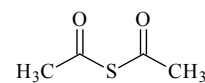


542 C₄H₆O₂SED, vibrational spectroscopy,
ab initio and DFT
calculations**Ethanethioic acid anhydrosulfide**Thioacetic acid anhydrosulfide
Diacetic thioanhydride**C_s assumed**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–H	1.109(9)	C–S–C	108.8(9)
C(1)=O	1.198(2) ^{b)}	S–C(1)=O	125.7(6) ^{b)}
C(1')=O	1.196(2) ^{b)}	S–C(1')=O	115.1(6) ^{b)}
C(1)–C(2)	1.483(4) ^{b)}	S–C(1)–C(2)	111.2(7) ^{b)}
C(1')–C(2')	1.472(4) ^{b)}	S–C(1')–C(2')	121.1(7) ^{b)}
S–C(1)	1.787(3) ^{b)}	H–C–H	109.8(20)
S–C(1')	1.808(3) ^{b)}	C(1')–S–C(1)=O ^{c)}	0 ^{d)}
		C(1)–S–C(1')=O ^{c)}	180 ^{d)}

The molecule was found to exist as a *syn-anti* conformer with C=O bonds in the *syn* and *anti* positions relative to the S–C bonds. Vibrational spectroscopic measurements suggested that any other conformer, if present in the vapor, was less than 1%.

Local C_{3v} symmetry was assumed for the CH₃ groups.

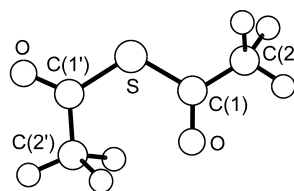
The nozzle temperature was 50 °C.

^{a)} Three times the estimated standard errors.

^{b)} Differences in the C=O, C–C and S–C bond lengths and in the S–C=O and S–C–C bond angles were constrained to the values from MP2/6-31+G* calculations.

^{c)} Torsional angle around the S–C bond.

^{d)} Assumed at the value from MP2/6-31+G* calculations.



Romano, R.M., Della Védova, C.O., Downs, A.J., Oberhammer, H., Parsons, S.: J. Am. Chem. Soc. **123** (2001) 12623.