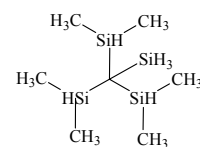


819 $C_7H_{24}Si_4$ ED, *ab initio*
calculations

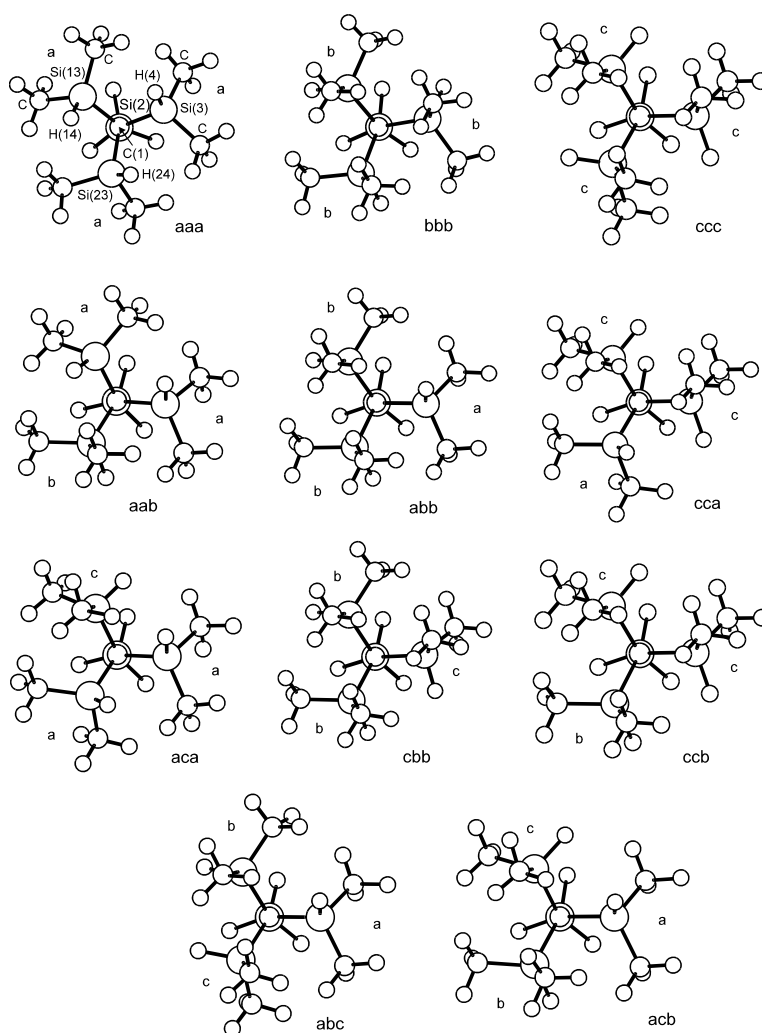
(Silylmethyldyne)tris(dimethylsilane)

Tris(dimethylsilyl)silylmethane

 C_3 (aaa) C_3 (bbb) C_3 (ccc) C_1 (eight remaining
conformers) (see comment)

