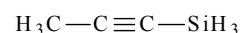


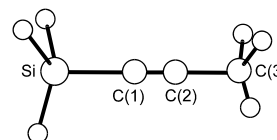
412 **C₃H₆Si**ED, *ab initio*
calculations**1-Propynylsilane**

1-Silabut-2-yne

(see comment)



$r_{\text{hl}}^{\text{a)}$	$\text{\AA}^{\text{b)}$
Si-C	1.814
C(1)≡C(2)	1.231
C(2)-C(3)	1.455
Si-H	1.534
C-H	1.065



The r_{a} parameters from a previous ED study [1] were converted to the r_{hl} values. According to the results of RHF/6-311G** and MP2/6-311G** calculations, the energy difference between the staggered and eclipsed conformations is less than 20 cal mol⁻¹, being evidence of virtually free internal rotation. The nozzle temperature was 298 K.

^{a)} Harmonic corrections were calculated taking into account nonlinear kinematic effects.

^{b)} Uncertainties were not estimated in the original paper.

Khaikin, L.S., Grikina, O.E., Sipachev, V.A., Traetteberg, M.: J. Mol. Struct. **567-568** (2001) 85.

[1] Cradock, S., Koprowski, J., Rankin, D.W.H.: J. Mol. Struct. **77** (1981) 113.

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