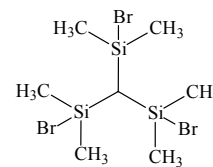


815 **C₇H₁₉Br₃Si₃**ED, *ab initio*
calculations**Methylidynetris(bromodimethylsilane)**

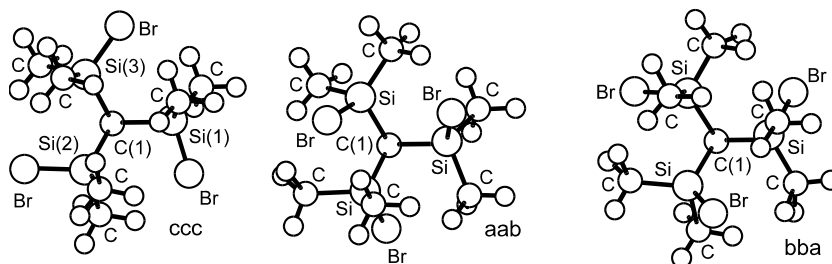
Tris(bromodimethylsilyl)methane

C₁ (ccc)**C₁ (aab)****C₁ (bba)**

| r_a | \AA^a | θ_a | deg^a |
|--------------|----------------|---------------------|-------------------------|
| C(1)–H | 1.089(10) | H–C(1)–Si | 104.6(7) |
| C–H (methyl) | 1.079(7) | Si–C–H(methyl) | 109.4(13) |
| Si–C(1) | 1.914(5) | C(1)–Si–C(methyl) | 109.1(9) ^{b)} |
| Si–C(methyl) | 1.889(5) | C(1)–Si–Br | 105.6(10) ^{b)} |
| Si–Br | 2.283(8) | Br–Si–C(methyl) | 102.5(13) ^{b)} |
| | | Si–C–Si (aa) | 119(3) |
| | | Si–C–Si (bb) | 110(3) |
| | | Si–C–Si (ba) | 115.2(12) |
| | | Si(1)–C–Si(2) (ccc) | 112.8(8) |
| | | Si(2)–C–Si(3) (ccc) | 114.6(9) |
| | | Si(3)–C–Si(1) (ccc) | 114.1(11) |
| | | τ^c (ccc) | –78(3) ^{b)} |
| | | τ_b^d (aab) | 40(3) |
| | | τ_a^d (aab) | 157(3) |
| | | τ_a^d (aab) | 160(3) |
| | | τ_b^d (bba) | 36(3) |
| | | τ_b^d (bba) | 48(3) |
| | | τ_a^d (bba) | 155(3) |



The potential energy surface was studied at HF/6-31G* and MP2/6-31G* levels. The minima of 11 conformers were found to lie within a range of 8.5 kJ mol^{–1}, predicting that three different conformers, ccc (76%), aab (9%) and bba (15%), may exist under conditions of the ED experiment. However, a satisfactory fit in the ED analysis could be obtained only by reducing the abundance of the ccc conformer to 33.3%, with the same weighting for aab and bba conformers. These conformers were described by three different branch types, a, b and c, with H–C(1)–Si–Br torsional angles of *ca.* 160, 40 and –80°, respectively. Local C_{3v} symmetry was assumed for the methyl groups. The H–C(1)–Si angle, the torsional angles involving hydrogen atoms and the differences in the C–H, Si–C, C(1)–Si–C(methyl), Br–Si–C and C(1)–Si–Br parameters were restrained to the values from MP2/6-31G* calculations. The nozzle temperature was 390 K.

^{a)} Estimated standard errors.^{b)} Average value.^{c)} Torsional angle H–C(1)–Si–Br from the *syn* position.^{d)} τ_a and τ_b are torsional angles H–C(1)–Si–Br in the a and b branches, respectively.

Morrison, C.A., Rankin, D.W.H., Robertson, H.E., Eaborn, C., Farook, A., Hitchcock, P.B., Smith, J.D.: J. Chem. Soc., Dalton Trans. (2000) 4312.