmark 5)*



More items... (Bookmark 7)

Visible	Ref. Code	Score	Compound Name	Displacement [°2Th.]	Scale Factor	Chemical Formula	Matched Lines	SemiQuant [%]
*	01-077-0388	34	Larnite	0,000	0,193	Ca ₂ Si O ₄	86	30
*	00-044-1481	66	Portlandite, syn	0,000	0,820	Ca (O H) ₂	19	31
*	01-072-0646	29	Ettringite	0,000	0,180	Ca ₆ (Al (O H) ₆) ₂ (S O ₄) ₃ (H ₂ O) _{25.7}	77	12
*	00-005-0586	51	Calcite, syn	0,000	0,483	Ca C O ₃	21	27

More items... (Bookmark 8)



Phase Larnite
Weight fraction/ % 30,0

Phase Portlandite, syn
Weight fraction/ % 31,0

Phase Ettringite
Weight fraction/ % 12,0

Phase Calcite, syn
Weight fraction/ % 27,0

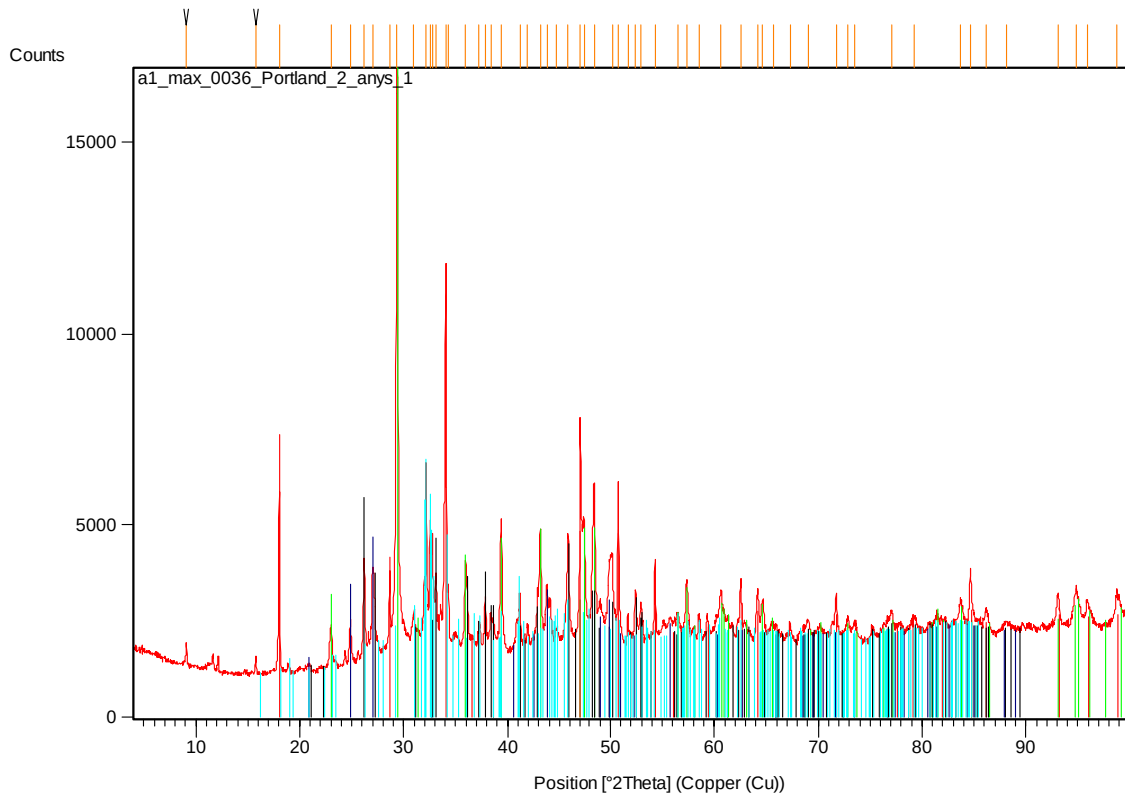
3.-INFORME DEL RESULTADO DEL ESTUDIO DEL DRX DE LA PASTA DE CEMENTO PORTLAND DE 2 AÑOS DE EDAD

Measurement Conditions: *(Bookmark 1)*

Dataset Name	a1_max_0036_Portland_2_anys_1
File name	F:\tfc\DRX\ a1_max_0036_Portland_2_anys_1.xrdml
Sample Identification	Portland_2_anys
Comment	Configuration=Sample Spinner, Owner=User-1, Creation date=6/30/2004 5:11:04 PM
	Goniometer=PW3050/60 (Theta/2Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001
	Sample stage=Spinner PW3064
	Diffraction system=XPRT-PRO
	Measurement program=max_riet_quan, Owner=User-1, Creation date=6/12/2009 7:06:33 PM
	Fine Calibration Offset for 2Theta = -0.010 deg
	Batch program=26-6-09_gb_max_c23, Owner=User-1, Creation date=6/26/2009 7:26:19 PM
	Laia_Haurie_(max)_Rietveld_quantitativ_juny-2009
Measurement Date / Time	26/06/2009 19:38:21
Operator	Univ. De Barcelona
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2Th.]	4,0173
End Position [°2Th.]	99,9823
Step Size [°2Th.]	0,0170
Scan Step Time [s]	510,5436
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2Th.]	2,11
Offset [°2Th.]	0,0000
Divergence Slit Type	Automatic
Irradiated Length [mm]	10,00
Specimen Length [mm]	10,00
Measurement Temperature [°C]	25,00
Anode Material	Cu
K-Alpha1 [Å]	1,54060
Generator Settings	40 mA, 45 kV
Diffraction Type	0000000085010818
Diffraction Number	0
Goniometer Radius [mm]	240,00
Dist. Focus-Diverg. Slit [mm]	100,00

Incident Beam Monochromator Yes
 Spinning Yes

Main Graphics, Analyze View: (Bookmark 2)



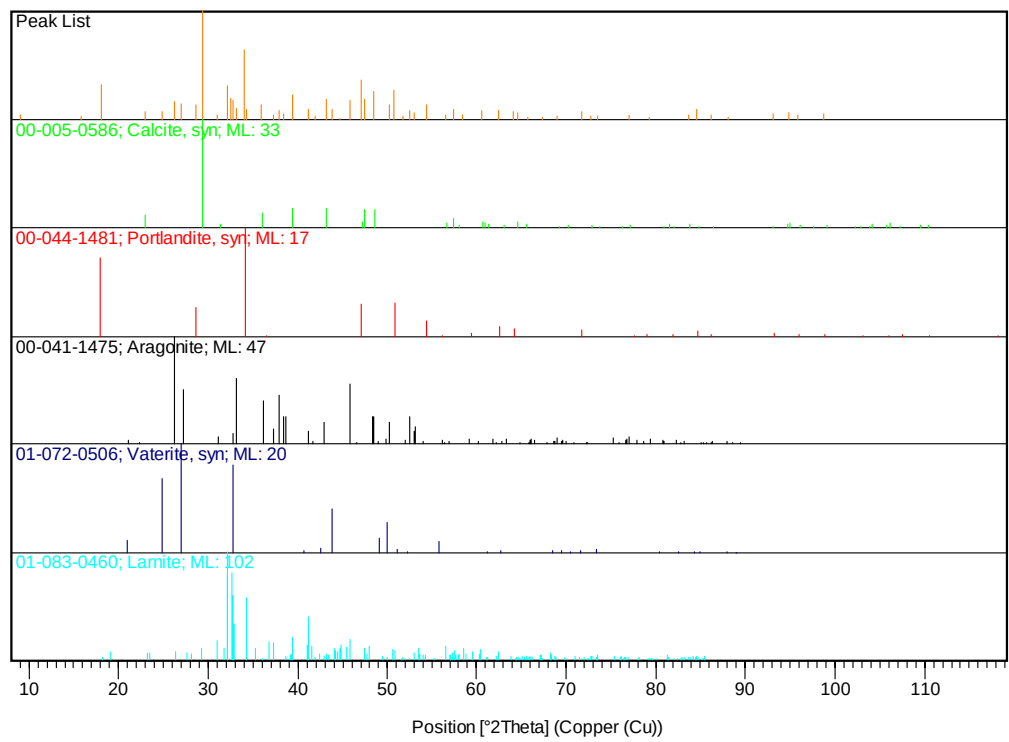
Peak List: (Bookmark 3)

Pos. [°2Th.]	Height [cts]	FWHM [°2Th.]	d-spacing [Å]	Rel. Int. [%]
9,0843	554,80	0,1632	9,72691	3,69
15,7653	386,20	0,2448	5,61669	2,57
18,0210	4731,18	0,1020	4,91842	31,47
23,0218	1087,15	0,2448	3,86009	7,23
24,8641	1098,95	0,1632	3,57810	7,31
26,1906	2507,50	0,1020	3,39981	16,68
27,0087	2170,86	0,2040	3,29866	14,44

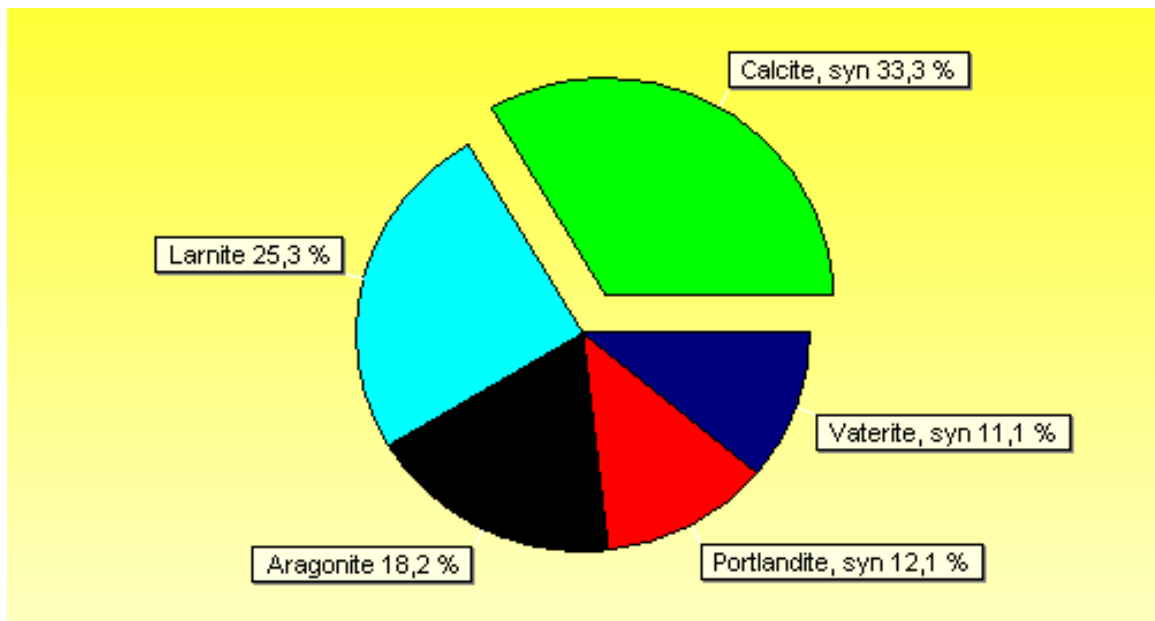
28,6495	1972,48	0,0816	3,11336	13,12
29,3711	15033,26	0,1428	3,03849	100,00
30,9622	575,19	0,3264	2,88587	3,83
32,1585	4583,61	0,0612	2,78120	30,49
32,5434	2979,13	0,0816	2,74918	19,82
32,7354	2593,69	0,1224	2,73349	17,25
33,1138	1496,77	0,1632	2,70311	9,96
34,0619	9642,24	0,1020	2,63001	64,14
34,3190	1352,81	0,1020	2,61090	9,00
35,9412	1973,62	0,2040	2,49668	13,13
37,2674	586,15	0,2040	2,41083	3,90
37,8747	1247,87	0,1224	2,37355	8,30
38,3756	797,89	0,3264	2,34372	5,31
39,3926	3379,39	0,1836	2,28552	22,48
41,1818	1280,96	0,1632	2,19026	8,52
41,9210	424,39	0,1632	2,15333	2,82
43,1525	2785,55	0,2040	2,09469	18,53
43,7836	1371,57	0,2040	2,06595	9,12
44,7299	140,76	0,3264	2,02442	0,94
45,8191	2564,49	0,1224	1,97879	17,06
47,0516	5352,83	0,1836	1,92979	35,61
47,4901	2779,73	0,1632	1,91299	18,49
48,4356	3864,94	0,1224	1,87783	25,71
50,1832	2028,26	0,2856	1,81646	13,49
50,7586	4075,59	0,1020	1,79721	27,11
51,7019	478,03	0,2448	1,76661	3,18
52,4293	1252,29	0,1836	1,74380	8,33

52,9405	859,04	0,2448	1,72816	5,71
54,3031	2049,96	0,1428	1,68797	13,64
56,4603	559,39	0,4896	1,62849	3,72
57,3398	1431,17	0,2448	1,60558	9,52
58,5308	601,03	0,2040	1,57572	4,00
60,6374	1179,09	0,1632	1,52592	7,84
62,5531	1272,34	0,1428	1,48371	8,46
64,1659	1089,72	0,2448	1,45026	7,25
64,6504	893,00	0,2448	1,44055	5,94
65,7115	298,44	0,6528	1,41984	1,99
67,3248	325,00	0,4896	1,38968	2,16
69,0393	439,80	0,3264	1,35930	2,93
71,7422	998,58	0,2040	1,31459	6,64
72,8383	475,27	0,3264	1,29748	3,16
73,5482	405,24	0,3264	1,28670	2,70
77,0618	569,09	0,3264	1,23656	3,79
79,2598	329,22	0,6528	1,20770	2,19
83,7359	620,60	0,4080	1,15415	4,13
84,6343	1419,75	0,1632	1,14418	9,44
86,1964	500,54	0,4080	1,12740	3,33
88,1389	218,56	0,9792	1,10750	1,45
93,0907	784,13	0,3264	1,06114	5,22
94,8206	825,76	0,4896	1,04629	5,49
95,9239	593,88	0,3264	1,03716	3,95
98,7481	723,85	0,5712	1,01492	4,81

Document History: *(Bookmark 5)*



Visible	Ref. Code	Score	Compound Name	Displacement [°2Th.]	Scale Factor	Chemical Formula	Matched Lines	SemiQuant [%]
*	00-005-0586	66	Calcite, syn	0,000	0,929	Ca C O3	33	33
*	00-044-1481	53	Portlandite, syn	0,000	0,504	Ca (O H)2	17	12
*	00-041-1475	46	Aragonite	0,000	0,245	Ca C O3	47	18
*	01-072-0506	39	Vaterite, syn	0,000	0,179	Ca C O3	20	11
*	01-083-0460	37	Larnite	0,000	0,268	Ca2 (Si O4)	102	25



Phase Calcite, syn	
Weight fraction/ %	33,0
Phase Portlandite, syn	
Weight fraction/ %	12,0
Phase Aragonite	
Weight fraction/ %	18,0
Phase Vaterite, syn	
Weight fraction/ %	11,0
Phase Larnite	
Weight fraction/ %	25,0

4.- Fichas de los componentes de la pasta de cemento portland de 7 días de edad.

PORTLANDITA

Name and formula

Reference code:	00-004-0733
Mineral name:	Portlandite, syn
PDF index name:	Calcium Hydroxide
Empirical formula:	CaH_2O_2
Chemical formula:	$\text{Ca}(\text{OH})_2$

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P-3m1
Space group number:	164
a (Å):	3,5930
b (Å):	3,5930
c (Å):	4,9090
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,24
Volume of cell (10 ⁶ pm ³):	54,88
Z:	1,00
RIR:	1,40

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Educational pattern Forensic NBS pattern Pharmaceutical
Quality:	Indexed (I)

Comments

General comments:	Levi, Giorn, <i>Chim. Ind. Applicata</i> , 6 333-7 (1924).
Analysis:	NBS analysis shows about 0.21% MgO, 0.1% Ba and no other impurities over 0.04%.
Temperature:	Pattern taken at 27 C.

