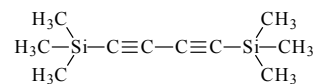


891 **C₁₀H₁₈Si₂**ED, *ab initio*
calculations**1,3-Butadiyne-1,4-diylbis(trimethylsilane)**

(see comment)

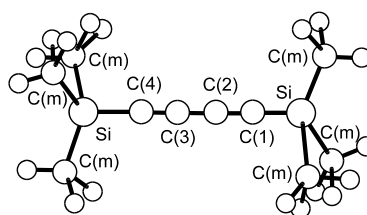
1,4-Bis(trimethylsilyl)-1,3-butadiyne



r_{hl} ^{a)}	Å ^{b)}	θ_{hl} ^{a)}	deg ^{b)}
Si-C(m)	1.875(1)	C(1,4)-Si-C(m)	107.8(3)
Si-C(1,4)	1.840(4)	Si-C-H ^{c)}	112.0(4)
C(1,3)≡C	1.236(2)		
C(2)-C(3)	1.373(3)		
C-H ^{c)}	1.113(2)		

The trimethylsilyl and the methyl groups were assumed to have local C_{3v} symmetry. Staggered conformation was assumed for the methyl groups. The nozzle temperature was 351 K.

According to the results of RHF/6-311G** calculations, the total energies of the D_{3d} and D_{3h} conformers differ by about 1 cal mol⁻¹, which implies virtually free internal rotation.



^{a)} Vibrational corrections were calculated taking into account the nonlinear relations between Cartesian and internal vibrational coordinates at the level of the first-order perturbation theory.

^{b)} Estimated standard errors.

^{c)} Average value.

Traetteberg, M., Khaikin, L.S., Grikina, O.E., Liebman, J.F., Hulce, M.: J. Mol. Struct. **559** (2001) 295.