

Ca ₂ [SiO ₄]	<i>hP</i> 14	(186) <i>P6₃mc</i> – <i>cb</i> ³ <i>a</i>
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Ca₂SiO₄ α [1]; Na₂MnO₄ [2]

Structural features: Ca atoms and SiO₄ tetrahedra in a distorted Ni₂In-type (ht-Co₂Ge) arrangement. Derivative of α-K₂SO₄.

Eysel W., Hahn T. (1970) [1]

Ca₂O₄Si

a = 0.5419, *c* = 0.7022 nm, *c/a* = 1.296, *V* = 0.1786 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.83	0.17	0.25		single atom Si
Ca2	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.05		pseudo Frank-Kasper O ₁₃ Si ₄ Ca ₃
O3	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.44		single atom Si
Si4	2 <i>b</i>	3 <i>m</i> .	¹ / ₃	² / ₃	0.66		tetrahedron O ₄
Ca5	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		6-vertex polyhedron O ₆

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.5

Remarks: Phase stable at *T* > 1723 K. In [2] the Schoenflies symbol for the space group is misprinted as C_{6v}⁶ instead of C_{6v}⁴ and the occupancy of former O2 as 4 atoms per cell instead of 6 atoms per cell.

References: [1] Eysel W., Hahn T. (1970), *Z. Kristallogr.* 131, 322-341. [2] Kopelev N.S., Val'kovskii M.D., Popov A.I., Chumaevskii N.A. (1991), *Russ. J. Inorg. Chem.* 36, 1246-1250 (*Zh. Neorg. Khim.* 36, 2210-2216).