

$\text{Ca}_3\text{Ge}[\text{CO}_3]_{0.92}[\text{SO}_4]_{1.08}[\text{OH}]_6[\text{H}_2\text{O}]_{12}$	<i>hP</i> 68	(176) $P6_3/m - i^3h^3f^3b$
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**$\text{Ca}_3\text{Ge}(\text{OH})_6(\text{CO}_3)_{0.92}(\text{SO}_4)_{1.08} \cdot 12\text{H}_2\text{O}$**  [1], carraraite

Structural features: Units of three edge-linked  $\text{Ca}([\text{OH}]_4[\text{OH}_2]_4)$  square antiprisms share edges with  $\text{Ge}(\text{OH})_6$  octahedra to form infinite chains parallel to [001];  $\text{SO}_4$  tetrahedra and  $\text{CO}_3$  trigonal units (substitutional disorder) between the chains.

Merlino S., Orlandi P. (2001) [1]

$\text{C}_{0.92}\text{Ca}_3\text{GeH}_{30}\text{O}_{25.08}\text{S}_{1.08}$

$a = 1.1056$ ,  $c = 1.0629$  nm,  $c/a = 0.961$ ,  $V = 1.1252$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12i	1	0.1269	0.1349	0.111		single atom Ge
O2	12i	1	0.3461	0.0153	0.0705		single atom Ca
O3	12i	1	0.6224	0.196	0.0379		
Ca4	6h	m..	0.2098	0.0122	$\frac{1}{4}$		square antiprism O <sub>8</sub>
O5	6h	m..	0.2348	0.3985	$\frac{1}{4}$		single atom Ca
O6	6h	m..	0.4054	0.2593	$\frac{1}{4}$		single atom Ca
S7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.011	0.54	
O8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1473	0.54	single atom S
C9	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5379	0.46	
Ge10	2b	-3..	0	0	0		octahedron O <sub>6</sub>
H11	12i	1	0.068	0.36	0.055		
H12	12i	1	0.179	0.191	0.084		
H13	12i	1	0.424	0.276	0.178		
H14	12i	1	0.465	0.108	0.07		
H15	6h	m..	0.229	0.503	$\frac{1}{4}$		
H16	6h	m..	0.253	0.326	$\frac{1}{4}$		

Transformation from published data:  $y, x, -z$ ; origin shift  $0\ 0\ \frac{1}{2}$

Experimental: twinned crystal, diffractometer, X-rays, R = 0.094

Remarks: Natural specimen from Gioia quarry, Colonnata valley, Carrara basin, Apuan Alps, Italy. 35.70 wt.% CaO, 18.15 wt.% GeO<sub>2</sub>, and 16.19 wt.% SO<sub>3</sub> were found by electron microprobe analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Merlino S., Orlandi P. (2001), Am. Mineral. 86, 1293-1301.