

Name and formula

Reference code: 01-089-1305

Mineral name: Calcite, magnesium, syn
ICSD name: Magnesium Calcium Carbonate

Empirical formula: $\text{CCa}_{0.94}\text{Mg}_{0.06}\text{O}_3$
Chemical formula: $(\text{Mg}_{0.06}\text{Ca}_{0.94})(\text{CO}_3)$

Crystallographic parameters

Crystal system: Rhombohedral
Space group: R-3c
Space group number: 167

a (Å): 4.9630
b (Å): 4.9630
c (Å): 16.9570
Alpha (°): 90.0000
Beta (°): 90.0000
Gamma (°): 120.0000

Calculated density (g/cm³): 2.73
Volume of cell (10⁶ pm³): 361.72
Z: 6.00

RIR: 3.07

Subfiles and Quality

Subfiles: Inorganic
Mineral
ICSD Pattern

Quality: Calculated (C)

Comments

Analysis: (Mg0.055 Ca0.945) C O3
Additional pattern: See PDF 00-043-0697.
ICSD collection code: 086162

References

Primary reference: *Calculated from ICSD using POWD-12++*
Structure: Falini, G., Fermani, S., Gazzano, M., Ripamonti, A., *J. Mater. Chem.* **8**, 1061, (1998)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	1	2	3.83362	23.183	9.3
2	1	0	4	3.01819	29.573	100.0
3	0	0	6	2.82616	31.633	2.1
4	1	1	0	2.48150	36.169	13.6
5	1	1	3	2.27217	39.634	17.6

6	2	0	2	2.08317	43.403	14.5
7	0	2	4	1.91681	47.390	6.2
8	0	1	8	1.90103	47.807	18.1
9	1	1	6	1.86470	48.799	18.9
10	2	1	1	1.61712	56.893	2.9
11	1	2	2	1.59550	57.736	8.2
12	1	0	10	1.57738	58.463	1.0
13	2	1	4	1.51695	61.034	4.8
14	2	0	8	1.50909	61.386	2.1
15	1	1	9	1.50059	61.772	2.2
16	1	2	5	1.46511	63.439	1.8
17	3	0	0	1.43269	65.049	5.4
18	0	0	12	1.41308	66.066	2.9
19	2	1	7	1.34922	69.629	1.0
20	0	2	10	1.33120	70.711	1.7
21	1	2	8	1.28938	73.371	2.5
22	3	0	6	1.27787	74.141	0.6
23	2	2	0	1.24075	76.754	1.0
24	1	1	12	1.22795	77.703	1.7
25	2	2	3	1.21190	78.931	0.1
26	1	3	1	1.18914	80.749	0.1
27	3	1	2	1.18046	81.467	0.4
28	2	1	10	1.17307	82.090	1.9
29	0	1	14	1.16581	82.713	0.3
30	1	3	4	1.14757	84.326	3.5
31	2	2	6	1.13609	85.379	1.5
32	3	1	5	1.12462	86.462	0.1
33	1	2	11	1.11822	87.080	0.4

Stick Pattern



