

1175
MW

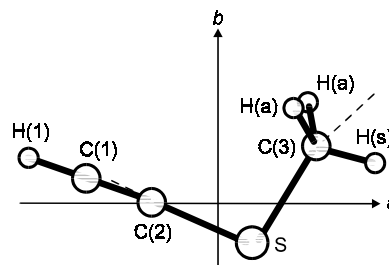
C₃H₄S

(Methylthio)ethyne

C_s
H₃C–S–C≡CH

r_s	Å	θ_s	deg
C(1)–H(1)	1.061(6)	H(s)–C(3)–H(a)	109.9(4)
C(1)≡C(2)	1.205(7)	C(3)–S–C(2)	99.9(2)
C(2)–S	1.685(5)	C(1)≡C(2)–S ^a	182.0(5)
S–C(3)	1.813(2)	H(1)–C(1)≡C(2)	180 ^b
C(3)–H(s)	1.079(10)	tilt (CH ₃) ^c	2.5(20)
C(3)–H(a)	1.090(10)		

Atom	a_s [Å]	b_s [Å]	c_s [Å]
H(1)	–3.1552	0.6990	0.00
S	0.5676	–0.6188	0.00
C(3)	1.4893	0.9425	0.00
H(s)	2.5375	0.6880	0.00
H(a)	1.2479	1.5202	±0.8918



The CH₃ conformation is staggered with respect to the S–C bond.

^a) Bent away from CH₃ group.

^b) Assumed.

^c) Tilt angle of the methyl group (see figure).

Den Engelsen, D.: J. Mol. Spectrosc. **30** (1969) 474.

See also: Den Engelsen, D.: J. Mol. Spectrosc. **22** (1967) 426.