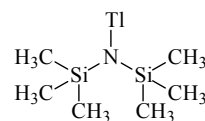
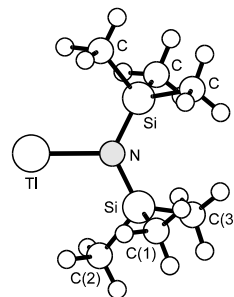


759 **C₆H₁₈NSi₂Tl**ED, *ab initio* and DFT
calculations**Thallium bis(trimethylsilyl)amide**1,1,1-Trimethyl-*N*-(trimethylsilyl)-
silanamine thallium salt**C₂ assumed**

r_a	Å ^{a)}	θ_a	deg ^{a)}
Tl–N	2.164(13)	Tl–N–Si	116.3(5)
Si–N	1.718(5)	Si–N–Si	127.4(9)
Si–C	1.873(3)	C–Si–C	101.6(10)
C–H	1.097(4)	N–Si–C(1)	116.7(10)
		N–Si–C(2)	114.9(10)
		N–Si–C(3)	118.0(10)
		Si–C–H	111.2 ^{b)}
		τ^c	23(2)
		tilt(Si(CH ₃) ₃) ^{d)}	1.8(11)

The Si(CH₃)₃ groups were assumed to have local C_{3v} symmetry with the C₃ axis lying in the TlNSi₂ plane and the methyl groups in staggered orientations. The nozzle temperature was 80(5) °C.



^{a)} Three times the estimated standard errors including a systematic error.

^{b)} Assumed at the value from DFT (BPW91) calculations.

^{c)} Torsional angle Tl–N–Si–C(2), zero degree for the *syn* position.

^{d)} Tilt angle of the Si(CH₃)₃ group between the symmetry axis of the Si(CH₃)₃ group and the Si–N bond, defined positive when it serves to increase the shorter distances between the methyl groups in different Si(CH₃)₃ fragments.

Haaland, A., Shorokhov, D.J., Volden, H.V., Klinkhammer, K.W.: Inorg. Chem. **38** (1999) 1118.