References

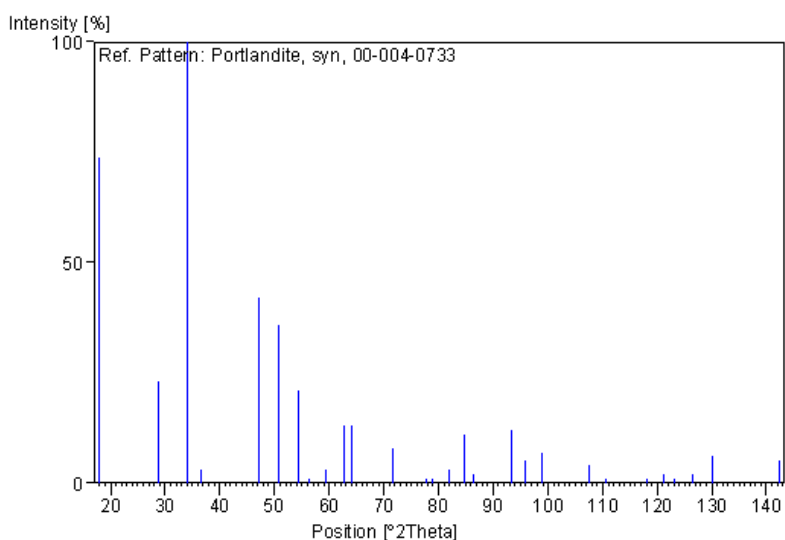
Primary reference:

Swanson, Tatge., *Natl. Bur. Stand. (U.S.), Circ. 539, I, 58,*
(1953)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	0	1	4,90000	18,089	74,0
2	1	0	0	3,11200	28,662	23,0
3	1	0	1	2,62800	34,089	100,0
4	0	0	2	2,44700	36,697	3,0
5	1	0	2	1,92700	47,124	42,0
6	1	1	0	1,79600	50,795	36,0
7	1	1	1	1,68700	54,337	21,0
8	0	0	3	1,63400	56,253	1,0
9	2	0	0	1,55700	59,304	3,0
10	2	0	1	1,48400	62,540	13,0
11	1	1	2	1,44900	64,228	13,0
12	2	0	2	1,31400	71,779	8,0
13	0	0	4	1,22800	77,699	1,0
14	1	1	3	1,21100	79,001	1,0
15	2	1	0	1,17620	81,825	3,0
16	2	1	1	1,14320	84,724	11,0
17	2	0	3	1,12750	86,187	2,0
18	2	1	2	1,05990	93,232	12,0
19	3	0	0	1,03660	95,993	5,0
20	3	0	1	1,01430	98,830	7,0
21	2	1	3	0,95510	107,513	4,0
22	1	0	5	0,93690	110,607	1,0
23	2	2	0	0,89790	118,161	1,0
24	2	2	1	0,88380	121,285	2,0
25	3	0	3	0,87600	123,125	1,0
26	3	1	0	0,86230	126,584	2,0
27	2	1	4	0,84950	130,125	6,0
28	3	1	2	0,81400	142,281	5,0

Stick Pattern



ETTRINGITA

Name and formula

Reference code:	01-072-0646
Mineral name:	Ettringite
ICSD name:	Calcium Aluminum Hydroxide Sulfate Hydrate
Empirical formula:	$\text{Al}_2\text{Ca}_6\text{H}_{63.4}\text{O}_{49.7}\text{S}_3$
Chemical formula:	$\text{Ca}_6(\text{Al}(\text{OH})_6)_2(\text{SO}_4)_3(\text{H}_2\text{O})_{25.7}$

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P31c
Space group number:	159
a (Å):	11,2600
b (Å):	11,2600
c (Å):	21,4800
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	1,76
Measured density (g/cm ³):	1,77
Volume of cell (10 ⁶ pm ³):	2358,53
Z:	2,00
RIR:	1,66

Subfiles and Quality

Subfiles:	Inorganic Mineral Corrosion Modelled additional pattern
Quality:	Calculated (C)

Comments

Sample source:	Specimen from Scawt Hill, Northern Ireland.
Additional pattern:	See PDF 41-1451.
ICSD collection code:	016045

References

Primary reference:	<i>Calculated from ICSD using POWD-12++</i>
Structure:	Moore, A.E., Taylor, H.F.W., <i>Acta Crystallogr., Sec. B</i> , 26 , 386, (1970)

Peak list

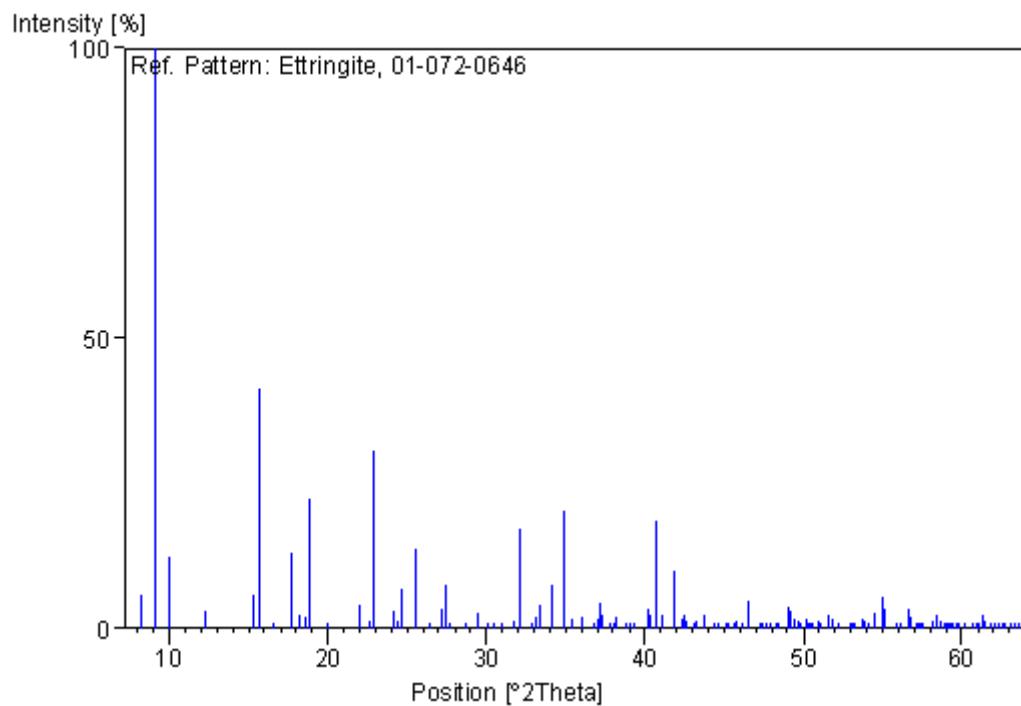
No.	h	k	l	d [Å]	2Theta[deg]	I [%]
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1	0	0	2	10,74000	8,226	5,9
2	1	0	0	9,75145	9,061	100,0
3	1	0	1	8,87929	9,954	12,4
4	1	0	2	7,21956	12,250	3,0
5	1	0	3	5,77134	15,340	5,8
6	1	1	0	5,63000	15,728	41,4
7	0	0	4	5,37000	16,494	0,2
8	-1	-1	2	4,98641	17,773	13,0
9	2	0	0	4,87572	18,180	2,4
10	2	0	1	4,75477	18,647	1,9
11	1	0	4	4,70391	18,850	22,5
12	2	0	2	4,43964	19,983	0,7
13	2	0	3	4,03005	22,039	4,1
14	1	0	5	3,93140	22,599	1,2
15	-1	-1	4	3,88583	22,867	30,8
16	2	1	0	3,68570	24,127	2,9
17	-2	-1	1	3,63261	24,485	1,4
18	2	0	4	3,60978	24,642	6,7
19	-2	-1	2	3,48613	25,531	13,9
20	1	0	6	3,36068	26,501	0,2
21	-2	-1	3	3,27701	27,191	3,5
22	3	0	0	3,25048	27,417	7,4
23	3	0	1	3,21389	27,735	0,6
24	3	0	2	3,11112	28,671	0,4
25	-1	-1	6	3,02097	29,545	2,6
26	3	0	3	2,95976	30,171	0,1
27	1	0	7	2,92707	30,516	0,2
28	2	0	6	2,88567	30,964	0,1
29	2	2	0	2,81500	31,762	1,2
30	3	0	4	2,78074	32,164	17,3
31	2	2	2	2,72302	32,865	0,8
32	3	1	0	2,70456	33,096	2,0
33	0	0	8	2,68500	33,344	4,0
34	3	1	2	2,62268	34,160	7,5
35	-2	-1	6	2,56800	34,911	20,4
36	-3	-1	3	2,53008	35,451	1,8
37	-2	-2	4	2,49321	35,993	2,0
38	4	0	0	2,43786	36,839	0,6
39	-1	-1	8	2,42350	37,065	1,7
40	-3	-1	4	2,41551	37,193	4,5
41	3	0	6	2,40652	37,337	2,4
42	4	0	2	2,37738	37,811	0,1
43	-2	-1	7	2,35824	38,130	0,7
44	2	0	8	2,35196	38,236	1,9
45	1	0	9	2,31824	38,814	0,4
46	4	0	3	2,30776	38,998	0,5
47	-3	-1	5	2,28877	39,334	0,2
48	3	2	0	2,23713	40,281	3,4
49	3	0	7	2,23135	40,390	2,2
50	-2	-2	6	2,21284	40,743	18,7
51	-3	-2	2	2,19013	41,184	2,3
52	-3	-1	6	2,15798	41,827	9,8
53	-3	-2	3	2,13533	42,291	1,6
54	4	1	0	2,12794	42,445	2,2
55	4	0	5	2,12026	42,607	1,2
56	1	0	10	2,09771	43,087	0,2
57	-4	-1	2	2,08736	43,312	1,3
58	-3	-2	4	2,06510	43,803	2,3
59	-4	-1	3	2,03976	44,375	0,2
60	-3	-1	7	2,02897	44,624	0,2
61	-1	-1	10	2,00690	45,142	0,7

62	-2	-1	9	2,00333	45,227	0,5
63	-3	-2	5	1,98422	45,687	0,5
64	-4	-1	4	1,97828	45,832	1,4
65	2	0	10	1,96570	46,142	0,1
66	5	0	0	1,95029	46,528	4,7
67	3	0	9	1,92378	47,208	0,2
68	5	0	2	1,91891	47,335	0,2
69	1	0	11	1,91471	47,445	0,2
70	-3	-1	8	1,90546	47,689	0,9
71	-3	-2	6	1,89717	47,911	0,5
72	5	0	3	1,88173	48,329	0,3
73	3	3	0	1,87667	48,468	0,7
74	-2	-1	10	1,85583	49,047	3,8
75	-3	-3	2	1,84866	49,250	2,9
76	4	2	0	1,84285	49,416	1,5
77	5	0	4	1,83314	49,695	1,4
78	-4	-1	6	1,82920	49,810	0,9
79	-4	-2	2	1,81631	50,188	1,5
80	2	0	11	1,81275	50,293	0,9
81	-3	-2	7	1,80772	50,443	0,6
82	4	0	8	1,80489	50,527	0,9
83	0	0	12	1,79000	50,978	1,4
84	-4	-2	3	1,78468	51,141	0,9
85	-3	-3	4	1,77160	51,546	2,2
86	1	0	12	1,76058	51,892	1,5
87	5	1	0	1,75141	52,184	0,9
88	-4	-1	7	1,74863	52,274	0,5
89	-5	-1	2	1,72858	52,927	0,8
90	-2	-1	11	1,72551	53,028	0,5
91	-3	-2	8	1,71873	53,254	0,1
92	1	1	12	1,70586	53,688	1,8
93	-5	-1	3	1,70125	53,845	1,3
94	4	2	5	1,69360	54,108	0,1
95	3	1	10	1,68204	54,511	2,8
96	-4	-1	8	1,66770	55,019	5,5
97	-5	-1	4	1,66509	55,112	3,5
98	5	0	7	1,64598	55,808	0,1
99	-4	-2	6	1,63851	56,084	0,2
100	6	0	0	1,62524	56,583	3,5
101	5	1	5	1,62181	56,714	1,9
102	-2	-1	12	1,61015	57,162	0,3
103	6	0	2	1,60695	57,287	0,2
104	4	3	0	1,60313	57,436	0,9
105	-4	-3	1	1,59868	57,611	0,5
106	-4	-3	2	1,58556	58,133	1,2
107	5	0	8	1,57795	58,440	2,5
108	-5	-1	6	1,57323	58,632	1,3
109	3	0	12	1,56797	58,848	0,5
110	-4	-3	3	1,56439	58,996	0,6
111	5	2	0	1,56148	59,117	0,4
112	-5	-2	1	1,55737	59,289	0,2
113	6	0	4	1,55556	59,365	0,2
114	-3	-2	10	1,54942	59,624	0,2
115	-5	-2	2	1,54523	59,802	0,5
116	-4	-3	4	1,53614	60,192	0,2
117	4	0	11	1,52408	60,718	0,2
118	-4	-2	8	1,51940	60,925	0,7
119	1	0	14	1,51564	61,093	0,4
120	-2	-2	12	1,51049	61,323	2,2
121	-2	-1	13	1,50773	61,448	1,2
122	-5	-2	4	1,49938	61,827	0,9

123	-3	-1	12	1,49268	62,136	0,5
124	6	1	0	1,48708	62,396	0,2
125	-6	-1	1	1,48353	62,562	0,1
126	1	1	14	1,48030	62,714	0,2
127	-3	-2	11	1,47113	63,150	0,3
128	-5	-1	8	1,46692	63,352	0,7
129	4	3	6	1,46313	63,535	1,0

Stick Pattern



CALCITE

Name and formula

Reference code:	01-072-1652
Mineral name:	Calcite
ICSD name:	Calcium Carbonate
Empirical formula:	CCaO ₃
Chemical formula:	CaCO ₃

Crystallographic parameters

Crystal system:	Rhombohedral
Space group:	R-3c
Space group number:	167
a (Å):	4,9900
b (Å):	4,9900
c (Å):	17,0020
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,72
Volume of cell (10 ⁶ pm ³):	366,63
Z:	6,00
RIR:	3,20

Subfiles and Quality

Subfiles:	Inorganic Mineral Modelled additional pattern Pharmaceutical
Quality:	Calculated (C)

Comments

Additional pattern:	See PDF 85-1108.
ICSD collection code:	018166
Test from ICSD:	At least one TF missing.

References

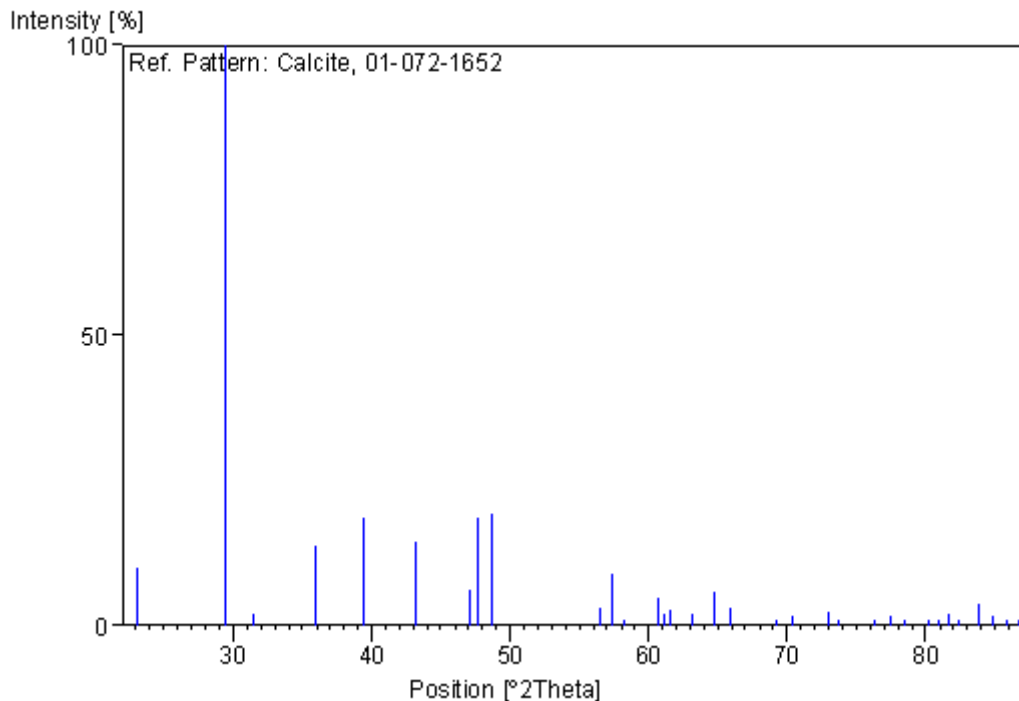
Primary reference:	<i>Calculated from ICSD using POWD-12++, (1997)</i>
Structure:	Chessin, H., Hamilton, W.C., <i>Acta Crystallogr.</i> , 18 , 689, (1965)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	1	2	3,85229	23,069	9,8

2	1	0	4	3,03034	29,452	100,0
3	0	0	6	2,83367	31,547	2,1
4	1	1	0	2,49500	35,966	13,9
5	1	1	3	2,28351	39,429	18,4
6	2	0	2	2,09415	43,164	14,5
7	0	2	4	1,92614	47,146	6,3
8	0	1	8	1,90710	47,646	18,4
9	1	1	6	1,87258	48,580	19,3
10	2	1	1	1,62588	56,559	3,2
11	1	2	2	1,60402	57,401	8,8
12	1	0	10	1,58215	58,270	1,0
13	2	1	4	1,52466	60,693	4,8
14	2	0	8	1,51517	61,114	2,1
15	1	1	9	1,50610	61,521	2,6
16	1	2	5	1,47231	63,093	2,0
17	3	0	0	1,44049	64,654	5,7
18	0	0	12	1,41683	65,869	3,2
19	2	1	7	1,35539	69,267	1,1
20	0	2	10	1,33615	70,410	1,8
21	1	2	8	1,29507	72,996	2,4
22	3	0	6	1,28410	73,722	0,5
23	2	2	0	1,24750	76,264	1,0
24	1	1	12	1,23204	77,397	1,7
25	2	2	3	1,21833	78,434	0,1
26	1	3	1	1,19559	80,224	0,1
27	3	1	2	1,18682	80,939	0,5
28	2	1	10	1,17788	81,683	2,1
29	0	1	14	1,16914	82,426	0,3
30	1	3	4	1,15357	83,788	3,7
31	2	2	6	1,14175	84,856	1,8
32	3	1	5	1,13039	85,914	0,1
33	1	2	11	1,12266	86,650	0,5

Stick Pattern



BROWNMILLERITA

Name and formula

Reference code:	01-074-1346
Mineral name:	Brownmillerite
ICSD name:	Iron Aluminum Calcium Oxide
Empirical formula:	$\text{AlCa}_2\text{FeO}_5$
Chemical formula:	$\text{FeAlO}_3 (\text{CaO})_2$

Crystallographic parameters

Crystal system:	Orthorhombic
Space group:	Pcmn
Space group number:	62
a (Å):	5,5800
b (Å):	14,5000
c (Å):	5,3400
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	90,0000
Calculated density (g/cm ³):	3,73
Volume of cell (10 ⁶ pm ³):	432,06
Z:	4,00
RIR:	1,87

Subfiles and Quality

Subfiles: Inorganic
Mineral
Corrosion
Modelled additional pattern
Quality: Calculated (C)

Comments

ICSD collection code: 027112
Test from ICSD: No R value given.
At least one TF missing.

