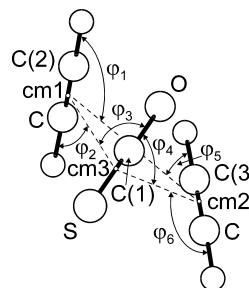


628
MW**C₅H₄OS****Carbonyl sulfide – ethyne (1/2)**Carbonyl sulfide – acetylene (1/2)
(weakly bound complex)**C₁**(effective symmetry class)
(large-amplitude motion)
OCS · 2(HC≡CH)

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
C(1)	1.0101	0.0472	0.6596
O	0.4112	0.2502	1.6389

Semi-empirical modeling predicted a structure that has the two acetylene monomers aligned in a geometry between the well-known T-shaped orientation of the acetylene dimer and a parallel intermediate. The measured rotational constants and dipole moment were consistent with this model.

Bond angles and distances were derived from a semi-empirical model. The dihedral angles derived from this model are $[C(3)-cm2...cm1-C(2)] = -34.6^\circ$, $[C(2)-cm1...cm3-C(1)] = -31.4^\circ$, $[C(1)-cm3...cm2-C(3)] = -40.3^\circ$ and $[C(1)-cm3...cm2...cm1] = -73.6^\circ$.



Peebles, S.A., Kuczkowski, R.L.: J. Mol. Struct. **500** (2000) 391.