

468  
MW $\text{C}_3\text{O}_5\text{S}$ 

Carbonyl sulfide – carbon dioxide (1/2)

(weakly bound complex)

 $\text{C}_1$ 

(effective symmetry class)

(large-amplitude motion)

 $\text{OCS} \cdot 2(\text{CO}_2)$ 

$r_0$	Å	$\theta_0$	deg
C(1)...C(2)	3.681(16)	C(1)...cm(3)...C(2) <sup>a)</sup>	58.9(2)
C(2)...C(3)	3.659(16)	O(8)=C(2)...cm(3) <sup>a)</sup>	101.8(35)
C(1)...C(3)	3.592(14)	O(7)=C(1)...C(2)	121.1(21)
C(1)...cm(3) <sup>a)</sup>	3.907(11)	S(4)=cm(3)...C(1) <sup>a)</sup>	129.9(10)
C(2)...cm(3) <sup>a)</sup>	3.548(12)	O(8)=C(2)...cm(3)...C(1) <sup>a) b)</sup>	124.6(17)
		O(7)=C(1)...C(2)...cm(3) <sup>a) b)</sup>	-100.9(34)
		S(4)=cm(3)...C(1)...C(2) <sup>a) b)</sup>	44.2(18)

$r_s$	Å <sup>c)</sup>
C(1)...C(2)	3.692(20)
C(2)...C(3)	3.627(20)
C(1)...C(3)	3.562(20)

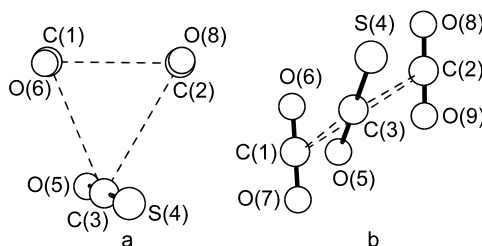
Atom	$a_0$ [Å]	$b_0$ [Å]	$c_0$ [Å]
C(1)	2.32378	0.21289	0.45474
C(2)	-0.44918	-2.05772	-0.37473
C(3)	-0.92758	1.56756	-0.24079
cm(3) <sup>a)</sup>	-1.37516	1.35330	-0.06603
S(4)	-2.25910	0.93016	0.27911
O(5)	0.05598	2.03839	-0.62482
O(6)	1.57453	-0.14621	1.27708
O(7)	3.07303	0.57199	-0.34761
O(8)	-1.16975	-2.56871	0.38019
O(9)	0.27140	-1.54673	-1.12965

The structure resembles a distorted triangular cylinder. It can be thought of as the slipped  $(\text{CO}_2)_2$  dimer with the OCS above the dimer and crossed about  $23^\circ$  to the axis of each  $\text{CO}_2$ . The distance between the carbon atoms on the  $\text{CO}_2$  is 3.68(5) Å. The distance between the carbon on each  $\text{CO}_2$  and the carbon on the OCS is 3.59(5) and 3.66(5) Å, respectively. The axes of the linear molecules are tilted  $30^\circ$ – $35^\circ$  from perpendicular relative to the edges of the C–C–C plane. The perspective in figure (a) places the carbon of OCS in the plane of the paper, the carbon of the left  $\text{CO}_2$  somewhat above the plane, and the carbon of the right  $\text{CO}_2$  somewhat below the plane. The perspective in (b) is obtained by rotating (a) by  $90^\circ$  in the plane of the paper. In perspective (b), the two  $\text{CO}_2$  monomers are almost coplanar.

<sup>a)</sup> cm(3) denotes the center of mass of the OCS.

<sup>b)</sup> Dihedral angle.

<sup>c)</sup> Uncertainties were not estimated in the original paper.



Peebles, S.A., Kuczkowski, R.L.: J. Chem. Phys. **109** (1998) 5276.