

Name and formula

Reference code: 01-085-0798

Mineral name: Quartz
ICSD name: Silicon Oxide

Empirical formula: O_2Si
Chemical formula: SiO_2

Crystallographic parameters

Crystal system: Hexagonal
Space group: P3221
Space group number: 154

a (Å): 4.9140
b (Å): 4.9140
c (Å): 5.4050
Alpha (°): 90.0000
Beta (°): 90.0000
Gamma (°): 120.0000

Calculated density (g/cm³): 2.65
Volume of cell (10⁶ pm³): 113.03
Z: 3.00

RIR: 3.34

Subfiles and Quality

Subfiles: Inorganic
Mineral
Alloy, metal or intermetallic
Corrosion
Pharmaceutical
ICSD Pattern

Quality: Calculated (C)

Comments

Additional pattern: See PDF 01-078-2315, PDF 00-033-1161 and PDF 00-046-1045.
ICSD collection code: 027834
Test from ICSD: At least one TF missing.

References

Primary reference: *Calculated from ICSD using POWD-12++*, (1997)
Structure: Young, R.A., Mackie, P.E., von Dreele, R.B., *J. Appl. Crystallogr.* **10**, 262, (1977)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	1	0	0	4.25565	20.857	11.8
2	0	1	1	3.34363	26.639	100.0

3	1	1	0	2.45700	36.542	7.3
4	1	0	2	2.28136	39.467	7.6
5	1	1	-1	2.23674	40.289	1.8
6	2	0	0	2.12782	42.448	2.5
7	0	2	1	1.97992	45.792	1.4
8	1	1	-2	1.81797	50.139	12.3
9	0	0	3	1.80167	50.624	0.3
10	0	2	2	1.67181	54.872	3.0
11	0	1	3	1.65911	55.328	1.2
12	2	1	0	1.60848	57.227	0.7
13	1	2	-1	1.54167	59.954	7.2
14	1	1	-3	1.45291	64.035	1.6
15	3	0	0	1.41855	65.779	0.2
16	2	1	-2	1.38219	67.739	2.7
17	2	0	3	1.37499	68.142	5.3
18	0	3	1	1.37208	68.307	4.9
19	1	0	4	1.28789	73.469	1.1
20	3	0	2	1.25603	75.654	2.1
21	2	2	0	1.22850	77.662	1.2
22	1	2	-3	1.19988	79.879	1.8
23	2	2	-1	1.19795	80.034	1.3
24	1	1	-4	1.18401	81.172	1.5
25	1	3	0	1.18030	81.480	2.5
26	3	1	-1	1.15313	83.827	0.9
27	2	0	4	1.14068	84.955	0.3
28	2	2	-2	1.11837	87.066	0.1
29	3	0	3	1.11454	87.440	0.1

Stick Pattern