References

Primary reference: *Calculated from ICSD using POWD-12++, (1997)*
Structure: Bertaut, F., Blum, P., Sagnieres, A., *Acta Crystallogr.*, **12**, 149, (1959)

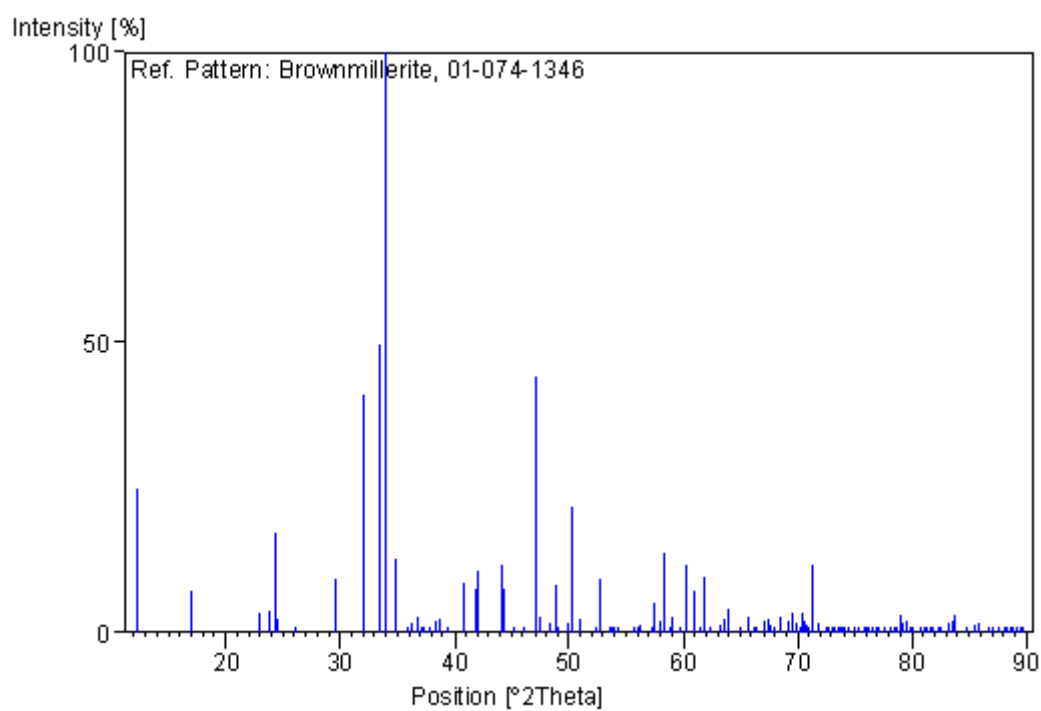
Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	2	0	7,25000	12,198	24,7
2	1	1	0	5,20770	17,012	7,3
3	1	0	1	3,85801	23,034	3,3
4	1	1	1	3,72829	23,847	3,6
5	1	3	0	3,65336	24,344	17,3
6	0	4	0	3,62500	24,537	2,3
7	1	2	1	3,40581	26,144	0,1
8	1	3	1	3,01523	29,603	9,1
9	2	0	0	2,79000	32,054	40,9
10	0	0	2	2,67000	33,537	49,6
11	1	4	1	2,64180	33,905	100,0
12	1	5	0	2,57323	34,837	12,7
13	0	2	2	2,50549	35,811	0,9
14	2	0	1	2,47283	36,300	1,8
15	2	1	1	2,43763	36,843	2,7
16	0	6	0	2,41667	37,174	0,6
17	1	0	2	2,40848	37,305	0,4
18	1	1	2	2,37593	37,835	0,1
19	2	2	1	2,34044	38,431	2,1
20	1	5	1	2,31813	38,816	2,5
21	1	2	2	2,28566	39,390	0,1
22	2	4	0	2,21097	40,779	8,5
23	1	3	2	2,15567	41,873	7,6
24	0	4	2	2,14980	41,993	10,8
25	1	6	1	2,04804	44,187	11,7
26	2	4	1	2,04279	44,306	7,4
27	1	4	2	2,00606	45,162	0,1
28	0	5	2	1,96426	46,178	0,1
29	2	0	2	1,92900	47,072	44,2
30	2	1	2	1,91216	47,512	2,8
31	2	5	1	1,88164	48,331	1,5
32	2	2	2	1,86415	48,814	8,1
33	1	5	2	1,85281	49,133	0,9
34	2	6	0	1,82668	49,883	1,6
35	0	8	0	1,81250	50,300	21,6
36	0	6	2	1,79173	50,925	2,2

37	3	1	1	1,74375	52,431	0,4
38	3	3	0	1,73590	52,686	9,2
39	3	2	1	1,70711	53,645	0,2
40	2	4	2	1,70291	53,788	0,2
41	1	0	3	1,69581	54,032	0,2
42	1	1	3	1,68433	54,430	0,6
43	1	2	3	1,65124	55,614	0,1
44	1	8	1	1,64048	56,011	1,1
45	0	7	2	1,63664	56,154	1,2
46	2	5	2	1,60613	57,319	0,3
47	1	3	3	1,60017	57,552	5,0
48	2	7	1	1,58792	58,038	2,1
49	3	4	1	1,58071	58,328	13,8
50	1	7	2	1,57048	58,745	0,6
51	3	5	0	1,56564	58,945	2,8
52	1	9	0	1,54788	59,689	0,9
53	1	4	3	1,53604	60,197	11,8
54	2	8	0	1,51993	60,902	7,3
55	2	6	2	1,50762	61,453	0,4
56	2	0	3	1,49961	61,817	9,6
57	1	9	1	1,48669	62,414	0,4
58	2	2	3	1,46946	63,230	1,2
59	1	5	3	1,46389	63,498	2,2
60	3	3	2	1,45535	63,915	4,1
61	2	3	3	1,43313	65,027	0,1
62	3	6	1	1,42084	65,659	2,6
63	2	7	2	1,41168	66,140	1,0
64	3	4	2	1,40660	66,409	0,7
65	4	0	0	1,39500	67,034	2,0
66	1	6	3	1,38814	67,410	2,4
67	3	7	0	1,38395	67,641	1,4
68	0	9	2	1,37944	67,893	0,2
69	4	2	0	1,36987	68,432	2,8
70	1	10	1	1,35730	69,155	1,9
71	3	5	2	1,35057	69,550	3,4
72	4	1	1	1,34390	69,945	1,8
73	3	7	1	1,33969	70,197	1,0
74	0	0	4	1,33500	70,480	3,4
75	2	5	3	1,33275	70,617	2,0
76	0	1	4	1,32938	70,823	1,3
77	4	2	1	1,32691	70,974	0,8
78	2	8	2	1,32090	71,347	11,7
79	0	2	4	1,31293	71,847	1,7
80	4	4	0	1,30192	72,550	0,1
81	4	3	1	1,29997	72,677	0,1
82	1	0	4	1,29836	72,781	0,1
83	1	1	4	1,29318	73,120	0,2
84	3	6	2	1,29040	73,303	0,2
85	2	10	0	1,28662	73,554	0,6
86	1	11	0	1,28287	73,804	0,4
87	3	1	3	1,28097	73,932	0,2
88	1	2	4	1,27803	74,131	0,2
89	2	6	3	1,27483	74,348	1,0
90	3	2	3	1,26624	74,939	0,3
91	3	8	1	1,26137	75,278	0,1
92	0	4	4	1,25275	75,887	0,2
93	2	10	1	1,25082	76,025	0,1
94	1	11	1	1,24738	76,273	0,3
95	3	3	3	1,24276	76,607	0,2
96	1	8	3	1,23832	76,932	0,3
97	2	9	2	1,23641	77,073	1,1

98	3	7	2	1,22870	77,647	0,4
99	4	5	1	1,22367	78,026	0,6
100	4	2	2	1,21882	78,396	0,6
101	2	7	3	1,21524	78,672	0,8
102	0	5	4	1,21199	78,924	3,0
103	0	12	0	1,20816	79,223	1,7
104	2	0	4	1,20424	79,532	2,0
105	2	1	4	1,20011	79,861	1,0
106	4	3	2	1,19784	80,043	0,4
107	2	2	4	1,18796	80,846	0,1
108	1	5	4	1,18501	81,089	0,2
109	0	11	2	1,18198	81,340	0,1
110	4	6	1	1,17838	81,641	0,1
111	3	5	3	1,17560	81,876	0,1
112	4	4	2	1,17022	82,333	0,9
113	1	9	3	1,16802	82,522	0,7
114	2	10	2	1,15906	83,302	1,8
115	1	11	2	1,15632	83,544	2,1
116	1	12	1	1,15310	83,830	2,9
117	2	4	4	1,14283	84,758	0,9
118	3	6	3	1,13527	85,456	1,4
119	4	7	1	1,13083	85,872	1,7
120	0	7	4	1,12214	86,700	0,6
121	3	10	1	1,11821	87,081	0,3
122	5	1	0	1,11271	87,621	0,2
123	3	9	2	1,10798	88,091	0,2
124	4	8	0	1,10548	88,342	1,0
125	1	10	3	1,10206	88,688	0,7
126	4	6	2	1,10012	88,886	0,4
127	2	9	3	1,09798	89,105	0,4
128	4	1	3	1,09485	89,428	0,4
129	1	13	0	1,09375	89,542	0,4
130	3	7	3	1,09257	89,665	0,4

Stick Pattern



LARNITA

Name and formula

Reference code:	01-077-0388
Mineral name:	Larnite
ICSD name:	Calcium Silicate
Empirical formula:	Ca ₂ O ₄ Si
Chemical formula:	Ca ₂ SiO ₄

Crystallographic parameters

Crystal system:	Monoclinic
Space group:	P21/n
Space group number:	14
a (Å):	5,5100
b (Å):	6,7600
c (Å):	9,3200
Alpha (°):	90,0000
Beta (°):	94,5000
Gamma (°):	90,0000
Calculated density (g/cm ³):	3,29
Volume of cell (10 ⁶ pm ³):	346,08
Z:	4,00
RIR:	0,72

Status, subfiles and quality

Status:	Marked as deleted by ICDD
Subfiles:	Inorganic Mineral Modelled additional pattern
Quality:	Calculated (C)

Comments

Additional pattern:	See PDF 33-302.
ICSD collection code:	039006
Test from ICSD:	At least one TF missing. Charge sum slightly deviates from zero.

References

Primary reference:	<i>Calculated from ICSD using POWD-12++, (1997)</i>
Structure:	Udagawa, S., Urabe, K., <i>Semento Gijutsu Nempo</i> , 32 , 35, (1978)

Peak list

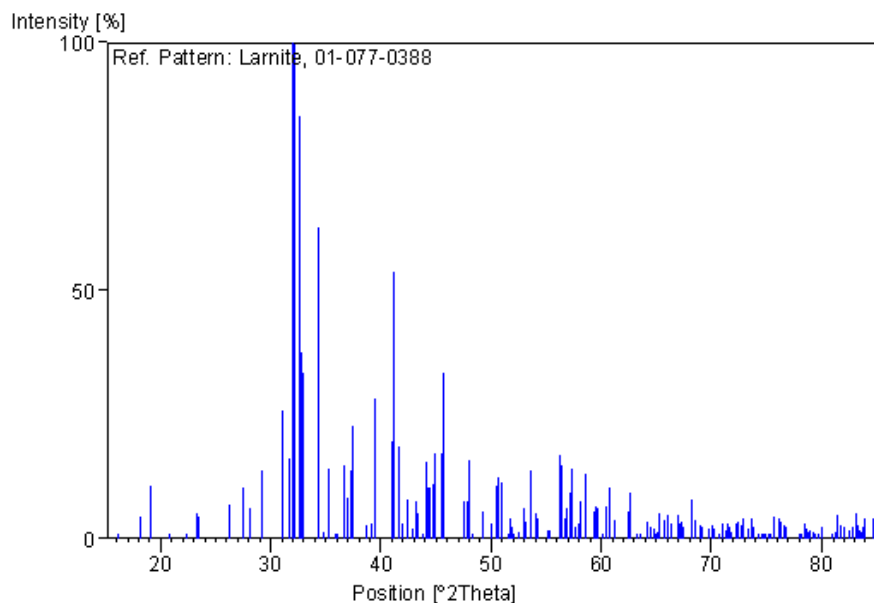
No.	h	k	l	d [Å]	2Theta[deg]	I [%]
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1	0	1	1	5,46630	16,202	0,1
2	-1	0	1	4,89989	18,090	4,4
3	0	0	2	4,64564	19,089	10,7
4	1	1	0	4,26305	20,820	1,0
5	-1	1	1	3,96731	22,392	0,2
6	0	1	2	3,82869	23,213	5,0
7	1	1	1	3,78822	23,465	4,3
8	0	2	0	3,38000	26,347	6,8
9	-1	1	2	3,24083	27,500	10,2
10	0	2	1	3,17635	28,070	6,0
11	1	1	2	3,04984	29,259	13,8
12	1	2	0	2,87868	31,042	25,9
13	0	1	3	2,81565	31,755	16,0
14	-1	0	3	2,79321	32,017	100,0
15	-1	2	1	2,78226	32,146	99,9
16	2	0	0	2,74651	32,576	85,3
17	0	2	2	2,73315	32,740	37,4
18	1	2	1	2,71831	32,923	33,4
19	1	0	3	2,61158	34,310	62,8
20	-1	1	3	2,58151	34,722	1,2
21	2	1	0	2,54451	35,243	14,2
22	-2	1	1	2,50090	35,879	0,9
23	-1	2	2	2,49331	35,992	0,8
24	-2	0	2	2,44995	36,651	14,8
25	1	1	3	2,43611	36,867	8,1
26	2	1	1	2,40993	37,282	13,8
27	1	2	2	2,40314	37,391	22,7
28	0	0	4	2,32282	38,735	2,7
29	-2	1	2	2,30334	39,075	3,2
30	2	0	2	2,28345	39,430	28,3
31	0	1	4	2,19675	41,055	19,7
32	0	3	1	2,18985	41,190	53,8
33	2	1	2	2,16633	41,658	18,6
34	-1	2	3	2,15313	41,925	3,0
35	2	2	0	2,13152	42,371	7,8
36	-2	2	1	2,10569	42,916	1,9
37	-1	1	4	2,09396	43,168	7,4
38	1	3	0	2,08474	43,369	5,1
39	1	2	3	2,06658	43,770	0,7
40	2	2	1	2,05052	44,130	15,4
41	-1	3	1	2,04723	44,205	10,3
42	-2	1	3	2,04015	44,367	10,3
43	0	3	2	2,02743	44,660	10,9
44	1	3	1	2,02135	44,801	17,2
45	1	1	4	1,98943	45,560	17,2
46	-2	2	2	1,98366	45,700	33,3
47	0	2	4	1,91435	47,454	7,6
48	2	1	3	1,89951	47,848	7,6
49	2	2	2	1,89411	47,993	15,7
50	1	3	2	1,88120	48,343	0,9
51	-2	0	4	1,84644	49,314	5,3
52	-3	0	1	1,82210	50,017	3,2
53	-2	2	3	1,80803	50,434	10,7
54	-1	0	5	1,80374	50,562	12,4
55	0	1	5	1,79179	50,923	11,3
56	1	2	4	1,77245	51,519	0,6
57	3	1	0	1,76732	51,680	4,2
58	-3	1	1	1,76084	51,884	2,5
59	-1	3	3	1,75380	52,108	0,6
60	-1	1	5	1,74277	52,463	1,2
61	-2	3	1	1,72787	52,950	6,3

