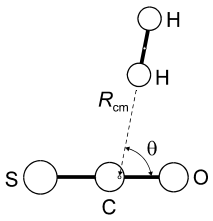
103 **CH_2OS** **Carbonyl sulfide – dihydrogen (1/1)** **C_s**
IR (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
$O{=}C{=}S \cdot H_2$

Isotopic species	State	$r_0(R_{cm})$ [Å] [a]	θ_0 [deg] [a] [b]
OCS · *para*H_2	v=0, j_H=0	3.719(5)	69.2(5)
OCS · *ortho*H_2	v=0, j_H=1	3.819(5)	67.0(5)
OCS · *ortho*D_2	v=0, j_H=0	3.590(5)	71.7(5)
OCS · *para*D_2	v=0, j_H=1	3.609(5)	70.5(5)
OCS · HD	v=0, j_H=0	3.643(5)	71.2(5)



The complex has a T-shaped configuration. The structure was determined from the rotationally resolved IR spectrum in the region of the ν_1 fundamental band of OCS under the assumption that the bond lengths of the monomers are unchanged upon complexation.

[a]) Uncertainties were not given in the original paper.
[b]) Angle between the OCS axis and R_{cm}, see figure for the definition.

Tang, J., McKellar, A.R.W.: J. Chem. Phys. **116** (2002) 646.