

**814**      **C<sub>7</sub>H<sub>16</sub>Ge**ED, *ab initio*  
calculations**1,1,3,3-Tetramethylgermetane**

1,1,3,3-Tetramethylgermacyclobutane

**C<sub>s</sub>**, assumed

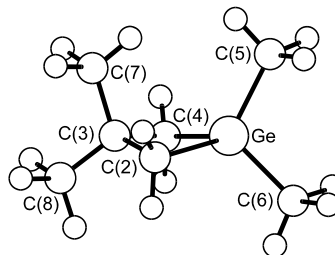
$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
Ge–C(2)	1.975(3)	C(2)–Ge–C(4)	75.3(2)
Ge–C(5)	1.959(3)	C(2)–Ge–C(5)	118.1(3)
Ge–C(6)	1.958(3)	C(2)–Ge–C(6)	116.8(3)
C(2)–C(3)	1.567(2)	C(5)–Ge–C(6)	108.8(8)
C(3)–C(7)	1.530(2)	Ge–C(2)–C(3)	89.5(2)
C(3)–C(8)	1.527(2)	C(2)–C(3)–C(4)	100.7(3)
C–H (mean)	1.111(2)	C(2)–C(3)–C(7)	109.9(3)
		C(2)–C(3)–C(8)	113.1(3)
		C(7)–C(3)–C(8)	109.9(10)
		Ge–C(5)–H	111.4(8)
		C–C–H	110.9 <sup>b)</sup>
		$\phi^c)$	24(2)

The differences between symmetry inequivalent Ge–C and C–C bond distances were assumed at the values from HF/6-31G\* calculations. The barrier to planarity of the ring was estimated to be  $V_0 = 4.2(8)$  kJ mol<sup>−1</sup> by the method of pseudoconformers. The nozzle temperature was 25 °C.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.

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

<sup>c)</sup> Ring puckering angle between the C(2)GeC(4) and C(2)C(3)C(4) planes.



Haaland, A., Samdal, S., Strand, T.G., Tafipolsky, M.A., Volden, H.V., van de Heisteeg, B.J.J., Akkerman, O.S., Bickelhaupt, F.: J. Organomet. Chem. **536-537** (1997) 217.