62	1	0	5	1,71977	53,219	3,4
63	2	0	4	1,70796	53,616	13,9
64	2	3	1	1,69699	53,991	5,1
65	0	4	0	1,69000	54,233	4,1
66	0	4	1	1,66272	55,198	1,6
67	-2	3	2	1,65851	55,350	1,7
68	-3	0	3	1,63330	56,279	16,9
69	0	2	5	1,62838	56,465	14,8
70	-2	2	4	1,62042	56,767	4,0
71	1	4	0	1,61528	56,964	6,0
72	3	1	2	1,60995	57,170	9,2
73	2	3	2	1,60505	57,361	14,0
74	-1	4	1	1,59764	57,652	2,5
75	-1	2	5	1,59133	57,902	3,2
76	0	4	2	1,58818	58,028	7,6
77	1	4	1	1,58525	58,145	6,3
78	-1	3	4	1,57499	58,561	13,1
79	-2	1	5	1,55549	59,368	5,5
80	-2	3	3	1,55170	59,527	6,5
81	0	0	6	1,54854	59,661	6,0
82	-1	4	2	1,53672	60,167	0,7
83	1	3	4	1,52903	60,501	6,5
84	2	2	4	1,52463	60,694	10,3
85	1	4	2	1,51488	61,126	3,9
86	3	1	3	1,48705	62,397	5,3
87	-1	1	6	1,48351	62,563	9,1
88	-3	2	3	1,47060	63,175	0,1
89	-3	1	4	1,46082	63,647	0,9
90	2	1	5	1,45127	64,116	3,5
91	-1	4	3	1,44496	64,430	2,5
92	2	4	0	1,43934	64,712	2,0
93	0	3	5	1,43364	65,001	0,6
94	-2	4	1	1,43130	65,120	1,2
95	-2	3	4	1,42819	65,279	5,0
96	3	3	0	1,42102	65,650	1,7
97	1	4	3	1,41884	65,764	3,8
98	2	4	1	1,41361	66,038	4,8
99	-1	3	5	1,40783	66,344	3,1
100	-2	0	6	1,39660	66,947	4,8
101	3	3	1	1,39207	67,194	3,0
102	-2	4	2	1,39113	67,246	3,3
103	-1	2	6	1,38776	67,431	2,5
104	4	0	0	1,37325	68,241	8,0
105	-2	1	6	1,36772	68,555	3,7
106	2	3	4	1,36152	68,911	2,6
107	-3	0	5	1,35782	69,125	2,3
108	-4	0	2	1,34577	69,834	2,0
109	1	2	6	1,34094	70,122	2,6
110	0	5	1	1,33791	70,304	1,9
111	-3	1	5	1,33199	70,663	0,2
112	-2	4	3	1,32628	71,013	3,0
113	-3	3	3	1,32244	71,251	1,7
114	-4	1	2	1,32003	71,401	3,0
115	4	1	1	1,31757	71,555	2,2
116	-1	0	7	1,31394	71,783	1,4
117	2	0	6	1,30579	72,301	2,9
118	-2	3	5	1,30370	72,436	3,4
119	0	5	2	1,29814	72,796	2,7
120	1	5	1	1,29654	72,900	4,0
121	-2	2	6	1,29076	73,279	2,1
122	2	4	3	1,28523	73,646	4,2

123	3	2	4	1,28243	73,834	2,4
124	0	3	6	1,27623	74,253	0,4
125	-4	2	1	1,27299	74,474	0,5
126	-4	1	3	1,27050	74,644	0,3
127	1	0	7	1,26768	74,839	0,2
128	3	3	3	1,26274	75,182	0,4
129	-1	3	6	1,26123	75,288	0,7
130	3	0	5	1,25591	75,663	4,4
131	-4	2	2	1,25027	76,065	4,2
132	-3	3	4	1,24643	76,341	3,4
133	3	4	0	1,24187	76,672	2,6
134	-3	4	1	1,23962	76,837	2,4
135	-4	0	4	1,22497	77,928	0,8
136	3	4	1	1,22241	78,122	0,9
137	2	2	6	1,21805	78,455	3,2
138	-3	4	2	1,21600	78,613	2,1
139	-2	1	7	1,21356	78,802	1,2
140	-3	1	6	1,21105	78,997	1,7
141	-2	5	1	1,20810	79,228	1,4
142	-4	1	4	1,20534	79,445	1,0
143	4	1	3	1,20099	79,791	0,7
144	2	5	1	1,19748	80,072	2,3
145	-2	3	6	1,18695	80,929	0,7
146	3	4	2	1,18372	81,196	1,4
147	3	3	4	1,18060	81,455	4,9
148	3	2	5	1,17727	81,735	2,7
149	-3	4	3	1,17445	81,973	2,4
150	0	5	4	1,16848	82,483	1,7
151	2	5	2	1,16383	82,885	2,5
152	0	0	8	1,16141	83,096	5,2
153	-2	2	7	1,15883	83,322	2,6
154	-3	2	6	1,15664	83,515	1,7
155	-4	3	2	1,15550	83,616	1,4
156	4	3	1	1,15385	83,763	2,2
157	-1	5	4	1,15167	83,957	4,0
158	0	3	7	1,14366	84,682	4,2

Stick Pattern



HATRURITA

Name and formula

Reference code:	01-086-0402
Mineral name:	Hatrurite, syn
ICSD name:	Calcium Silicon Oxide
Empirical formula:	$\text{Ca}_3\text{O}_5\text{Si}$
Chemical formula:	Ca_3SiO_5

Crystallographic parameters

Crystal system:	Monoclinic
Space group:	Cm
Space group number:	8
a (Å):	12,2350
b (Å):	7,0730
c (Å):	9,2980
Alpha (°):	90,0000
Beta (°):	116,3100
Gamma (°):	90,0000
Calculated density (g/cm ³):	3,15
Volume of cell (10 ⁶ pm ³):	721,28
Z:	6,00
RIR:	0,93

Subfiles and Quality

Subfiles:	Inorganic
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Quality: Mineral
Modelled additional pattern
Calculated (C)

Comments

Additional pattern: See PDF 49-442.
ICSD collection code: 081100

References

Primary reference: *Calculated from ICSD using POWD-12++, (1997)*
Structure: Mumme, W.G., *Neues Jahrb. Mineral., Monatsh.*, **1995**, 145, (1995)

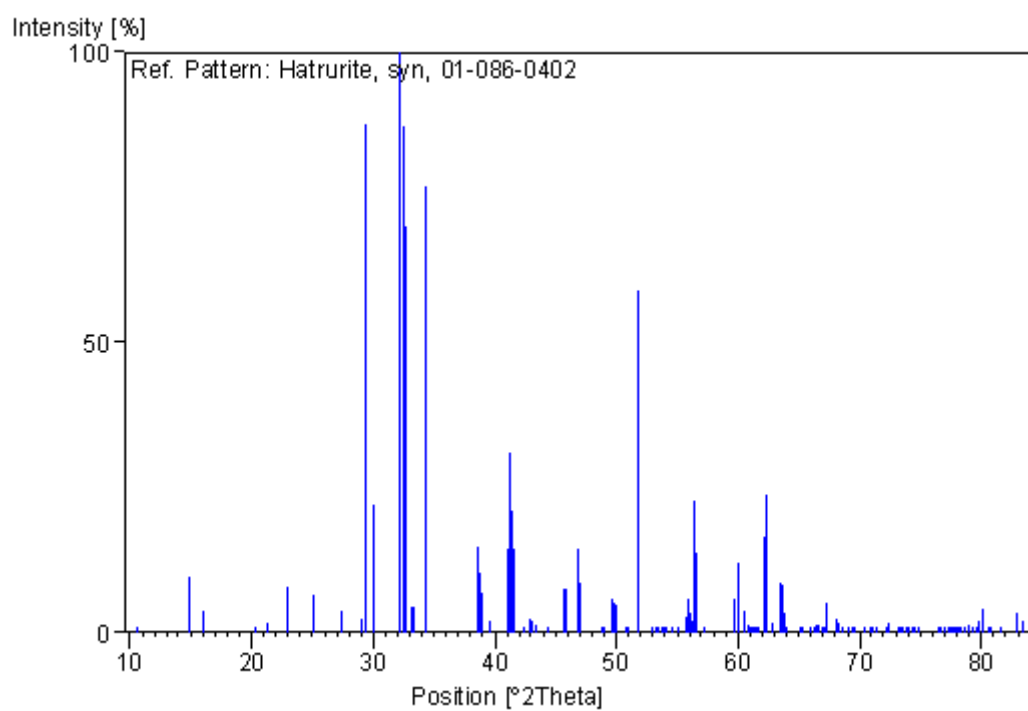
Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	0	1	8,33481	10,606	0,7
2	-2	0	1	5,94412	14,892	9,7
3	-1	1	1	5,50481	16,088	3,7
4	-2	0	2	4,36874	20,311	0,3
5	0	0	2	4,16741	21,303	1,8
6	-1	1	2	3,87820	22,913	7,7
7	0	2	0	3,53304	25,186	6,4
8	-3	1	2	3,25808	27,352	3,8
9	3	1	0	3,24768	27,441	3,9
10	1	1	2	3,08201	28,947	2,2
11	-2	2	1	3,03995	29,357	87,6
12	-4	0	1	3,03420	29,414	85,2
13	-4	0	2	2,97206	30,043	21,9
14	0	0	3	2,77827	32,193	100,0
15	-2	2	2	2,75241	32,504	87,4
16	4	0	0	2,74189	32,632	70,0
17	-3	1	3	2,70085	33,142	4,4
18	3	1	1	2,68902	33,292	4,4
19	-4	0	3	2,61532	34,259	37,4
20	2	2	1	2,60821	34,355	77,0
21	-2	2	3	2,32760	38,652	14,8
22	-2	0	4	2,31746	38,828	10,3
23	1	1	3	2,31281	38,909	7,0
24	-1	3	1	2,27642	39,557	1,9
25	-5	1	1	2,27195	39,638	1,8
26	-4	0	4	2,19172	41,153	14,3
27	0	2	3	2,18437	41,298	31,1
28	3	1	2	2,17921	41,400	20,9
29	-5	1	3	2,17228	41,538	14,6
30	4	2	0	2,16690	41,646	14,5
31	-1	1	4	2,13282	42,344	1,1
32	2	0	3	2,12722	42,460	0,8
33	-4	2	3	2,10278	42,978	2,3
34	5	1	0	2,09508	43,144	1,9
35	0	0	4	2,08370	43,392	1,3
36	-3	3	1	2,04113	44,344	0,7
37	-3	3	2	1,98373	45,699	7,5
38	-6	0	1	1,97838	45,829	7,5
39	-2	2	4	1,93910	46,812	14,4
40	4	0	2	1,93105	47,019	8,4
41	-4	2	4	1,86296	48,847	0,1
42	5	1	1	1,85470	49,079	0,1

43	-3	3	3	1,83494	49,643	5,9
44	-4	0	5	1,82793	49,847	5,2
45	2	2	3	1,82286	49,995	4,9
46	-3	1	5	1,79831	50,725	0,5
47	0	2	4	1,79526	50,818	0,6
48	3	1	3	1,79132	50,937	0,7
49	0	4	0	1,76652	51,705	59,2
50	0	4	1	1,72969	52,890	0,3
51	-6	2	1	1,72658	52,993	0,2
52	-1	1	5	1,71577	53,353	0,5
53	2	0	4	1,71209	53,477	0,5
54	-5	1	5	1,70186	53,824	0,2
55	1	3	3	1,69794	53,958	0,2
56	4	2	2	1,69484	54,065	0,3
57	-7	1	3	1,68250	54,494	0,2
58	0	0	5	1,66696	55,045	0,6
59	-6	0	5	1,64792	55,736	2,8
60	3	3	2	1,64291	55,921	5,7
61	-5	3	3	1,63994	56,031	3,4
62	-7	1	1	1,63548	56,198	2,1
63	-2	2	5	1,63058	56,382	22,7
64	0	4	2	1,62778	56,487	14,3
65	4	0	3	1,62449	56,612	13,8
66	-7	1	4	1,60926	57,197	0,3
67	5	3	0	1,60595	57,326	0,2
68	-4	0	6	1,54580	59,778	5,7
69	2	2	4	1,54100	59,983	11,9
70	-4	4	1	1,52775	60,557	3,9
71	-4	4	2	1,51997	60,900	1,2
72	-8	0	2	1,51710	61,027	1,0
73	1	1	5	1,51331	61,197	0,8
74	-3	1	6	1,51018	61,337	0,6
75	0	2	5	1,50785	61,442	0,5
76	3	1	4	1,50500	61,571	0,6
77	-7	1	5	1,49371	62,088	15,0
78	0	4	3	1,49174	62,179	16,4
79	5	3	1	1,48969	62,274	12,0
80	6	2	1	1,48771	62,366	23,6
81	1	3	4	1,47873	62,788	1,8
82	4	2	3	1,47620	62,908	1,3
83	-4	4	3	1,46486	63,451	8,5
84	-8	0	1	1,46040	63,668	8,2
85	3	3	3	1,45625	63,871	3,3
86	6	0	2	1,45366	63,998	0,9
87	-1	1	6	1,43101	65,135	0,7
88	2	0	5	1,42843	65,267	0,5
89	-4	2	6	1,41641	65,891	0,4
90	-1	3	5	1,41478	65,976	0,4
91	5	1	3	1,41022	66,217	0,5
92	-8	0	5	1,40854	66,306	0,7
93	-2	4	4	1,40577	66,454	1,4
94	-8	2	3	1,40155	66,680	1,2
95	-1	5	1	1,39595	66,983	0,3
96	-8	2	2	1,39339	67,122	0,9
97	0	0	6	1,38914	67,355	5,2
98	-4	4	4	1,37620	68,074	2,3
99	8	0	0	1,37095	68,371	1,7
100	-7	3	1	1,36874	68,497	0,9
101	2	4	3	1,35980	69,010	0,1
102	-7	3	4	1,35305	69,404	0,7
103	-6	2	6	1,34983	69,593	0,8

104	-3	5	1	1,33648	70,391	0,3
105	-4	0	7	1,32822	70,894	0,5
106	2	2	5	1,32447	71,125	1,0
107	-9	1	4	1,31839	71,503	1,1
108	-8	0	6	1,30766	72,182	0,7
109	7	3	0	1,30410	72,410	1,7
110	-3	3	6	1,29273	73,149	0,8
111	3	3	4	1,28948	73,364	0,5
112	-2	0	7	1,28736	73,505	0,4
113	-7	3	5	1,28276	73,812	0,2
114	8	2	0	1,27826	74,115	0,2
115	-3	5	3	1,27322	74,458	0,5
116	-4	4	5	1,27127	74,592	1,1
117	8	0	1	1,26589	74,963	0,4
118	-4	2	7	1,24342	76,559	0,1
119	-1	3	6	1,24202	76,661	0,2
120	5	1	4	1,23836	76,929	0,2
121	-7	1	7	1,23323	77,309	0,1
122	2	4	4	1,23001	77,549	0,1
123	5	3	3	1,22836	77,672	0,1
124	-8	2	6	1,22650	77,812	0,3
125	-1	1	7	1,22473	77,946	0,4
126	2	0	6	1,22337	78,049	0,3
127	7	3	1	1,22212	78,144	0,4
128	-5	5	1	1,21854	78,418	0,2
129	-6	2	7	1,21509	78,684	0,1
130	-2	2	7	1,21019	79,064	1,2
131	4	0	5	1,20663	79,344	1,1
132	-5	5	3	1,20242	79,677	0,9
133	-8	0	7	1,20007	79,864	2,1
134	4	4	3	1,19629	80,168	4,0
135	0	0	7	1,18984	80,691	0,3
136	5	5	0	1,18882	80,775	0,3
137	-9	3	3	1,17768	81,700	0,5
138	-4	4	6	1,16380	82,887	3,4
139	8	0	2	1,15873	83,331	1,9

Stick Pattern



5.- Fichas de los componentes de la pasta de cemento portland de 28 días de edad.

PORTLANDITA

Name and formula

Reference code:	00-044-1481
Mineral name:	Portlandite, syn
PDF index name:	Calcium Hydroxide
Empirical formula:	CaH_2O_2
Chemical formula:	$\text{Ca}(\text{OH})_2$

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P-3m1
Space group number:	164
a (Å):	3,5899
b (Å):	3,5899
c (Å):	4,9160
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,24
Volume of cell (10 ⁶ pm ³):	54,87
Z:	1,00
RIR:	2,90

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Forensic Pharmaceutical
Quality:	Star (S)

Comments

Deleted by:	Deleted by 4-733 which is satisfactory.
Color:	White
General comments:	Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2.2%.
Sample source:	Sample obtained from Sigma Chemical Co.
Optical data:	A=1.545, B=1.574, Sign=-
Additional pattern:	Validated by a calculated pattern.

