05-0586 Quality: Quality Data

Ca C O3
Calcium Carbonate
Calcite, Syn

Rad:CuKa1 Lambda:1.5405 Filter:Beta filter used d sp:
Cutoff: Int: I/Icor:2
Ref:Swanson, Fuyat., II 51, (1953)

Sys:Rhombohedral S.G.:R-3c
a:4.989 b: c:17.062
α: β: γ: Z:6 mp
Ref2
Dx:2.711 Dm:2.711 SS/FOM: F30=57.1(0.0159,33) Volume[CD]:367.78

εα:1.487 ηω β:1.659 εγ: Sign:- 2V:
Ref3

Color:Colorless

Sample from Mallinckrodt Chemical Works. 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. Pattern taken at 26 C. Other form: aragonite. Pattern reviewed by Parks, J., McCarthy, G.,* North Dakota State Univ., Fargo, ND, USA, \ITICDD Grant-in-Aid\RG (1992). Agrees well with experimental and calculated patterns. Additional weak reflections [indicated by brackets] were observed.

45 reflections in pattern.

d A	Int.	h	k	l	d A	Int.	h	k	l	d A	Int.	h	k	l	d A	Int.	h	k	l
3.8600	12	0	1	2	1.5250	5	2	1	4	1.1869	1	3	1	2	0.9895	1	3	2	1
3.0350	100	1	0	4	1.5180	4	2	0	8	1.1795	3	2	1	10	0.9846	1	2	3	2
2.8450	3	0	0	6	1.5100	3	1	1	9	1.1728	1	0	1	14	0.9782	1	1	3	10
2.4950	14	1	1	0	1.4730	2	1	2	5	1.1538	3	1	3	4	0.9767	3	1	2	14
2.2850	18	1	1	3	1.4400	5	3	0	0	1.1425	1	2	2	6	0.9655	2	3	2	4
2.0950	18	2	0	2	1.4220	3	0	0	12	1.1244	1	1	2	11	0.9636	4	0	4	8
1.9270	5	0	2	4	1.3560	1	2	1	7	1.0613	1	2	0	14	0.9562	1	0	2	16
1.9130	17	0	1	8	1.3390	2	0	2	10	1.0473	3	4	0	4	0.9429	2	4	1	0
1.8750	17	1	1	6	1.2970	2	1	2	8	1.0447	4	3	1	8	0.9376	2	2	2	12
1.6260	4	2	1	1	1.2840	1	3	0	6	1.0352	2	1	0	16					
1.6040	8	1	2	2	1.2470	1	2	2	0	1.0234	1	2	1	13					
1.5870	2	1	0	10	1.2350	2	1	1	12	1.0118	2	3	0	12					

33-1161 Quality: Quality Data

SiO2
Silicon Oxide
Quartz, Syn

Rad:CuKa1 Lambda:1.540598 Filter:Monochromator crystal used d sp:Diffractometer
Cutoff: Int:Diffractometer I/Icor:3.6
Ref:Swanson, Fuyat., 18 61, (1981)

Sys:Hexagonal S.G.:P3221
a:4.9133±0.0002 b: c:5.4053±0.0004
α: β: γ: Z:3 mp
Ref2
Dx:2.649 Dm:2.649 SS/FOM: F30=76.6(0.0126,31) Volume[CD]:113

εα: ηω β:1.544 εγ:1.553 Sign:+ 2V:
Ref3

Color:Colorless

Sample from the Glass Section at NBS, Gaithersburg, MD, USA, ground single-crystals of optical quality. To replace 5-490 and validated by calculated pattern. Plus 6 additional reflections to 0.9089. Pattern taken at 25 C. Pattern reviewed by Holzer, J., McCarthy, G., North Dakota State Univ., Fargo, ND, USA, \ITICDD Grant-in-Aid\RG (1990). Agrees well with experimental and calculated patterns. Deleted by 46-1045, higher F#N, more complete, LRB 1/95.

39 reflections in pattern.

d A	Int.	h	k	l	d A	Int.	h	k	l	d A	Int.	h	k	l	d A	Int.	h	k	l
4.2570	22	1	0	0	1.6591	2	1	0	3	1.2285	1	2	2	0	1.0476	1	1	0	5
3.3420	100	1	0	1	1.6082	1	2	1	0	1.1999	2	2	1	3	1.0438	1	4	0	1
2.4570	8	1	1	0	1.5418	9	2	1	1	1.1978	1	2	2	1	1.0347	1	2	1	4
2.2820	8	1	0	2	1.4536	1	1	1	3	1.1843	3	1	1	4	1.0150	1	2	2	3
2.2370	4	1	1	1	1.4189	1	3	0	0	1.1804	3	3	1	0	0.9898	1	4	0	2
2.1270	6	2	0	0	1.3820	6	2	1	2	1.1532	1	3	1	1	0.9873	1	3	1	3
1.9792	4	2	0	1	1.3752	7	2	0	3	1.1405	1	2	0	4	0.9783	1	3	0	4
1.8179	14	1	1	2	1.3718	8	3	0	1	1.1143	1	3	0	3	0.9762	1	3	2	0
1.8021	1	0	0	3	1.2880	2	1	0	4	1.0813	2	3	1	2	0.9636	1	2	0	5
1.6719	4	2	0	2	1.2558	2	3	0	2	1.0635	1	4	0	0					