

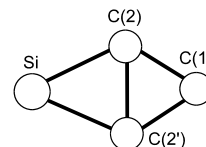
470  
MW $C_3Si$ 

Silicon tricarbonide

 $C_{2v}$  (ground electronic state)

$r_0$	Å
Si–C(2)	1.834(2)
C(1)–C(2)	1.435(2)
C(2)–C(2')	1.490(2)

The molecule has a closed-shell singlet electronic ground state and a planar rhomboidal geometry that consists of atoms in the shape of a distorted four-membered ring with a transannular carbon-carbon bond.



McCarthy, M.C., Apponi, A.J., Thaddeus, P.: J. Chem. Phys. **110** (1999) 10645.

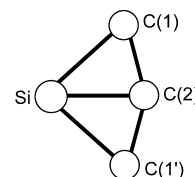
See also: Apponi, A.J., McCarthy, M.C., Gottlieb, C.A., Thaddeus, P.: J. Chem. Phys. **111** (1999) 3911.

MW

 $C_{2v}$  (first excited electronic state)

$r_0$	Å
Si–C(1) <sup>a)</sup>	2.022(1)
C(1)–C(2)	1.344(1)
Si–C(2) <sup>b)</sup>	1.893(1)

A second low-lying cyclic isomer, which is calculated to lie *ca.* 5 kcal mol<sup>−1</sup> (21 kJ mol<sup>−1</sup>) above the ground state rhomboid, is also a planar rhomboid with a transannular bond,  $C_{2v}$  symmetry, and a singlet electronic ground state. The transannular bond, however, is between the Si and the opposite C.



<sup>a)</sup> Peripheral bond.

<sup>b)</sup> Transannular bond.

McCarthy, M.C., Apponi, A.J., Thaddeus, P.: J. Chem. Phys. **111** (1999) 7175.