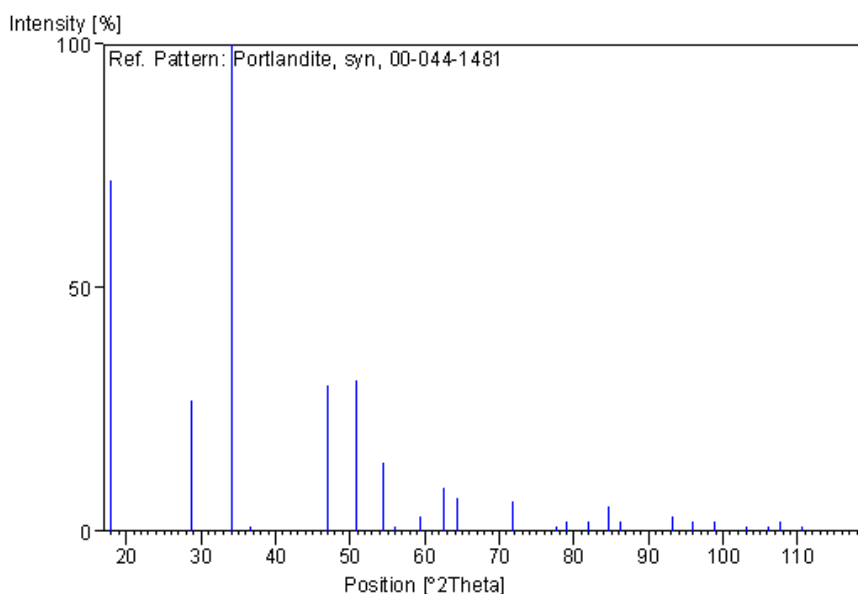
References

Primary reference: Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA., *ICDD Grant-in-Aid*, (1992)
Optical data: Winchell, A., Winchell, H., *Microscopic Character of Artificial Inorg. Solid Sub.*, 69, (1964)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	0	1	4,92200	18,008	72,0
2	1	0	0	3,11100	28,672	27,0
3	1	0	1	2,62700	34,102	100,0
4	0	0	2	2,45800	36,527	1,0
5	1	0	2	1,92710	47,121	30,0
6	1	1	0	1,79540	50,813	31,0
7	1	1	1	1,68640	54,358	14,0
8	0	0	3	1,63830	56,092	1,0
9	2	0	0	1,55410	59,426	3,0
10	2	0	1	1,48200	62,634	9,0
11	1	0	3	1,44890	64,233	7,0
12	2	0	2	1,31350	71,811	6,0
13	0	0	4	1,22860	77,654	1,0
14	1	1	3	1,20980	79,095	2,0
15	2	1	0	1,17520	81,910	2,0
16	1	0	4	1,14290	84,751	5,0
17	2	0	3	1,12740	86,197	2,0
18	2	1	2	1,06010	93,209	3,0
19	3	0	0	1,03630	96,030	2,0
20	1	1	4	1,01390	98,882	2,0
21	0	0	5	0,98330	103,143	1,0
22	2	0	4	0,96410	106,066	1,0
23	2	1	3	0,95470	107,579	2,0
24	1	0	5	0,93739	110,521	1,0
25	2	2	0	0,89740	118,268	1,0

Stick Pattern



CALCITA

Name and formula

Reference code:	00-005-0586
Mineral name:	Calcite, syn
PDF index name:	Calcium Carbonate
Empirical formula:	CCaO ₃
Chemical formula:	CaCO ₃

Crystallographic parameters

Crystal system:	Rhombohedral
Space group:	R-3c
Space group number:	167
a (Å):	4,9890
b (Å):	4,9890
c (Å):	17,0620
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,71
Measured density (g/cm ³):	2,71
Volume of cell (10 ⁶ pm ³):	367,78
Z:	6,00
RIR:	2,00

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Educational pattern Forensic NBS pattern Pharmaceutical Superconducting Material
Quality:	Star (S)

Comments

Color:	Colorless
General comments:	Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, <i>ICDD Grant-in-Aid</i> (1992). Agrees well with experimental and calculated patterns. Additional weak reflections [indicated by brackets] were observed.
Sample source:	Sample from Mallinckrodt Chemical Works.

Analysis: Spectroscopic analysis: <0.1% Sr; <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na, Si, Sn; <0.0001% Ag, Cr, Fe, Li, Mn.
Optical data: A=1.487, B=1.659, Sign=-
Additional pattern: See ICSD 16710, 20179, 28827, 18164, 18165 and 18166 (PDF 72-1214 and 72-1937); ICSD 73446 (PDF 81-2027); ICSD 79673 (PDF 83-577); ICSD 79674 (PDF 83-578).
Temperature: Pattern taken at 26 C.

References

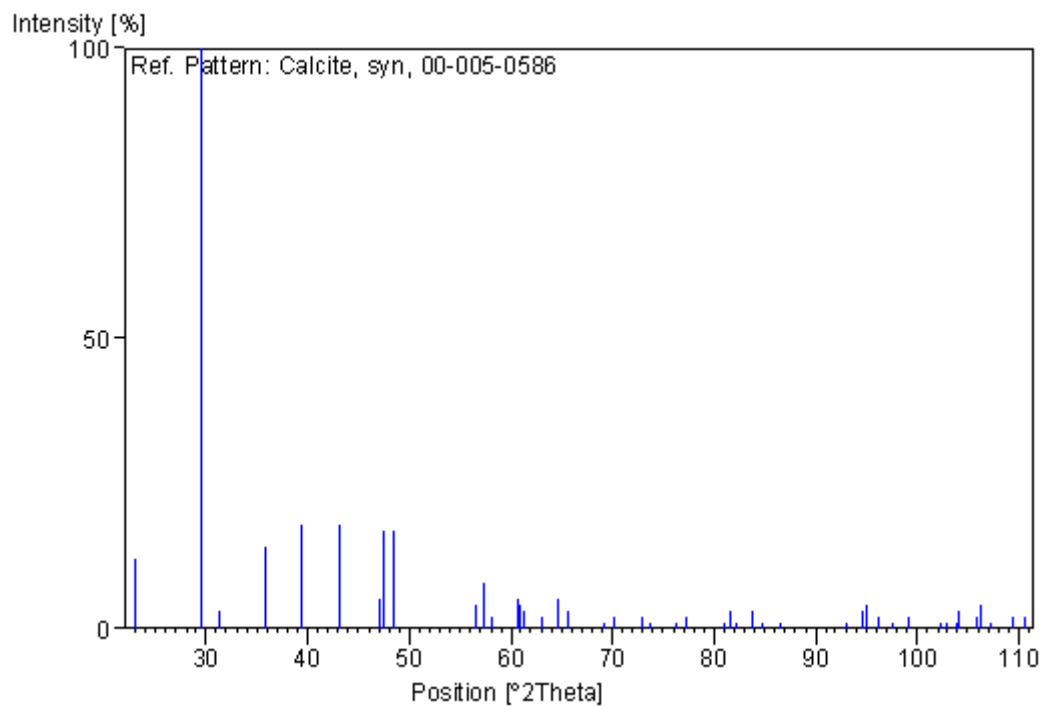
Primary reference: Swanson, Fuyat., *Natl. Bur. Stand. (U.S.), Circ. 539, II*, 51, (1953)
Optical data: *Dana's System of Mineralogy, 7th Ed., II*, 142

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	1	2	3,86000	23,022	12,0
2	1	0	4	3,03500	29,406	100,0
3	0	0	6	2,84500	31,418	3,0
4	1	1	0	2,49500	35,966	14,0
5	1	1	3	2,28500	39,402	18,0
6	2	0	2	2,09500	43,146	18,0
7	0	2	4	1,92700	47,124	5,0
8	0	1	8	1,91300	47,490	17,0
9	1	1	6	1,87500	48,514	17,0
10	2	1	1	1,62600	56,555	4,0
11	1	2	2	1,60400	57,402	8,0
12	1	0	10	1,58700	58,075	2,0
13	2	1	4	1,52500	60,678	5,0
14	2	0	8	1,51800	60,987	4,0
15	1	1	9	1,51000	61,345	3,0
16	1	2	5	1,47300	63,060	2,0
17	3	0	0	1,44000	64,678	5,0
18	0	0	12	1,42200	65,599	3,0
19	2	1	7	1,35600	69,231	1,0
20	0	2	10	1,33900	70,238	2,0
21	1	2	8	1,29700	72,870	2,0
22	3	0	6	1,28400	73,729	1,0
23	2	2	0	1,24700	76,300	1,0
24	1	1	12	1,23500	77,177	2,0
25	3	1	2	1,18690	80,933	1,0
26	2	1	10	1,17950	81,547	3,0
27	0	1	14	1,17280	82,113	1,0
28	1	3	4	1,15380	83,767	3,0
29	2	2	6	1,14250	84,788	1,0
30	1	2	11	1,12440	86,483	1,0
31	2	0	14	1,06130	93,072	1,0
32	4	0	4	1,04730	94,701	3,0
33	3	1	8	1,04470	95,011	4,0
34	1	0	16	1,03520	96,165	2,0
35	2	1	13	1,02340	97,647	1,0
36	3	0	12	1,01180	99,161	2,0
37	3	2	1	0,98950	102,242	1,0
38	2	3	2	0,98460	102,952	1,0
39	1	3	10	0,97820	103,899	1,0
40	1	2	14	0,97670	104,124	3,0
41	3	2	4	0,96550	105,846	2,0
42	0	4	8	0,96360	106,145	4,0
43	0	2	16	0,95620	107,334	1,0

44	4	1	0	0,94290	109,561	2,0
45	2	2	12	0,93760	110,484	2,0

Stick Pattern



ETTRINGITA

Name and formula

Reference code:	01-072-0646
Mineral name:	Ettringite
ICSD name:	Calcium Aluminum Hydroxide Sulfate Hydrate
Empirical formula:	$\text{Al}_2\text{Ca}_6\text{H}_{63.4}\text{O}_{49.7}\text{S}_3$
Chemical formula:	$\text{Ca}_6(\text{Al}(\text{OH})_6)_2(\text{SO}_4)_3(\text{H}_2\text{O})_{25.7}$

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P31c
Space group number:	159

a (Å):	11,2600
b (Å):	11,2600
c (Å):	21,4800
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000

Calculated density (g/cm ³):	1,76
Measured density (g/cm ³):	1,77
Volume of cell (10 ⁶ pm ³):	2358,53
Z:	2,00

RIR:	1,66
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Subfiles and Quality

Subfiles:	Inorganic Mineral Corrosion Modelled additional pattern
Quality:	Calculated (C)

Comments

Sample source:	Specimen from Scawt Hill, Northern Ireland.
Additional pattern:	See PDF 41-1451.
ICSD collection code:	016045

References

Primary reference:	<i>Calculated from ICSD using POWD-12++</i>
Structure:	Moore, A.E., Taylor, H.F.W., <i>Acta Crystallogr., Sec. B</i> , 26 , 386, (1970)

Peak list

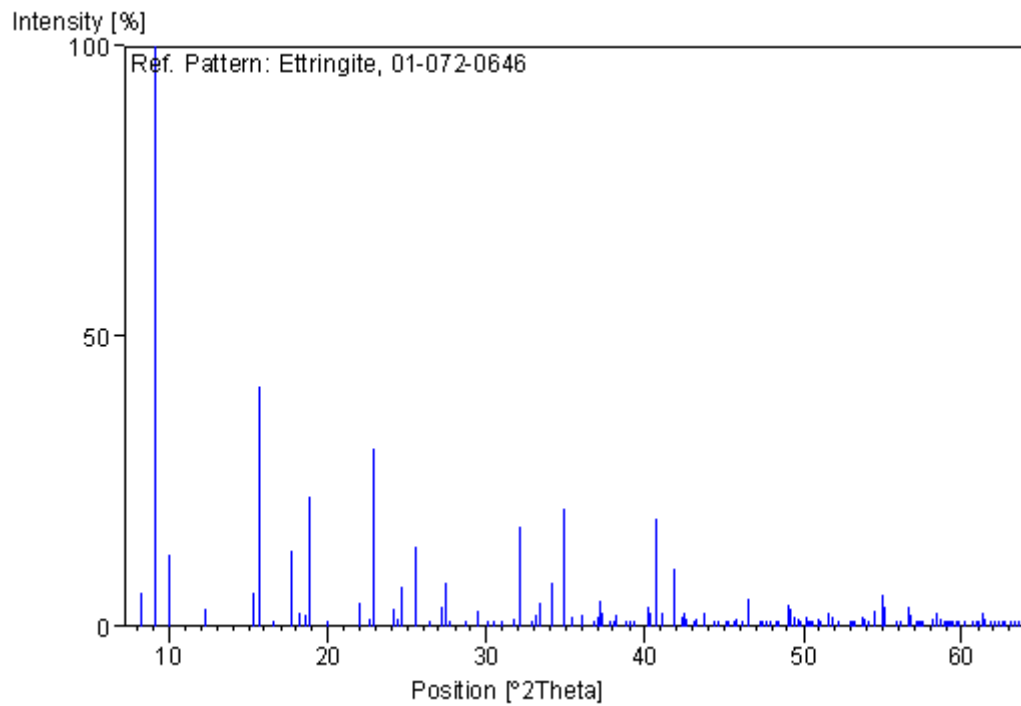
No.	h	k	l	d [Å]	2Theta[deg]	I [%]
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1	0	0	2	10,74000	8,226	5,9
2	1	0	0	9,75145	9,061	100,0
3	1	0	1	8,87929	9,954	12,4
4	1	0	2	7,21956	12,250	3,0
5	1	0	3	5,77134	15,340	5,8
6	1	1	0	5,63000	15,728	41,4
7	0	0	4	5,37000	16,494	0,2
8	-1	-1	2	4,98641	17,773	13,0
9	2	0	0	4,87572	18,180	2,4
10	2	0	1	4,75477	18,647	1,9
11	1	0	4	4,70391	18,850	22,5
12	2	0	2	4,43964	19,983	0,7
13	2	0	3	4,03005	22,039	4,1
14	1	0	5	3,93140	22,599	1,2
15	-1	-1	4	3,88583	22,867	30,8
16	2	1	0	3,68570	24,127	2,9
17	-2	-1	1	3,63261	24,485	1,4
18	2	0	4	3,60978	24,642	6,7
19	-2	-1	2	3,48613	25,531	13,9
20	1	0	6	3,36068	26,501	0,2
21	-2	-1	3	3,27701	27,191	3,5
22	3	0	0	3,25048	27,417	7,4
23	3	0	1	3,21389	27,735	0,6
24	3	0	2	3,11112	28,671	0,4
25	-1	-1	6	3,02097	29,545	2,6
26	3	0	3	2,95976	30,171	0,1
27	1	0	7	2,92707	30,516	0,2
28	2	0	6	2,88567	30,964	0,1
29	2	2	0	2,81500	31,762	1,2
30	3	0	4	2,78074	32,164	17,3
31	2	2	2	2,72302	32,865	0,8
32	3	1	0	2,70456	33,096	2,0
33	0	0	8	2,68500	33,344	4,0
34	3	1	2	2,62268	34,160	7,5
35	-2	-1	6	2,56800	34,911	20,4
36	-3	-1	3	2,53008	35,451	1,8
37	-2	-2	4	2,49321	35,993	2,0
38	4	0	0	2,43786	36,839	0,6
39	-1	-1	8	2,42350	37,065	1,7
40	-3	-1	4	2,41551	37,193	4,5
41	3	0	6	2,40652	37,337	2,4
42	4	0	2	2,37738	37,811	0,1
43	-2	-1	7	2,35824	38,130	0,7
44	2	0	8	2,35196	38,236	1,9
45	1	0	9	2,31824	38,814	0,4
46	4	0	3	2,30776	38,998	0,5
47	-3	-1	5	2,28877	39,334	0,2
48	3	2	0	2,23713	40,281	3,4
49	3	0	7	2,23135	40,390	2,2
50	-2	-2	6	2,21284	40,743	18,7
51	-3	-2	2	2,19013	41,184	2,3
52	-3	-1	6	2,15798	41,827	9,8
53	-3	-2	3	2,13533	42,291	1,6
54	4	1	0	2,12794	42,445	2,2
55	4	0	5	2,12026	42,607	1,2
56	1	0	10	2,09771	43,087	0,2
57	-4	-1	2	2,08736	43,312	1,3
58	-3	-2	4	2,06510	43,803	2,3
59	-4	-1	3	2,03976	44,375	0,2
60	-3	-1	7	2,02897	44,624	0,2
61	-1	-1	10	2,00690	45,142	0,7