$r_a^a)$	$\text{\AA}^b)$	$\theta_a^a)$	$\text{deg}^b)$
C–H	1.089(4)	Si–C–H (branch)	109.8(5)
Si–C (silyl, middle, branch) ^{c)}	1.884(1)	C(1)–Si–C (branch)	113.8(4)
$\Delta_1(\text{Si–C})^d)$	0.013(2)	C(1)–Si–H (branch)	106.4(9)
$\Delta_2(\text{Si–C})$ (branch – silyl)	0.005(2)	H–Si–C (branch)	107.1(7)
Si–H (branch, silyl) ^{c)}	1.502(12)	Si(2)–C(1)–Si (a, b, c)	107.0(6)
$\Delta(\text{Si–H})$ (branch – silyl)	0.010(5)	$\Delta_1[\text{Si}(2)–\text{C}(1)–\text{Si}]^e)$	1.6(4)
Si–C (silyl) ^{f)}	1.878(1)	$\Delta_2[\text{Si}(2)–\text{C}(1)–\text{Si}]$ (b – c)	–1.5(5)
Si–C (middle) ^{f)}	1.893(2)	Si(branch)–C–Si(branch) ^{c)}	109.9(9)
Si–C (branch) ^{f)}	1.883(1)	$\Delta_1[\text{Si–C}(1)–\text{Si}]^g)$	2.7(4)
Si–H (silyl) ^{f)}	1.497(12)	$\Delta_2[\text{Si–C}(1)–\text{Si}]^h)$	–2.6(5)
Si–H (branch) ^{f)}	1.508(12)	$\Delta_3[\text{Si–C}(1)–\text{Si}]$ (ab – bb)	0.7(5)
		$\Delta_4[\text{Si–C}(1)–\text{Si}]^i)$	1.8(5)
		$\Delta_5[\text{Si–C}(1)–\text{Si}]$ (cc – aa)	0.2(5)
		$\Delta_6[\text{Si–C}(1)–\text{Si}]$ (ac – bc)	0.9(5)
		C(1)–Si(2)–H	109.0(9)
		Si(2)–C(1)–Si ^{f)} (a)	108.1(6)
		Si(2)–C(1)–Si ^{f)} (b)	105.7(6)
		Si(2)–C(1)–Si ^{f)} (c)	107.2(6)
		Si–C(1)–Si ^{f)} (aa)	109.6(10)
		Si–C(1)–Si ^{f)} (ab)	110.3(10)
		Si–C(1)–Si ^{f)} (ac)	107.4(10)
		Si–C(1)–Si ^{f)} (bb)	111.0(10)
		Si–C(1)–Si ^{f)} (bc)	108.3(10)
		Si–C(1)–Si ^{f)} (cb)	113.2(10)
		Si–C(1)–Si ^{f)} (cc)	109.8(10)
		$\tau^j)$ (aaa)	158.7(18)
		$\tau^j)$ (bbb)	43.8(18)
		$\tau^j)$ (ccc)	–79.8(18)
		$\tau_1^k)$ (aab)	163.7(18)
		$\tau_2^l)$ (aab)	154.8(18)
		$\tau_3^m)$ (aab)	45.6(18)
		$\tau_1^k)$ (aca)	158.2(18)
		$\tau_2^l)$ (aca)	–76.5(18)
		$\tau_3^m)$ (aca)	161.2(18)
		$\tau_1^k)$ (abb)	163.4(18)
		$\tau_2^l)$ (abb)	43.2(18)
		$\tau_3^m)$ (abb)	44.8(18)
		$\tau_1^k)$ (cbb)	–78.0(18)
		$\tau_2^l)$ (cbb)	43.4(18)
		$\tau_3^m)$ (cbb)	40.7(18)
		$\tau_1^k)$ (cca)	–75.8(17)

τ_2^1) (cca)	-79.9(18)
τ_3^m) (cca)	164.4(18)
τ_1^k) (ccb)	-78.3(18)
τ_2^1) (ccb)	-79.6(18)
τ_3^m) (ccb)	40.4(17)
τ_1^k) (abc)	161.6(18)
τ_2^1) (abc)	39.7(18)
τ_3^m) (abc)	-77.4(18)
τ_1^k) (acb)	165.3(18)
τ_2^1) (acb)	-77.2(18)
τ_3^m) (acb)	43.3(18)
twist(SiH ₃) ⁿ)	-80.5(18)



The potential energy surface was studied by MP2/6-31G* and HF/6-31G* calculations. The minima were found to lie within a range of only *ca.* 3 kJ mol⁻¹, predicting that all eleven conformers, aaa (3%), bbb (4%), ccc (5%), aab (11%), aca (13%), abb (8%), cbb (9%), cca (16%), ccb (11%), acb (14%) and abc (6%), exist in the gas phase.

All eleven conformers were described in the ED analysis by just three different branch types a, b and c with Si(2)–C(1)–Si–H torsional angles of *ca.* 160°, 40° and –80°, respectively. Local C_{3v} symmetry was assumed for the CH₃ and SiH₃ groups. The groups were assumed to be perfectly staggered with respect to the H(4), H(14) and H(24) atoms. Some structural parameters or their differences were constrained to the values from MP2/6-31G* calculations. The nozzle temperature was *ca.* 373 K.

^a) silyl = $r[\text{Si}(2)\text{--C}]$, middle = $r[\text{Si}(3,13,23)\text{--C}]$, branch = $r[\text{Si--C}(\text{methyl})]$.

^b) Estimated standard errors.

^c) Average value.

^d) $[\text{middle} - (\text{branch, silyl})_{\text{average}}]$.

^e) $[a - (\text{b,c})_{\text{average}}]$.

^f) Dependent parameter.

^g) $[(\text{ab, bb, cb})_{\text{average}} - (\text{aa, ac, bc, cc})_{\text{average}}]$.

^h) $[(\text{ab, bb})_{\text{average}} - \text{cb}]$.

ⁱ) $[(\text{aa, cc})_{\text{average}} - (\text{ac, bc})_{\text{average}}]$.

^j) Torsional angle Si(2)–C(1)–Si–H.

^k) Torsional angle Si(2)–C(1)–Si(3)–H(4).

^l) Torsional angle Si(2)–C(1)–Si(13)–H(14).

^m) Torsional angle Si(2)–C(1)–Si(23)–H(24).

ⁿ) Torsional angle H–Si(2)–C(1)–Si from the *syn* position.

Morrison, C.A., Rankin, D.W.H., Robertson, H.E., Lickiss, P.D., Masangane, P.C.: J. Chem. Soc., Dalton Trans. (1999) 2293.