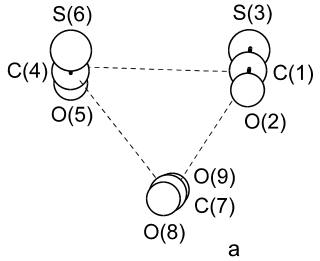
467 **$C_3O_4S_2$** **Carbon dioxide – carbonyl sulfide (1/2)** **C_1**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
$CO_2 \cdot 2(OCS)$

r_0	Å
C(1)...C(7)	3.773(8)
C(4)...C(7)	3.574(6)
C(1)...C(4)	3.757(9)
C(7)...cm(1) [a])	3.616(9)
C(7)...cm(4) [a])	3.891(8)
cm(1)...cm(4) [a])	3.652(12)

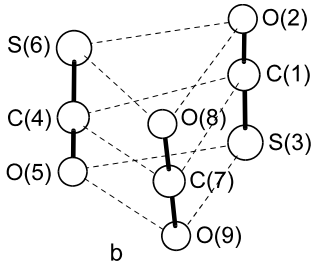
θ_0	deg
C(4)...C(7)...C(1)	61.4(1)
O(5)=C(4)...C(7)	56.2(7)
O(2)=C(1)...C(4)	102.3(4)
O(8)=C(7)...C(1)	60.1(14)
O(5)=C(4)...C(7)...C(1) [b])	133.2(9)
O(2)=C(1)...C(4)...C(7) [b])	–107.4(7)
O(8)=C(7)...C(1)...C(4) [b]) [c])	–79.0

r_s	Å [d])
C(1)...C(7)	3.767(10)
C(4)...C(7)	3.567(7)
C(1)...C(4)	3.744(10)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)	0.04891	2.05879	0.20495
C(4)	–1.37246	–1.35454	–0.45910
C(7)	2.01710	–1.12875	0.65188
cm(1) [a])	0.29146	1.92066	–0.24099
O(2)	–0.48411	2.36231	1.18491
S(3)	0.77049	1.64788	–1.12170
cm(4) [a])	–1.77114	–1.09265	–0.23721
O(5)	–0.49634	–1.93007	–0.94670
S(6)	–2.55852	–0.57541	0.20101
O(8)	1.25771	–0.79718	1.46652
O(9)	2.77649	–1.46032	–0.16276



a



b

The structure resembles a distorted triangular cylinder with the three monomers aligned roughly parallel. The trimer may be thought of as a slightly perturbed $(OCS)_2$ dimer with the CO_2 lying above the dimer and crossed at 12° and 20° to the axes of the two OCS molecules, respectively. The perspective in figure (a) places the carbon of the left-hand OCS in the plane of the paper, the carbon of the right-hand OCS slightly behind this plane, and the carbon of the CO_2 slightly in front of the plane. The perspective in (b) is obtained by rotating (a) by 90°, placing C(1) and C(4) in the plane of the paper and C(7) above the plane.

[a]) cm(1) and cm(4) are the centers of mass of the OCS molecules and are bound to the C(1) and C(4) atoms, respectively.
[b]) Dihedral angle.
[c]) Dependent parameter.
[d]) Uncertainties were not estimated in the original paper.

Peebles, S.A., Kuczkowski, R.L.: J. Phys. Chem. A **102** (1998) 8091.