62	-2	-1	9	2,00333	45,227	0,5
63	-3	-2	5	1,98422	45,687	0,5
64	-4	-1	4	1,97828	45,832	1,4
65	2	0	10	1,96570	46,142	0,1
66	5	0	0	1,95029	46,528	4,7
67	3	0	9	1,92378	47,208	0,2
68	5	0	2	1,91891	47,335	0,2
69	1	0	11	1,91471	47,445	0,2
70	-3	-1	8	1,90546	47,689	0,9
71	-3	-2	6	1,89717	47,911	0,5
72	5	0	3	1,88173	48,329	0,3
73	3	3	0	1,87667	48,468	0,7
74	-2	-1	10	1,85583	49,047	3,8
75	-3	-3	2	1,84866	49,250	2,9
76	4	2	0	1,84285	49,416	1,5
77	5	0	4	1,83314	49,695	1,4
78	-4	-1	6	1,82920	49,810	0,9
79	-4	-2	2	1,81631	50,188	1,5
80	2	0	11	1,81275	50,293	0,9
81	-3	-2	7	1,80772	50,443	0,6
82	4	0	8	1,80489	50,527	0,9
83	0	0	12	1,79000	50,978	1,4
84	-4	-2	3	1,78468	51,141	0,9
85	-3	-3	4	1,77160	51,546	2,2
86	1	0	12	1,76058	51,892	1,5
87	5	1	0	1,75141	52,184	0,9
88	-4	-1	7	1,74863	52,274	0,5
89	-5	-1	2	1,72858	52,927	0,8
90	-2	-1	11	1,72551	53,028	0,5
91	-3	-2	8	1,71873	53,254	0,1
92	1	1	12	1,70586	53,688	1,8
93	-5	-1	3	1,70125	53,845	1,3
94	4	2	5	1,69360	54,108	0,1
95	3	1	10	1,68204	54,511	2,8
96	-4	-1	8	1,66770	55,019	5,5
97	-5	-1	4	1,66509	55,112	3,5
98	5	0	7	1,64598	55,808	0,1
99	-4	-2	6	1,63851	56,084	0,2
100	6	0	0	1,62524	56,583	3,5
101	5	1	5	1,62181	56,714	1,9
102	-2	-1	12	1,61015	57,162	0,3
103	6	0	2	1,60695	57,287	0,2
104	4	3	0	1,60313	57,436	0,9
105	-4	-3	1	1,59868	57,611	0,5
106	-4	-3	2	1,58556	58,133	1,2
107	5	0	8	1,57795	58,440	2,5
108	-5	-1	6	1,57323	58,632	1,3
109	3	0	12	1,56797	58,848	0,5
110	-4	-3	3	1,56439	58,996	0,6
111	5	2	0	1,56148	59,117	0,4
112	-5	-2	1	1,55737	59,289	0,2
113	6	0	4	1,55556	59,365	0,2
114	-3	-2	10	1,54942	59,624	0,2
115	-5	-2	2	1,54523	59,802	0,5
116	-4	-3	4	1,53614	60,192	0,2
117	4	0	11	1,52408	60,718	0,2
118	-4	-2	8	1,51940	60,925	0,7
119	1	0	14	1,51564	61,093	0,4
120	-2	-2	12	1,51049	61,323	2,2
121	-2	-1	13	1,50773	61,448	1,2
122	-5	-2	4	1,49938	61,827	0,9

123	-3	-1	12	1,49268	62,136	0,5
124	6	1	0	1,48708	62,396	0,2
125	-6	-1	1	1,48353	62,562	0,1
126	1	1	14	1,48030	62,714	0,2
127	-3	-2	11	1,47113	63,150	0,3
128	-5	-1	8	1,46692	63,352	0,7
129	4	3	6	1,46313	63,535	1,0

Stick Pattern



LARNITA

Name and formula

Reference code:	01-077-0388
Mineral name:	Larnite
ICSD name:	Calcium Silicate
Empirical formula:	Ca ₂ O ₄ Si
Chemical formula:	Ca ₂ SiO ₄

Crystallographic parameters

Crystal system:	Monoclinic
Space group:	P21/n
Space group number:	14
a (Å):	5,5100
b (Å):	6,7600
c (Å):	9,3200
Alpha (°):	90,0000
Beta (°):	94,5000
Gamma (°):	90,0000
Calculated density (g/cm ³):	3,29
Volume of cell (10 ⁶ pm ³):	346,08
Z:	4,00
RIR:	0,72

Status, subfiles and quality

Status:	Marked as deleted by ICDD
Subfiles:	Inorganic Mineral Modelled additional pattern
Quality:	Calculated (C)

Comments

Additional pattern:	See PDF 33-302.
ICSD collection code:	039006
Test from ICSD:	At least one TF missing. Charge sum slightly deviates from zero.

References

Primary reference:	<i>Calculated from ICSD using POWD-12++, (1997)</i>
Structure:	Udagawa, S., Urabe, K., <i>Semento Gijutsu Nempo</i> , 32 , 35, (1978)

Peak list

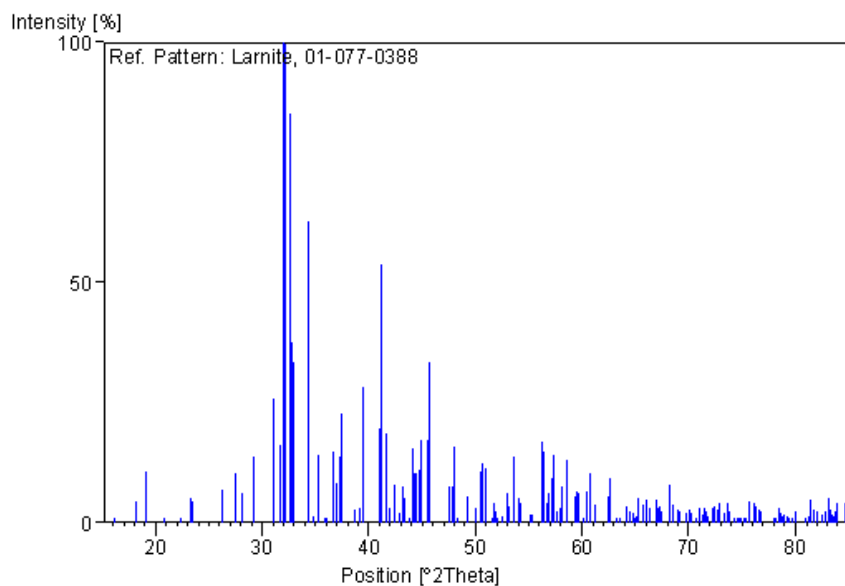
No.	h	k	l	d [Å]	2Theta[deg]	I [%]
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1	0	1	1	5,46630	16,202	0,1
2	-1	0	1	4,89989	18,090	4,4
3	0	0	2	4,64564	19,089	10,7
4	1	1	0	4,26305	20,820	1,0
5	-1	1	1	3,96731	22,392	0,2
6	0	1	2	3,82869	23,213	5,0
7	1	1	1	3,78822	23,465	4,3
8	0	2	0	3,38000	26,347	6,8
9	-1	1	2	3,24083	27,500	10,2
10	0	2	1	3,17635	28,070	6,0
11	1	1	2	3,04984	29,259	13,8
12	1	2	0	2,87868	31,042	25,9
13	0	1	3	2,81565	31,755	16,0
14	-1	0	3	2,79321	32,017	100,0
15	-1	2	1	2,78226	32,146	99,9
16	2	0	0	2,74651	32,576	85,3
17	0	2	2	2,73315	32,740	37,4
18	1	2	1	2,71831	32,923	33,4
19	1	0	3	2,61158	34,310	62,8
20	-1	1	3	2,58151	34,722	1,2
21	2	1	0	2,54451	35,243	14,2
22	-2	1	1	2,50090	35,879	0,9
23	-1	2	2	2,49331	35,992	0,8
24	-2	0	2	2,44995	36,651	14,8
25	1	1	3	2,43611	36,867	8,1
26	2	1	1	2,40993	37,282	13,8
27	1	2	2	2,40314	37,391	22,7
28	0	0	4	2,32282	38,735	2,7
29	-2	1	2	2,30334	39,075	3,2
30	2	0	2	2,28345	39,430	28,3
31	0	1	4	2,19675	41,055	19,7
32	0	3	1	2,18985	41,190	53,8
33	2	1	2	2,16633	41,658	18,6
34	-1	2	3	2,15313	41,925	3,0
35	2	2	0	2,13152	42,371	7,8
36	-2	2	1	2,10569	42,916	1,9
37	-1	1	4	2,09396	43,168	7,4
38	1	3	0	2,08474	43,369	5,1
39	1	2	3	2,06658	43,770	0,7
40	2	2	1	2,05052	44,130	15,4
41	-1	3	1	2,04723	44,205	10,3
42	-2	1	3	2,04015	44,367	10,3
43	0	3	2	2,02743	44,660	10,9
44	1	3	1	2,02135	44,801	17,2
45	1	1	4	1,98943	45,560	17,2
46	-2	2	2	1,98366	45,700	33,3
47	0	2	4	1,91435	47,454	7,6
48	2	1	3	1,89951	47,848	7,6
49	2	2	2	1,89411	47,993	15,7
50	1	3	2	1,88120	48,343	0,9
51	-2	0	4	1,84644	49,314	5,3
52	-3	0	1	1,82210	50,017	3,2
53	-2	2	3	1,80803	50,434	10,7
54	-1	0	5	1,80374	50,562	12,4
55	0	1	5	1,79179	50,923	11,3
56	1	2	4	1,77245	51,519	0,6
57	3	1	0	1,76732	51,680	4,2
58	-3	1	1	1,76084	51,884	2,5
59	-1	3	3	1,75380	52,108	0,6
60	-1	1	5	1,74277	52,463	1,2
61	-2	3	1	1,72787	52,950	6,3

62	1	0	5	1,71977	53,219	3,4
63	2	0	4	1,70796	53,616	13,9
64	2	3	1	1,69699	53,991	5,1
65	0	4	0	1,69000	54,233	4,1
66	0	4	1	1,66272	55,198	1,6
67	-2	3	2	1,65851	55,350	1,7
68	-3	0	3	1,63330	56,279	16,9
69	0	2	5	1,62838	56,465	14,8
70	-2	2	4	1,62042	56,767	4,0
71	1	4	0	1,61528	56,964	6,0
72	3	1	2	1,60995	57,170	9,2
73	2	3	2	1,60505	57,361	14,0
74	-1	4	1	1,59764	57,652	2,5
75	-1	2	5	1,59133	57,902	3,2
76	0	4	2	1,58818	58,028	7,6
77	1	4	1	1,58525	58,145	6,3
78	-1	3	4	1,57499	58,561	13,1
79	-2	1	5	1,55549	59,368	5,5
80	-2	3	3	1,55170	59,527	6,5
81	0	0	6	1,54854	59,661	6,0
82	-1	4	2	1,53672	60,167	0,7
83	1	3	4	1,52903	60,501	6,5
84	2	2	4	1,52463	60,694	10,3
85	1	4	2	1,51488	61,126	3,9
86	3	1	3	1,48705	62,397	5,3
87	-1	1	6	1,48351	62,563	9,1
88	-3	2	3	1,47060	63,175	0,1
89	-3	1	4	1,46082	63,647	0,9
90	2	1	5	1,45127	64,116	3,5
91	-1	4	3	1,44496	64,430	2,5
92	2	4	0	1,43934	64,712	2,0
93	0	3	5	1,43364	65,001	0,6
94	-2	4	1	1,43130	65,120	1,2
95	-2	3	4	1,42819	65,279	5,0
96	3	3	0	1,42102	65,650	1,7
97	1	4	3	1,41884	65,764	3,8
98	2	4	1	1,41361	66,038	4,8
99	-1	3	5	1,40783	66,344	3,1
100	-2	0	6	1,39660	66,947	4,8
101	3	3	1	1,39207	67,194	3,0
102	-2	4	2	1,39113	67,246	3,3
103	-1	2	6	1,38776	67,431	2,5
104	4	0	0	1,37325	68,241	8,0
105	-2	1	6	1,36772	68,555	3,7
106	2	3	4	1,36152	68,911	2,6
107	-3	0	5	1,35782	69,125	2,3
108	-4	0	2	1,34577	69,834	2,0
109	1	2	6	1,34094	70,122	2,6
110	0	5	1	1,33791	70,304	1,9
111	-3	1	5	1,33199	70,663	0,2
112	-2	4	3	1,32628	71,013	3,0
113	-3	3	3	1,32244	71,251	1,7
114	-4	1	2	1,32003	71,401	3,0
115	4	1	1	1,31757	71,555	2,2
116	-1	0	7	1,31394	71,783	1,4
117	2	0	6	1,30579	72,301	2,9
118	-2	3	5	1,30370	72,436	3,4
119	0	5	2	1,29814	72,796	2,7
120	1	5	1	1,29654	72,900	4,0
121	-2	2	6	1,29076	73,279	2,1
122	2	4	3	1,28523	73,646	4,2

123	3	2	4	1,28243	73,834	2,4
124	0	3	6	1,27623	74,253	0,4
125	-4	2	1	1,27299	74,474	0,5
126	-4	1	3	1,27050	74,644	0,3
127	1	0	7	1,26768	74,839	0,2
128	3	3	3	1,26274	75,182	0,4
129	-1	3	6	1,26123	75,288	0,7
130	3	0	5	1,25591	75,663	4,4
131	-4	2	2	1,25027	76,065	4,2
132	-3	3	4	1,24643	76,341	3,4
133	3	4	0	1,24187	76,672	2,6
134	-3	4	1	1,23962	76,837	2,4
135	-4	0	4	1,22497	77,928	0,8
136	3	4	1	1,22241	78,122	0,9
137	2	2	6	1,21805	78,455	3,2
138	-3	4	2	1,21600	78,613	2,1
139	-2	1	7	1,21356	78,802	1,2
140	-3	1	6	1,21105	78,997	1,7
141	-2	5	1	1,20810	79,228	1,4
142	-4	1	4	1,20534	79,445	1,0
143	4	1	3	1,20099	79,791	0,7
144	2	5	1	1,19748	80,072	2,3
145	-2	3	6	1,18695	80,929	0,7
146	3	4	2	1,18372	81,196	1,4
147	3	3	4	1,18060	81,455	4,9
148	3	2	5	1,17727	81,735	2,7
149	-3	4	3	1,17445	81,973	2,4
150	0	5	4	1,16848	82,483	1,7
151	2	5	2	1,16383	82,885	2,5
152	0	0	8	1,16141	83,096	5,2
153	-2	2	7	1,15883	83,322	2,6
154	-3	2	6	1,15664	83,515	1,7
155	-4	3	2	1,15550	83,616	1,4
156	4	3	1	1,15385	83,763	2,2
157	-1	5	4	1,15167	83,957	4,0
158	0	3	7	1,14366	84,682	4,2

Stick Pattern



6.- Fichas de los componentes de la pasta de cemento portland de 2 años de edad.

CALCITA

Name and formula

Reference code:	00-005-0586
Mineral name:	Calcite, syn
PDF index name:	Calcium Carbonate
Empirical formula:	CCaO ₃
Chemical formula:	CaCO ₃

Crystallographic parameters

Crystal system:	Rhombohedral
Space group:	R-3c
Space group number:	167
a (Å):	4,9890
b (Å):	4,9890
c (Å):	17,0620
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,71
Measured density (g/cm ³):	2,71
Volume of cell (10 ⁶ pm ³):	367,78
Z:	6,00
RIR:	2,00

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Educational pattern Forensic NBS pattern Pharmaceutical Superconducting Material
Quality:	Star (S)

Comments

Color:	Colorless
General comments:	Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G., North Dakota State Univ., Fargo, North Dakota, USA, <i>ICDD Grant-in-Aid</i>

(1992).
 Agrees well with experimental and calculated patterns.
 Additional weak reflections [indicated by brackets] were observed.
 Sample source: Sample from Mallinckrodt Chemical Works.
 Analysis: Spectroscopic analysis: <0.1% Sr; <0.01% Ba; <0.001% Al, B, Cs, Cu, K, Mg, Na, Si, Sn; <0.0001% Ag, Cr, Fe, Li, Mn.
 Optical data: A=1.487, B=1.659, Sign=-
 Additional pattern: See ICSD 16710, 20179, 28827, 18164, 18165 and 18166 (PDF 72-1214 and 72-1937); ICSD 73446 (PDF 81-2027); ICSD 79673 (PDF 83-577); ICSD 79674 (PDF 83-578).
 Temperature: Pattern taken at 26 C.

