

SiC	<i>hP</i> 12	(186) $P6_3mc - b^4a^2$
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**SiC 6H** [2], moissanite-6H, carborundum II, Strukturbericht notation B6; ZnS 6H [3]

Structural features: Close-packed Si layers in  $hc_2$  stacking; C in tetrahedral voids (same stacking position as the preceding Si layer).  $CSi_4$  tetrahedra share vertices to form a 3D-framework.

Gomes De Mesquita A.H. (1967) [1]

CSi

$a = 0.308065$ ,  $c = 1.511738$  nm,  $c/a = 4.907$ ,  $V = 0.1243$  nm<sup>3</sup>,  $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.20778		tetrahedron C <sub>4</sub>
C2	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.33298		tetrahedron Si <sub>4</sub>
Si3	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.54134		tetrahedron C <sub>4</sub>
C4	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.66647		tetrahedron Si <sub>4</sub>
C5	<i>2a</i>	<i>3m.</i>	0	0	0.00000		tetrahedron Si <sub>4</sub>
Si6	<i>2a</i>	<i>3m.</i>	0	0	0.37461		tetrahedron C <sub>4</sub>

Transformation from published data: origin shift 0 0 0.12539

Experimental: single crystal, diffractometer, X-rays,  $wR = 0.021$

Remarks: Zhdanov notation (33). Cell parameters from [4].

References: [1] Gomes De Mesquita A.H. (1967), Acta Crystallogr. 23, 610-617. [2] Ott H. (1931), Z. Kristallogr. 61, 515-531. [3] Frondel C., Palache C. (1948), Science (Washington D.C.) 107, 602. [4] Taylor A., Jones R.M. (1959), Proc. Conf. Silicon Carbide High Temp. Semicond., 1959, New York: Pergamon Press, p. 147.