

497
MW $C_4H_2O_2S_2$

Acetylene – carbonyl sulfide (1/2)

Ethyne – carbonyl sulfide (1/2)
(weakly bound complex) C_1 (effective symmetry class)
(large-amplitude motion)
 $HC\equiv CH \cdot 2(OCS)$

r_0	\AA	θ_0	deg
C(2)...C(5)	3.703(30)	C(2)...C(5)...cm(9) ^{a)}	58.6(11)
C(2)...cm(9) ^{a)}	3.517(66)	C(5)...cm(9) \equiv C(10) ^{a)}	108.8(22)
C(5)...cm(9) ^{a)}	3.467(34)	C(2)...C(5)=O(4)	63.0(15)
		O(1)=C(2)...cm(9) ^{a)}	75.8(24)
		C(2)...C(5)...cm(9) \equiv C(10) ^{a) b)}	-65.9(23)
		cm(9)...C(2)...C(5)=O(4) ^{a) b)}	104.4(31)
		O(1)=C(2)...cm(9)...C(5) ^{a) b)}	111.0(18)
		O(1)=C(2)...C(5)=O(4) ^{b) c)}	38.0
		O(1)=C(2)...cm(9) \equiv C(8) ^{a) b) c)}	48.9
		O(4)=C(5)...cm(9) \equiv C(8) ^{a) b) c)}	54.3

r_s	$\text{\AA}^d)$
C(2)...C(5)	3.678(30)

Atom	$a_0 [\text{\AA}]$	$b_0 [\text{\AA}]$	$c_0 [\text{\AA}]$
O(1)	2.2946	-0.7333	0.9871
C(2)	2.0611	0.1575	0.2882
S(3)	1.7450	1.3635	-0.6580
O(4)	-0.9597	0.0997	1.7139
C(5)	-1.6028	0.3524	0.7870
S(6)	-2.4734	0.6945	-0.4678
H(7)	-0.8038	-2.8745	0.6657
C(8)	-0.3782	-2.5556	-0.2524
cm(9) ^{a)}	-0.1370	-2.3748	-0.7729
C(10)	0.1043	-2.1940	-1.2934
H(11)	0.5298	-1.8751	-2.2116

The observed spectroscopic constants are consistent with a nonplanar, triangular-twisted structure of C_1 symmetry which aligns the three monomer axes approximately $3\sim 27^\circ$ away from perpendicular to a triangle formed by the center of HCCH and the carbons of OCS. The OCS dimer portion of the trimer has the two OCS monomers aligned in an almost parallel fashion such that the monomer dipole moments reinforce, rather than in the antiparallel arrangement observed in the well-known OCS dimer.

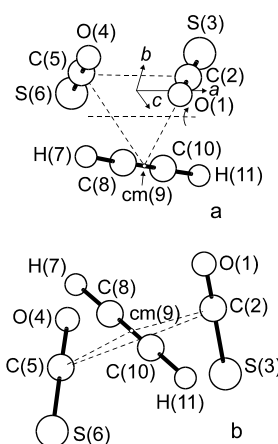
The perspective in figure (a) places the carbon of the left-hand OCS molecule slightly in front of the plane of the paper and the carbon of the right-hand OCS slightly behind the plane of the paper. The perspective in (b) is obtained by rotating the view in (a) by 90° about the arrow in the direction shown. This will place C(2) and C(5) in the plane of the paper and the HCCH molecule above this plane.

^{a)} cm(9) denotes the center of mass of the HCCH.

^{b)} Dihedral angle.

^{c)} Dependent parameter.

^{d)} Uncertainty was not estimated in the original paper.



Peebles, S.A., Kuczkowski, R.L.: J. Chem. Phys. **111** (1999) 10511.