References

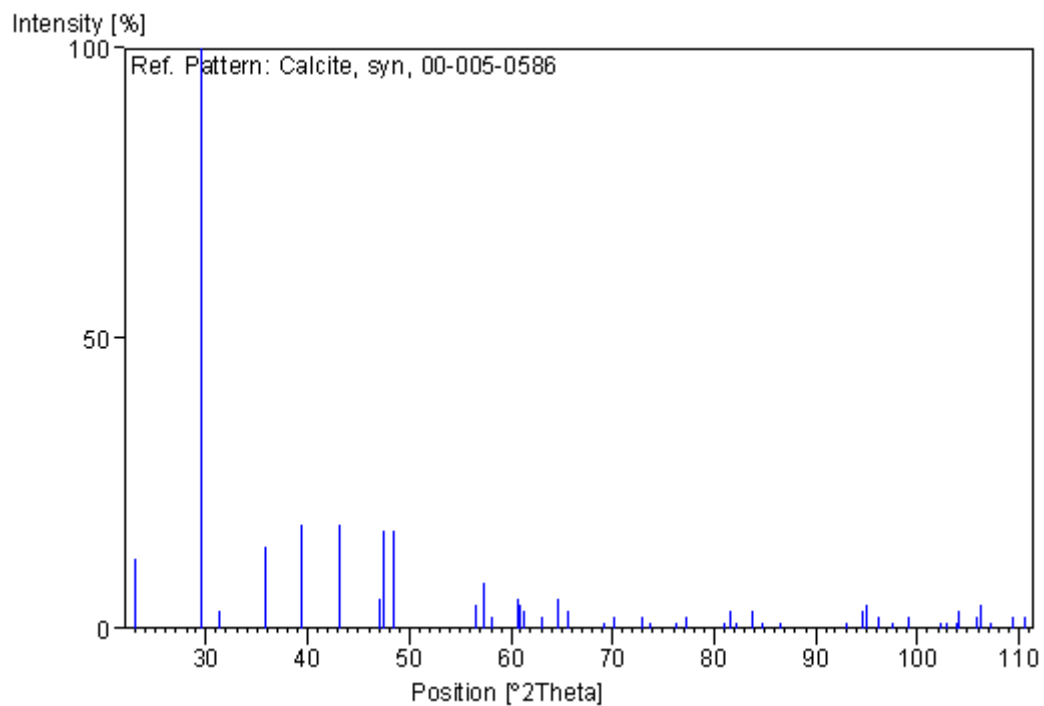
Primary reference: Swanson, Fuyat., *Natl. Bur. Stand. (U.S.), Circ. 539, II*, 51, (1953)
 Optical data: *Dana's System of Mineralogy, 7th Ed., II*, 142

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	1	2	3,86000	23,022	12,0
2	1	0	4	3,03500	29,406	100,0
3	0	0	6	2,84500	31,418	3,0
4	1	1	0	2,49500	35,966	14,0
5	1	1	3	2,28500	39,402	18,0
6	2	0	2	2,09500	43,146	18,0
7	0	2	4	1,92700	47,124	5,0
8	0	1	8	1,91300	47,490	17,0
9	1	1	6	1,87500	48,514	17,0
10	2	1	1	1,62600	56,555	4,0
11	1	2	2	1,60400	57,402	8,0
12	1	0	10	1,58700	58,075	2,0
13	2	1	4	1,52500	60,678	5,0
14	2	0	8	1,51800	60,987	4,0
15	1	1	9	1,51000	61,345	3,0
16	1	2	5	1,47300	63,060	2,0
17	3	0	0	1,44000	64,678	5,0
18	0	0	12	1,42200	65,599	3,0
19	2	1	7	1,35600	69,231	1,0
20	0	2	10	1,33900	70,238	2,0
21	1	2	8	1,29700	72,870	2,0
22	3	0	6	1,28400	73,729	1,0
23	2	2	0	1,24700	76,300	1,0
24	1	1	12	1,23500	77,177	2,0
25	3	1	2	1,18690	80,933	1,0
26	2	1	10	1,17950	81,547	3,0
27	0	1	14	1,17280	82,113	1,0
28	1	3	4	1,15380	83,767	3,0
29	2	2	6	1,14250	84,788	1,0
30	1	2	11	1,12440	86,483	1,0
31	2	0	14	1,06130	93,072	1,0
32	4	0	4	1,04730	94,701	3,0
33	3	1	8	1,04470	95,011	4,0
34	1	0	16	1,03520	96,165	2,0
35	2	1	13	1,02340	97,647	1,0
36	3	0	12	1,01180	99,161	2,0
37	3	2	1	0,98950	102,242	1,0
38	2	3	2	0,98460	102,952	1,0

39	1	3	10	0,97820	103,899	1,0
40	1	2	14	0,97670	104,124	3,0
41	3	2	4	0,96550	105,846	2,0
42	0	4	8	0,96360	106,145	4,0
43	0	2	16	0,95620	107,334	1,0
44	4	1	0	0,94290	109,561	2,0
45	2	2	12	0,93760	110,484	2,0

Stick Pattern



PORTLANDITA

Name and formula

Reference code:	00-044-1481
Mineral name:	Portlandite, syn
PDF index name:	Calcium Hydroxide
Empirical formula:	CaH ₂ O ₂
Chemical formula:	Ca (OH) ₂

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P-3m1
Space group number:	164
a (Å):	3,5899
b (Å):	3,5899
c (Å):	4,9160
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000
Calculated density (g/cm ³):	2,24
Volume of cell (10 ⁶ pm ³):	54,87
Z:	1,00
RIR:	2,90

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Forensic Pharmaceutical
Quality:	Star (S)

Comments

Deleted by:	Deleted by 4-733 which is satisfactory.
Color:	White
General comments:	Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2.2%.
Sample source:	Sample obtained from Sigma Chemical Co.
Optical data:	A=1.545, B=1.574, Sign=-
Additional pattern:	Validated by a calculated pattern.

References

Primary reference:	Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA., <i>ICDD Grant-in-Aid</i> , (1992)
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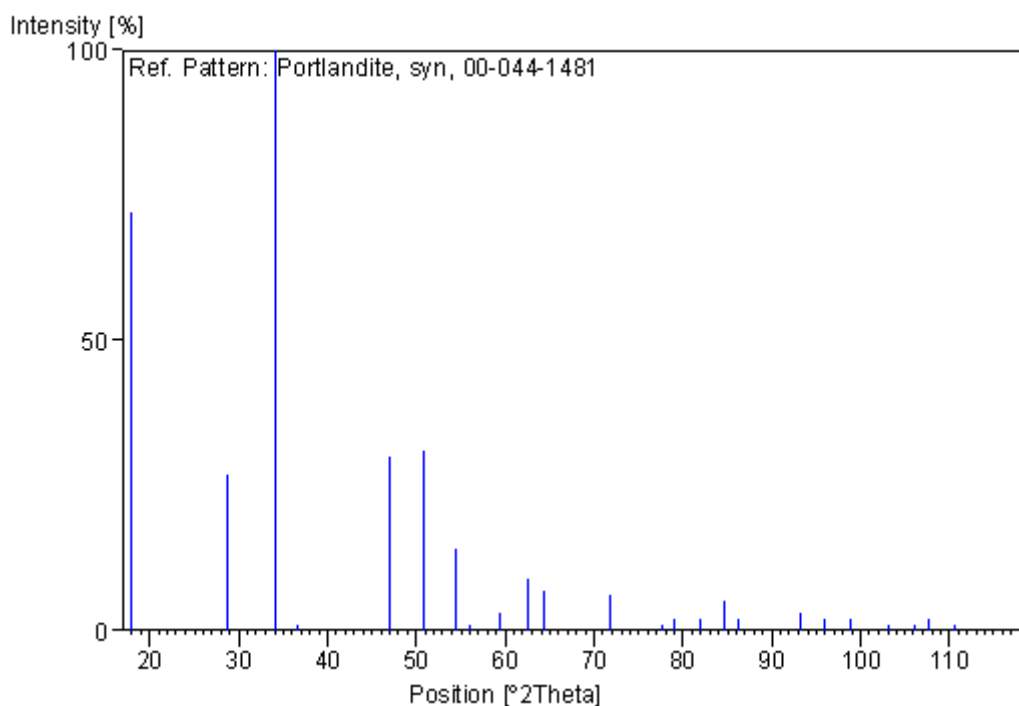
Optical data:

Winchell, A., Winchell, H., *Microscopic Character of Artificial Inorg. Solid Sub.*, 69, (1964)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	0	1	4,92200	18,008	72,0
2	1	0	0	3,11100	28,672	27,0
3	1	0	1	2,62700	34,102	100,0
4	0	0	2	2,45800	36,527	1,0
5	1	0	2	1,92710	47,121	30,0
6	1	1	0	1,79540	50,813	31,0
7	1	1	1	1,68640	54,358	14,0
8	0	0	3	1,63830	56,092	1,0
9	2	0	0	1,55410	59,426	3,0
10	2	0	1	1,48200	62,634	9,0
11	1	0	3	1,44890	64,233	7,0
12	2	0	2	1,31350	71,811	6,0
13	0	0	4	1,22860	77,654	1,0
14	1	1	3	1,20980	79,095	2,0
15	2	1	0	1,17520	81,910	2,0
16	1	0	4	1,14290	84,751	5,0
17	2	0	3	1,12740	86,197	2,0
18	2	1	2	1,06010	93,209	3,0
19	3	0	0	1,03630	96,030	2,0
20	1	1	4	1,01390	98,882	2,0
21	0	0	5	0,98330	103,143	1,0
22	2	0	4	0,96410	106,066	1,0
23	2	1	3	0,95470	107,579	2,0
24	1	0	5	0,93739	110,521	1,0
25	2	2	0	0,89740	118,268	1,0

Stick Pattern



ARAGONITA

Name and formula

Reference code:	00-041-1475
Mineral name:	Aragonite
PDF index name:	Calcium Carbonate
Empirical formula:	CCaO ₃
Chemical formula:	CaCO ₃

Crystallographic parameters

Crystal system:	Orthorhombic
Space group:	Pmcn
Space group number:	62
a (Å):	4,9623
b (Å):	7,9680
c (Å):	5,7439
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	90,0000
Calculated density (g/cm ³):	2,93
Measured density (g/cm ³):	2,95
Volume of cell (10 ⁶ pm ³):	227,11
Z:	4,00
RIR:	1,00

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Educational pattern Pharmaceutical Superconducting Material
Quality:	Star (S)

Comments

Color:	Colorless
General comments:	Optical data on specimen from Bilin, Bohemia, Czechoslovakia.
Sample source:	Specimen from Sefrou, Morocco.
Analysis:	Microprobe analyses (wt.%): major Ca, and trace Sr(<<1).
Optical data:	A=1.5300, B=1.6810, Q=1.6854, Sign=-, 2V=18(calc.)°
Additional pattern:	To replace 5-453 and validated by calculated pattern 24-25. See ICSD 15194 (PDF 71-2392); ICSD 34308 (PDF 76-606).

References

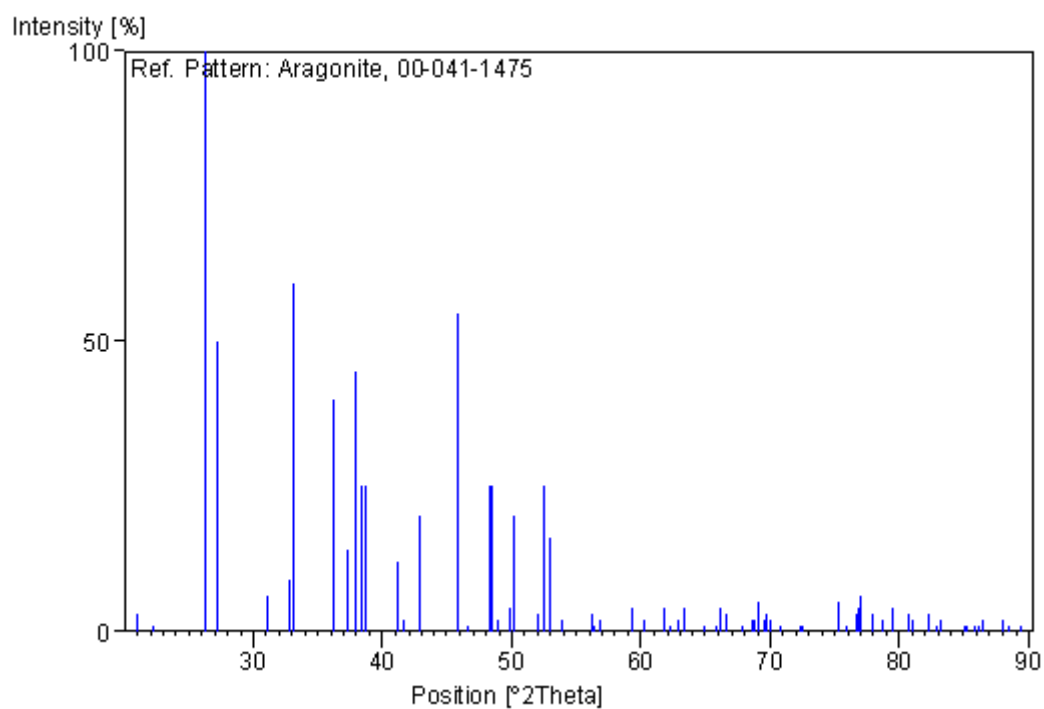
Primary reference: Keller, L., Rask, J., Buseck, P., Arizona State Univ., Tempe, AZ, USA., *ICDD Grant-in-Aid*, (1989)
 Structure: Jarosch, D., Heger, G., *Tschermaks Mineral. Petrogr. Mitt.*, **35**, 127, (1986)
 Optical data: *Dana's System of Mineralogy, 7th Ed.*, II, 182, (1951)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	1	0	4,21200	21,075	3,0
2	0	2	0	3,98400	22,297	1,0
3	1	1	1	3,39700	26,213	100,0
4	0	2	1	3,27400	27,216	50,0
5	0	0	2	2,87200	31,116	6,0
6	1	2	1	2,73300	32,741	9,0
7	0	1	2	2,70200	33,128	60,0
8	2	0	0	2,48100	36,176	40,0
9	0	3	1	2,41100	37,265	14,0
10	1	1	2	2,37300	37,884	45,0
11	1	3	0	2,34200	38,405	25,0
12	0	2	2	2,33000	38,610	25,0
13	2	1	1	2,19000	41,187	12,0
14	1	3	1	2,16800	41,624	2,0
15	1	2	2	2,10800	42,867	20,0
16	2	2	1	1,97740	45,853	55,0
17	0	3	2	1,95000	46,535	1,0
18	0	4	1	1,88210	48,319	25,0
19	2	0	2	1,87750	48,445	25,0
20	0	1	3	1,86160	48,886	2,0
21	2	1	2	1,82750	49,859	4,0
22	1	3	2	1,81490	50,229	20,0
23	1	4	1	1,75980	51,917	3,0
24	1	1	3	1,74300	52,455	25,0
25	2	3	1	1,72900	52,913	12,0
26	0	2	3	1,72570	53,022	16,0
27	2	2	2	1,69840	53,943	2,0
28	0	4	2	1,63690	56,145	3,0
29	1	2	3	1,63000	56,403	1,0
30	3	1	0	1,61980	56,791	2,0
31	3	1	1	1,55880	59,229	4,0
32	0	5	1	1,53570	60,211	2,0
33	2	4	1	1,49930	61,831	4,0
34	2	1	3	1,48910	62,302	1,0
35	3	2	1	1,47640	62,898	2,0
36	1	5	1	1,46720	63,338	4,0
37	0	0	4	1,43600	64,881	1,0
38	2	2	3	1,41670	65,876	1,0
39	0	1	4	1,41320	66,060	3,0
40	3	1	2	1,41070	66,192	4,0
41	3	3	0	1,40400	66,548	3,0
42	0	4	3	1,38040	67,839	1,0
43	2	4	2	1,36630	68,636	2,0
44	3	3	1	1,36390	68,774	2,0
45	1	1	4	1,35920	69,045	5,0
46	0	2	4	1,35070	69,542	2,0
47	3	2	2	1,34870	69,660	3,0
48	1	5	2	1,34160	70,082	2,0

49	1	4	3	1,32900	70,846	1,0
50	2	5	1	1,30580	72,301	1,0
51	1	2	4	1,30350	72,449	1,0
52	3	3	2	1,26150	75,269	5,0
53	1	6	1	1,25210	75,934	1,0
54	2	0	4	1,24270	76,612	3,0
55	4	0	0	1,24060	76,765	4,0
56	3	1	3	1,23650	77,066	6,0
57	0	5	3	1,22450	77,964	3,0
58	2	5	2	1,21490	78,698	2,0
59	2	4	3	1,20590	79,401	4,0
60	1	5	3	1,18900	80,760	3,0
61	2	2	4	1,18640	80,974	2,0
62	1	6	2	1,17110	82,258	3,0
63	0	4	4	1,16420	82,853	1,0
64	4	2	1	1,16000	83,219	2,0
65	4	0	2	1,13890	85,119	1,0
66	0	1	5	1,13700	85,295	1,0
67	3	3	3	1,13230	85,734	1,0
68	4	1	2	1,12740	86,197	1,0
69	2	3	4	1,12560	86,368	2,0
70	1	7	0	1,10890	87,999	2,0
71	0	2	5	1,10350	88,542	1,0
72	4	2	2	1,09500	89,412	1,0

Stick Pattern



VATERITA

Name and formula

Reference code:	01-072-0506
Mineral name:	Vaterite, syn
ICSD name:	Calcium Carbonate
Empirical formula:	CCaO ₃
Chemical formula:	CaCO ₃

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P63/mmc
Space group number:	194

a (Å):	4,1300
b (Å):	4,1300
c (Å):	8,4900
Alpha (°):	90,0000
Beta (°):	90,0000
Gamma (°):	120,0000

Calculated density (g/cm ³):	2,63
Measured density (g/cm ³):	2,60
Volume of cell (10 ⁶ pm ³):	125,41
Z:	2,00

RIR:	1,14
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Subfiles and Quality

Subfiles:	Inorganic Mineral Modelled additional pattern Pharmaceutical
Quality:	Calculated (C)

Comments

Sample preparation:	Prepared by ion diffusion for 4 days.
Additional pattern:	See PDF 33-268.
ICSD collection code:	015879
Test from ICSD:	Calc. density unusual but tolerable.

