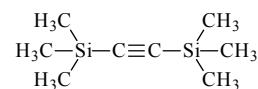


858 **C₈H₁₈Si₂**ED, *ab initio*
calculations**1,2-Ethynediylbis(trimethylsilane)**

Bis(trimethylsilyl)acetylene

(see comment)



$r_{\text{hl}}^{\text{a)}$	$\text{\AA}^{\text{b)}$	$\theta_{\text{hl}}^{\text{a)}$	$\text{deg}^{\text{b)}$
Si–C(m)	1.877(4)	C(1,2)–Si–C	109.2(2)
Si–C(1,2)	1.841(4)	C(m)–Si–C(m)	109.8(2)
C(1)≡C(2)	1.239(3)	Si–C–H	111.3(2) ^{c)}
C–H	1.108(3) ^{c)}	H–C–H	107.6(2) ^{c)}

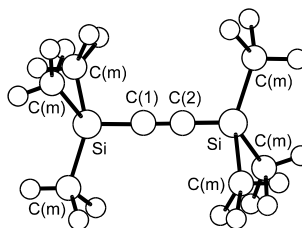
According to the results of *ab initio* (up to MP2/6-311G**) calculations [1], the energy difference between the D_{3d} and D_{3h} conformations of the molecule is less than 10 cal mol^{−1}, which implies virtually free internal rotation. Thus free internal rotation of the Si(CH₃)₃ groups about the linear Si–C≡C–Si fragment was described in the ED analysis using a one-dimensional dynamic model. It was assumed that the Si(CH₃)₃ groups have local C_{3v} symmetry and the methyl groups have the staggered conformation with respect to the Si–C(1,2) bonds. Nonlinear relations between Cartesian and internal vibrational coordinates at the first-order perturbation theory were used to obtain the so-called r_{hl} parameters, which are very close to r_{g} values in the case of bonded distances.

The nozzle temperature was 317...319 K.

^{a)} See comment for definition.

^{b)} 1.4 times the estimated standard errors including a systematic error.

^{c)} Average value.



Khaikin, L.S., Grikina, O.E., Sipachev, V.A., Belyakov, A.V., Bogoradovskii, E.T., Kolonits, M.: J. Mol. Struct. **523** (2000) 23.

[1] Sipachev, V.A., Khaikin, L.S., Grikina, O.E., Nikitin, V.S., Trætterberg, M.: J. Mol. Struct. **523** (2000) 1.

Replaces [II/25D \(3, 2618\)](#)