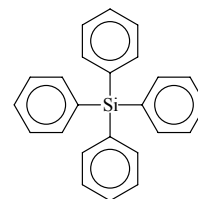


**948**      **C<sub>24</sub>H<sub>20</sub>Si**  
ED, *ab initio* and DFT  
calculations

**Tetraphenylsilane****S<sub>4</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
Si–C	1.881(4)	C(1)–Si–C(1')	108.6 <sup>b)</sup>
C–C <sup>c)</sup>	1.401(3)	C(1)–Si–C(1'')	109.9 <sup>d)</sup>
C(1)–C(2)	1.409 <sup>c)</sup>	C(2)–C(1)–C(6)	117.5 <sup>b)</sup>
C(2)–C(3)	1.397 <sup>c)</sup>	C(1)–C(2)–C(3)	121.4 <sup>d)</sup>
C(3)–C(4)	1.397 <sup>c)</sup>	C(2)–C(3)–C(4)	119.9 <sup>d)</sup>
C–H <sup>c)</sup>	1.102(3)	C(3)–C(4)–C(5)	119.9 <sup>d)</sup>
		$\tau^f$	40(2)
		$\varphi^g$	8(1)



The ED intensities from [1] were reanalyzed. Local C<sub>2v</sub> symmetry was assumed for the Si–C<sub>6</sub>H<sub>5</sub> groups. The bending of each phenyl group about the respective Si–C bond in a plane perpendicular to the plane of the ring was treated as a large-amplitude motion. The nozzle temperature was 573 K.

<sup>a)</sup> Estimated total errors.

including a systematic error.

<sup>b)</sup> Assumed at the value from B3LYP/6-31G\* calculations.

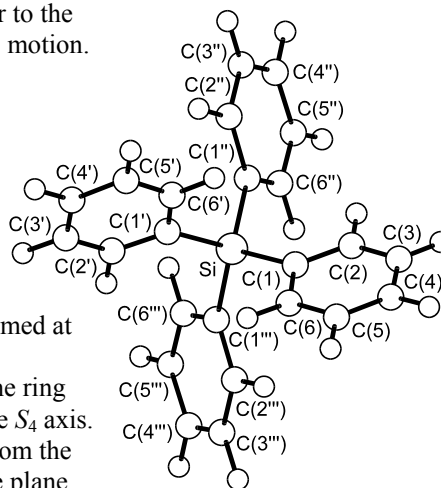
<sup>c)</sup> Average value.

<sup>d)</sup> Dependent parameter.

<sup>e)</sup> Differences in the C–C bond lengths were assumed at the values from B3LYP/6-31G\* calculations.

<sup>f)</sup> Dihedral angle between the plane of the benzene ring and the plane defined by the Si–C bond and the S<sub>4</sub> axis.

<sup>g)</sup> Effective bending angle of the Si–C(1) bond from the C(1) ... C(4) line in a plane perpendicular to the plane of the ring.



Campanelli, A.R., Ramondo, F., Domenicano, A., Hargittai, I.: J. Phys. Chem. A **105** (2001) 5933.

[1] Csákvári, É.; Shishkov, I.F.; Rozsondai, B.; Hargittai, I.: J. Mol. Struct. **239** (1990) 291.

Replaces [II/25D \(3, 2919\)](#)