References

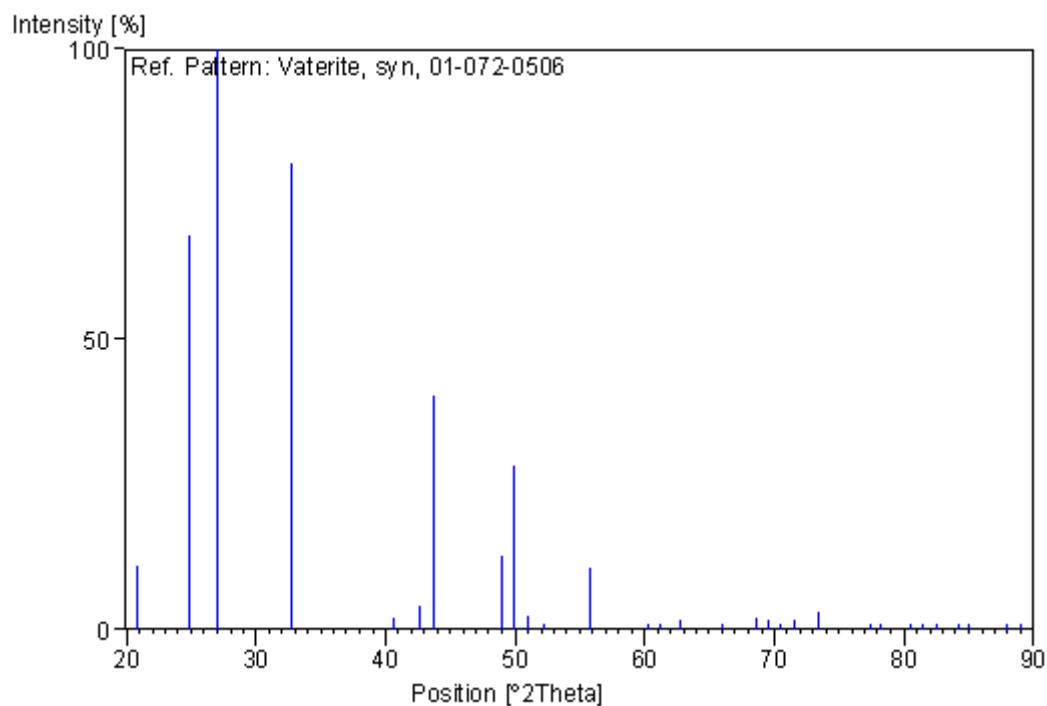
Primary reference:	<i>Calculated from ICSD using POWD-12++, (1997)</i>
Structure:	Kamhi, S.R., <i>Acta Crystallogr.</i> , 16 , 770, (1963)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
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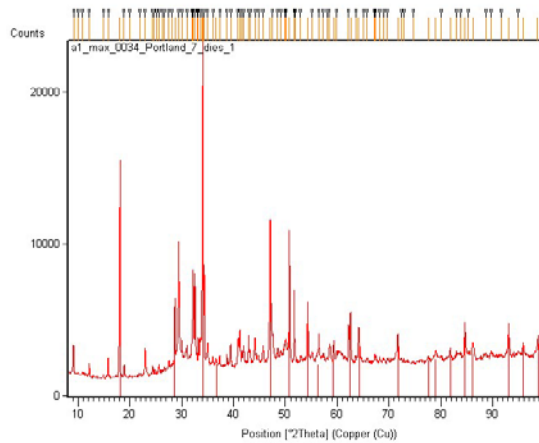
1	0	0	2	4,24500	20,910	10,9
2	1	0	0	3,57668	24,874	68,1
3	1	0	1	3,29613	27,030	100,0
4	1	0	2	2,73523	32,714	80,5
5	1	0	3	2,21932	40,619	1,9
6	0	0	4	2,12250	42,559	4,1
7	1	1	0	2,06500	43,805	40,2
8	1	1	2	1,85694	49,016	12,8
9	1	0	4	1,82530	49,923	28,1
10	2	0	0	1,78834	51,028	2,5
11	2	0	1	1,74994	52,232	0,5
12	2	0	2	1,64806	55,731	10,5
13	1	0	5	1,53392	60,288	0,1
14	2	0	3	1,51179	61,265	0,7
15	1	1	4	1,48009	62,724	1,5
16	0	0	6	1,41500	65,965	0,1
17	2	0	4	1,36761	68,561	2,1
18	2	1	0	1,35186	69,474	1,6
19	2	1	1	1,33504	70,478	0,6
20	1	0	6	1,31577	71,668	1,5
21	2	1	2	1,28812	73,454	3,2
22	2	0	5	1,23137	77,447	0,1
23	2	1	3	1,21983	78,319	0,1
24	3	0	0	1,19223	80,496	0,4
25	3	0	1	1,18064	81,452	0,1
26	1	1	6	1,16725	82,589	0,3
27	1	0	7	1,14782	84,304	0,6
28	2	1	4	1,14023	84,996	1,0
29	2	0	6	1,10966	87,923	0,5
30	3	0	3	1,09871	89,030	0,1

Stick Pattern

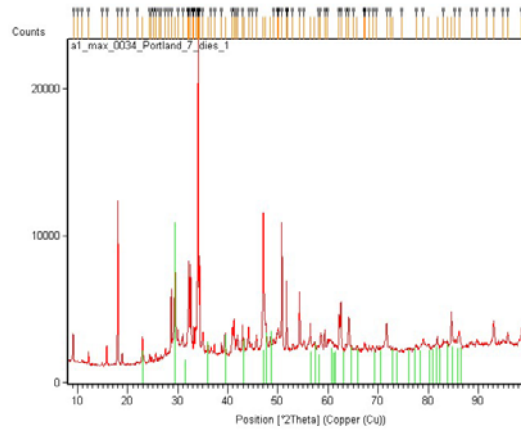


7.- ESQUEMAS DE INTERPRETACIÓN DE DIFRACTOGRAMA DE PASTA DE CEMENTO DE 7 DÍAS DE EDAD.

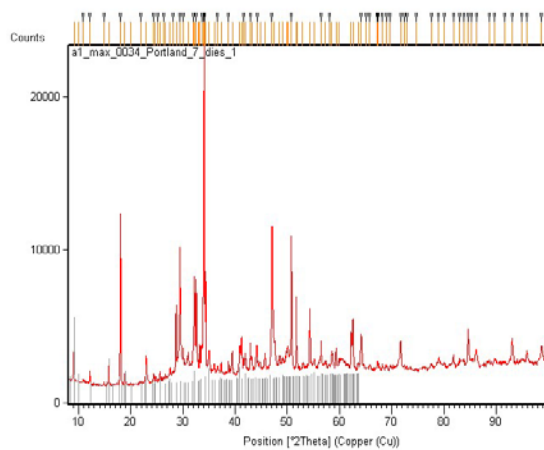
PORTLANDITA



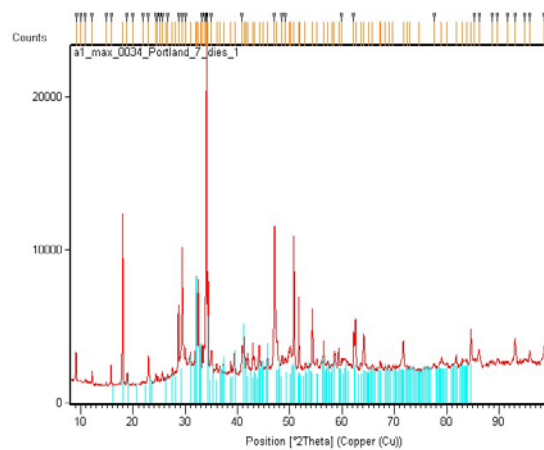
CALCITA



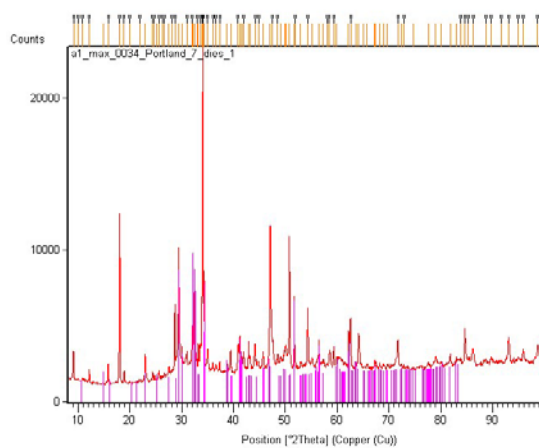
ETTRINGITA



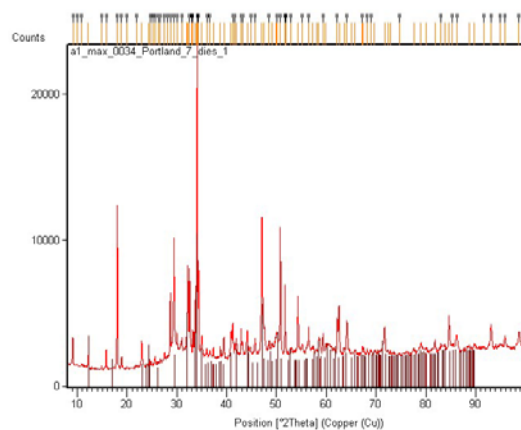
LARNITA



HATRURITA

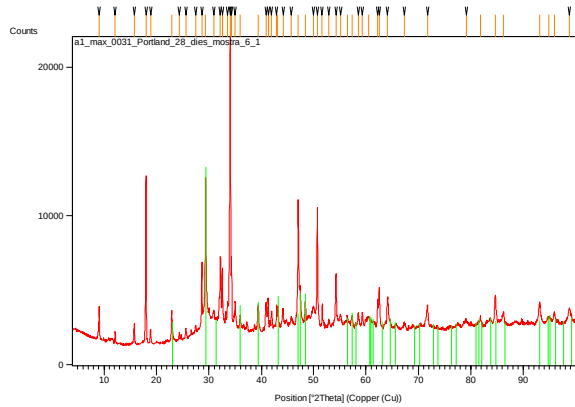


BROWNMILLERITA

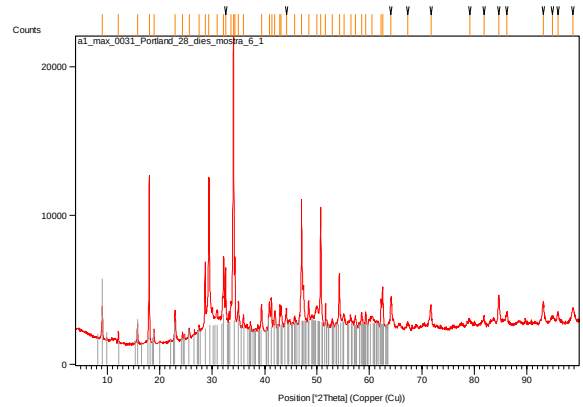


8.- ESQUEMAS DE INTERPRETACIÓN DE DIFRACTOGRAMA DE PASTA DE CEMENTO DE 28 DÍAS DE EDAD

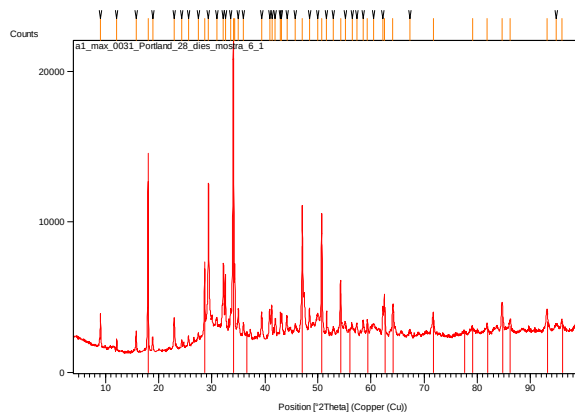
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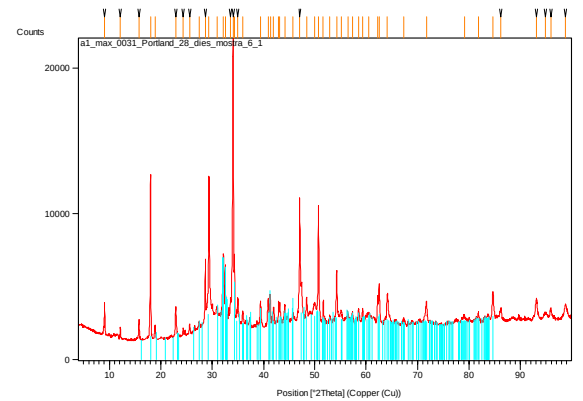
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PORTLANDITA

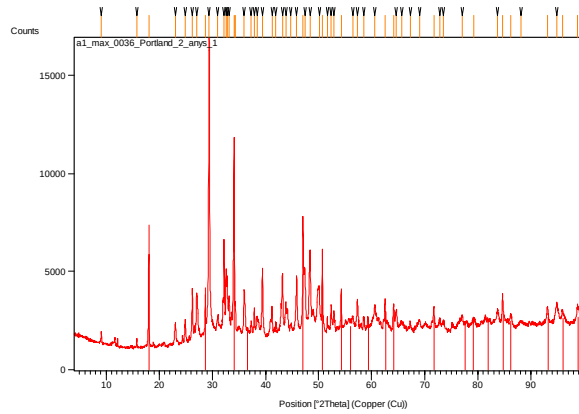


LARNITA

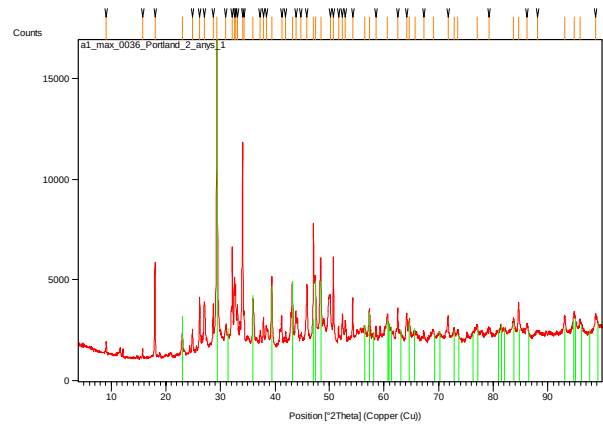


9.- ESQUEMAS DE INTERPRETACIÓN DE DIFRACTOGRAMA DE PASTA DE CEMENTO DE 2 AÑOS DE EDAD

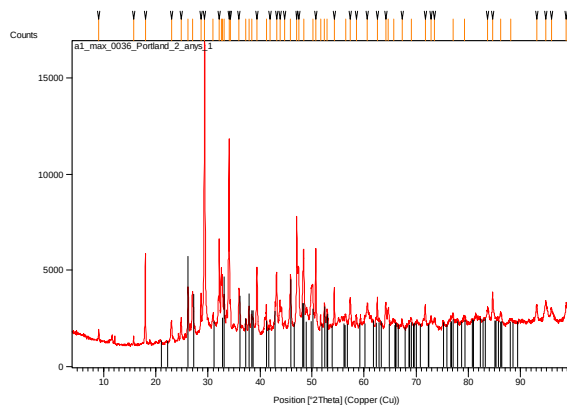
PORTLANDITA



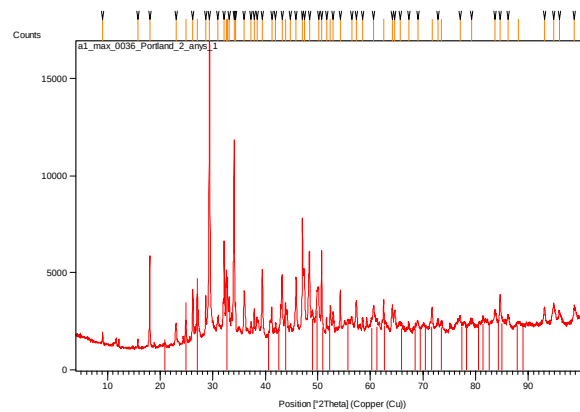
CALCITA



ARAGONITA



VATERITA



LARNITA

