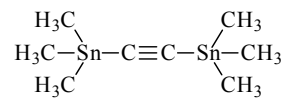


859 **C₈H₁₈Sn₂** **1,2-Ethynediylbis(trimethylstannane)** (see comment)
ED, *ab initio* calculations Bis(trimethylstannyl)acetylene

r_{hl} ^{a)}	Å ^{b)}	θ_{hl} ^{a)}	deg ^{b)}	
Sn–C(m)	2.129(5)	C(1,2)–Sn–C	108.7(4)	
Sn–C(1,2)	2.113(8)	Sn–C–H	113.8(3) ^{c)}	
C(1)≡C(2)	1.206(13)	H–C–H	104.8(4) ^{c)}	
C–H	1.111(5) ^{c)}			

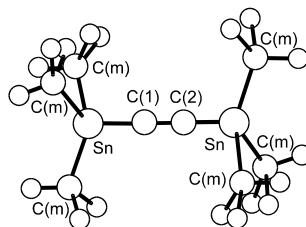
The results of *ab initio* (up to MP2/6-311G**) calculations [1] have shown that the molecule is a nonrigid system with free rotating Sn(CH₃)₃ groups around the linear Sn–C≡C–Sn fragment. The experimental ED data from [2] were reanalyzed using the one-dimensional dynamic model describing free internal rotation of the Sn(CH₃)₃ groups about the Sn–C≡C–Sn axis. It was assumed that the trimethylstannyl groups have local C_{3v} symmetry and the methyl groups have the staggered conformation with respect to the Sn–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 353 K.

^{a)} See comment for definition.

^{b)} 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.: Izv. Akad. Nauk, Ser. Khim. **49** No.4 (2000) 627; Russ. Chem. Bull. (Engl. Transl.) **49** No.4 (2000) 631.

[1] Khaikin, L.S., Grikina, O.E., Sipachev, V.A., Granovskii, A.A., Nikitin, V.S.: Izv. Akad. Nauk, Ser. Khim. **49** No.4 (2000) 616; Russ. Chem. Bull. (Engl. Transl.) **49** No.4 (2000) 620.

[2] Khaikin, L.S., Novikov, V.P., Vilkov, L.V.: J. Mol. Struct. **42** (1977) 129.

Replaces [II/25D \(3, 2619\)](#)