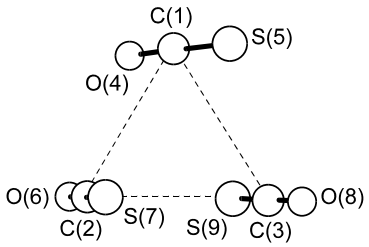
466 **$C_3O_3S_3$** **Carbonyl sulfide trimer** **C_1** (antiparallel)
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
3(OCS)

r_0	Å [a])
C(1)...C(2)	3.654(5)
C(1)...C(3)	3.797(5)
C(2)...C(3)	3.908(5)

θ_0	deg [a])
C(1)...C(2)...C(3)	60.2(5)
C(2)...C(3)...C(1)	56.6(5)
C(3)...C(1)...C(2)	63.2(5)
S(5)–C(1)...C(3)	70.9(5)
S(7)–C(2)...C(1)	82.8(5)
O(8)–C(3)...C(2)	116.5(5)
S(5)–C(1)...C(3)...C(2) [b])	136.4(5)
S(7)–C(2)...C(1)...C(3) [b])	80.0(5)
O(8)–C(3)...C(2)...C(1) [b])	89.9(5)
S(5)–C(1)...C(3)–S(9) [b])	–156.2(5)
S(7)–C(2)...C(1)–S(5) [b])	32.7(5)
S(9)–C(3)...C(2)–S(7) [b])	–178.8(5)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)	1.08070	1.68607	–0.64283
C(2)	–2.25260	0.31900	–0.03202
C(3)	0.88452	–1.98819	0.29479
O(4)	0.25388	1.92442	–1.41492
S(5)	2.20003	1.36340	0.40240
O(6)	–2.55231	0.16991	–1.13859
S(7)	–1.84685	0.52082	1.46604
O(8)	1.37954	–2.04039	1.33824
S(9)	0.21438	–1.91753	–1.11782
cm1 [c])	1.45697	1.57760	–0.29149
cm2 [c])	–2.11620	0.38684	0.47155
cm3 [c])	0.65925	–1.96444	–0.18006



The carbon atoms form a triangle with the axes of the monomer units roughly parallel to each other (barrel-like structure). The monomers have an antiparallel-like arrangement, with the dipole moment of one monomer opposing those of the other two monomers.

[a]) Uncertainties were not estimated in the original paper.
[b]) Dihedral angle.
[c]) The center of mass of OCS.

Peebles, R.A., Kuczkowski, R.L.: J. Phys. Chem. A **103** (1999) 6344.
See also: Connelly, J.P., Bauder, A., Chisholm, A., Howard, B.J.: Mol. Phys. **88** (1996) 915.