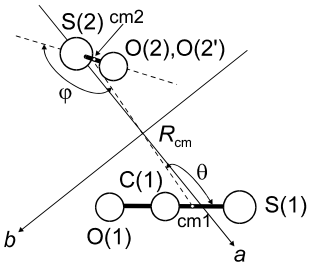
164 **CO_3S_2** **Carbonyl sulfide – sulfur dioxide (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
O=C=S · SO_2

r_0	Å
R_{cm}	3.7471(4)

θ_0	deg
θ [a])	123.8(5)
φ [a])	142.1(50)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)	1.58725	0.60427	0.0
O(1)	0.84807	1.49319	0.0
S(1)	2.58794	–0.59912	0.0
cm1 [b])	1.92363	0.19976	0.0
S(2)	–2.11196	0.00523	0.0
O(2)	–1.49515	–0.37970	1.29940
O(2')	–1.49515	–0.37970	–1.29940
cm2 [b])	–1.80348	–0.18729	0.0



The dimer has C_s symmetry with the oxygen atoms of the SO_2 straddling the OCS. The C_2 axis of SO_2 is nearly parallel to the OCS molecule orienting the dipole moments of the monomers approximately antiparallel.

[a]) See figure for the definition.
[b]) cm1 and cm2 denote the centers of mass for the OCS and SO_2 molecules, respectively.

Peebles, S.A., Sun, L.H., Ioannou, I.I., Kuczkowski, R.L.: J. Mol. Struct. **485-486** (1999) 211.