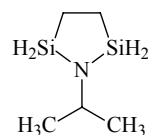


685 **C₅H₁₅NSi₂**ED, *ab initio*
calculations**1-(1-Methylethyl)-1-aza-2,5-disilacyclopentane**

1-Isopropyl-1-aza-2,5-disilacyclopentane

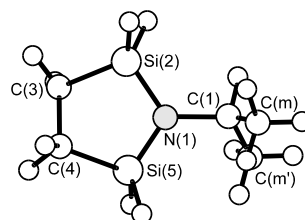
C₁

r_{α}	$\text{\AA}^a)$	θ_{α}	$\text{deg}^a)$
N(1)–Si(2)	1.721(3)	Si(2)–N(1)–Si(5)	111.8(4)
Si(2)–C(3)	1.868(4)	Si(2)–N(1)–C(1)	122.6(6)
C(3)–C(4)	1.528(9)	Si(5)–N(1)–C(1)	125.5(6)
C(4)–Si(5)	1.858(4)	N(1)–Si(2)–C(3)	102.8(5)
Si(5)–N(1)	1.720(3)	Si(2)–C(3)–C(4)	105.0(10)
N(1)–C(1)	1.458(4)	C(3)–C(4)–Si(5)	110.8(11)
C(1)–C(m)	1.504(6)	N(1)–Si(5)–C(4)	100.0(8)
C(1)–C(m')	1.502(4)	N(1)–C(1)–C(m)	112.3(8)
Si–H	1.460(3) ^{b)}	N(1)–C(1)–C(m')	112.7(8)
C–H	1.078(2)	N(1)–Si(2)–H	112.7(15)
		Si(2)–C(3)–H	106.7(13)
		C(1)–C(m)–H	110.0(10)
		N(1)–C(1)–H	107.3(16)
		C(m)–C(1)–C(m')	108.7(12)
		C(3)–Si(2)–N(1)–Si(5)	8.9(13)
		C(4)–Si(5)–N(1)–Si(2)	7.8(13)
		Si(2)–N(1)–C(1)–C(m)	93.3(32)
		Si(2)–N(1)–C(1)–C(m')	–122.5(15)
		Si(5)–N(1)–Si(2)–H	133.6(18)
		N(1)–Si(2)–C(3)–H	89.2(18)
		$\tau(\text{CH}_3)^c)$	–124.1(37)
		tilt(CH ₃) ^{d)}	–0.8(11)

Experimental data were augmented by restraints derived from MP2/6-31G* calculations.

The bond configuration at the ring nitrogen atom was found to be planar.

The nozzle temperature was 86 °C.

^{a)} Estimated standard errors.^{b)} Determined by gas-phase vibrational spectroscopy using the relationships between the stretching frequencies and the bond lengths.^{c)} Twist angle of the methyl groups from the staggered position with respect to the N–C bond.^{d)} Angle between the C₃ axis of the methyl group and the C(1)–C axis, positive value when the methyl groups are tilted away from one another.Mitzel, N.W., Schmidbaur, H., Rankin, D.W.H., Smart, B.A., Hofmann, M., Schleyer, P.v.R.: *Inorg. Chem.* **36** (1997) 4360.