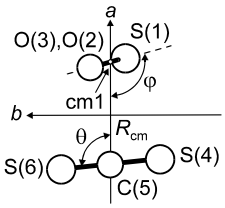
163 **CO_2S_3** **Carbon disulfide – sulfur dioxide (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
$CS_2 \cdot SO_2$

r_0	Å	Å
	I	II
R_{cm}	3.4287(1)	3.4287(2)

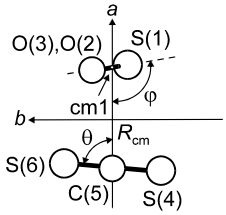
θ_0	deg	deg
	I	II
θ [a])	92.7(1)	87.0(2)
φ [a])	102.5(7)	104.1(9)

Atom	a_0 [Å]	a_0 [Å]	b_0 [Å]	b_0 [Å]	c_0 [Å]
	I	II	I	II	II
S(1)	1.9531	1.9416	–0.2880	–0.4057	0.0
O(2)	1.7668	1.7796	0.4256	0.3138	1.2226
O(3)	1.7668	1.7796	0.4256	0.3138	–1.2226
cm1 [b])	1.8599	1.8606	0.0689	–0.0458	0.0
C(5)	–1.5665	–1.5670	–0.0580	0.0386	0.0
S(6)	–1.6976	–1.4467	1.4884	1.5859	0.0
S(4)	–1.4353	–1.6874	–1.6045	–1.5087	0.0



I

The observed rotational constants are consistent with the SO_2 straddling the CS_2 molecule and C_s symmetry for the complex. Two structures I and II were found that are consistent with this symmetry which differ in the relative tilt of the CS_2 and SO_2. In both structures, the C_2 axis of the SO_2 is aligned close to parallel to the CS_2 molecular axis with the oxygen end of the SO_2 tipped closer to the CS_2 molecule. In one structure the deviation from parallel is 9.8(8)°, while in the other it is 17.7(11)°.



II

[a]) See figure for the definition.
[b]) Center of mass of the SO_2.

Peebles, S.A., Sun, L.H., Kuczkowski, R.L.: J. Chem. Phys. **110** (1999) 6804.