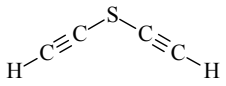
500 **C_4H_2S** **Ethynyl sulfide** **C_{2v}**

MW 1,1'-Thiobisethyne

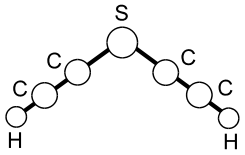


r_0	Å [a])
S–C	1.7230(50)
C≡C	1.2066(50)
C–H	1.0573(50)

θ_0	deg [a])
C–S–C	100.24(50)
S–C≡C	173.30(50) [b])
C≡C–H	174.80(50) [c])
S–C≡C–H [d])	180.00
C–S–C≡C [d])	180.00

r_e	Å [e])
S–C	1.708(20)
C≡C	1.211(10)
C–H	1.061(10)

θ_e	deg [e])
C–S–C	100.5(10)
S–C≡C	174.4(15) [b])
C≡C–H	177.0(25) [c])
S–C≡C–H [d])	180.00
C–S–C≡C [d])	180.00



The structure has planar C_{2v} symmetry.

[a]) Effective structure parameters by directly fitting the observed moments of inertia, namely the so-called r_0 structure parameters. Uncertainties were not estimated in the original paper.
[b]) Bent away from each other.
[c]) Bent toward each other.
[d]) Dihedral angle.
[e]) Average of the two sets of equilibrium structure; one was derived from the experimental moments of inertia, after being corrected for vibration-rotation interaction effects calculated by *ab initio* force fields, and the other was obtained by a high-level *ab initio* calculation at the CCSD(T) level with basis sets: cc-pwCVTZ for S and cc-pCVTZ for C and H atoms.

Matzger, A. J., Lewis, K.D., Nathan, C.E., Peebles, S.A., Peebles, R.A., Kuczkowski, R.L., Stanton, J.F., Oh, J.J.: J. Phys. Chem. A **106** (2002) 12110.