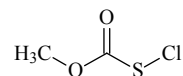


237 C₂H₃ClO₂SED, vibrational
spectroscopy, *ab initio*
and DFT calculations**Carbonothioic acid anhydrosulfide with
thiohypochlorous acid, *O*-methyl ester**Thiohypochlorous acid anhydrosulfide
with *O*-methyl thiocarbonate**C_s assumed (*syn-syn*)
C_s assumed (*syn-anti*)**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–H	1.093(16)	O(1)=C(1)–O(2)	129.1(7)
C=O(1)	1.185(3)	O(1)=C(1)–S	126.1(7)
O(2)–C ^{b)}	1.381(4)	C(1)–O(2)–C(2)	114.3(10)
O(2)–C(1)	1.329(7) ^{c)}	C(1)–S–Cl	99.1(3)
O(2)–C(2)	1.432(7) ^{c)}	H–C–H	111.1(34)
C–S	1.778(4)	tilt(CH ₃) ^{d)}	3.3 ^{e)}
S–Cl	1.999(2)	C(2)–O(2)–C(1)=O(1)	0 ^{e)}
		C(2)–O(2)–C(1)–S	180 ^{e)}
		Cl–S–C(1)=O(1)	0 ^{e)}
		Cl–S–C(1)–O(2)	180 ^{e)}

The molecule was found to exist as a mixture of *syn-syn* (72(8)%) and *syn-anti* (28(8)%) conformers. Differences between the parameters of the conformers were assumed at the values from MP2/6-311G* calculations. Local C_{3v} symmetry was assumed for the methyl group. The difference in the Gibbs energy, estimated from ED and IR (matrix) data, agreed well and gave $\Delta G^\circ[(\textit{syn-syn}) - (\textit{syn-anti})] = 0.67 \text{ kcal mol}^{-1}$.

The parameters are listed for the *syn-syn* conformer.

The nozzle was at room temperature.

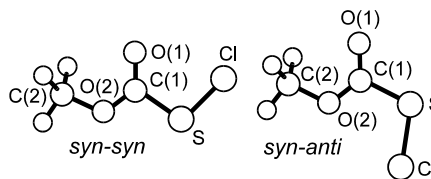
^{a)} Three times the estimated standard errors.

^{b)} Mean value.

^{c)} Difference between the O(2)–C(1,2) bond lengths was assumed at the value from MP2/6-311G* calculations.

^{d)} Tilt angle between the C₃ axis of the CH₃ group and the O(2)–C(2) bond direction, away from the O(1) atom.

^{e)} Assumed at the value from MP2/6-311G* calculations.



Erben, M.F., Della Védova, C.O., Romano, R.M., Boese, R., Oberhammer, H., Willner, H., Sala, O.: Inorg. Chem. **41** (2002) 1064.