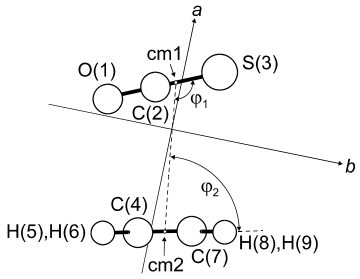
373 **C_3H_4OS** **Ethene – carbonyl sulfide (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)
$H_2C{=}CH_2 \cdot OCS$

r_0	Å
R_{cm}	3.660(2)

θ_0	deg
φ_1 [a])	106.6(3)
φ_2 [a])	85.2(17)

Atom	a_0 [$\lvert a_s \rvert$] [Å]	b_0 [$\lvert b_s \rvert$] [Å]	c_0 [$\lvert c_s \rvert$] [Å]
O(1)	0.4544	–1.6909	0.0
C(2)	0.9356	–0.6397	0.0
	[0.9495]	[0.6298]	[0.0]
S(3)	1.5872	0.7833	0.0
	[1.5502]	[0.8123]	[0.0]
C(4)	–2.6176	–0.3079	0.0
H(5),H(6)	–2.7411	–0.8545	±0.9291
	[2.6356]	[0.8982]	[0.8903]
C(7)	–2.3226	0.9982	0.0
H(8),H(9)	–2.1992	1.5449	±0.9291
	[2.0697]	[1.5184]	[0.8785]



The observed data are consistent with a stacked geometry in which the OCS lies above the ethene molecular plane, approximately parallel to the C=C bond. Two internal motions of the monomer subunits split each rotational transition into four components. The larger tunneling splittings were analyzed to give a twofold barrier for the internal motion of the ethene subunit about its *c* inertial axis of 16(3) cm^{-1}.

[a]) See figure for the definition.

Peebles, S.A., Kuczkowski, R.L.: Mol. Phys. **99** (2001) 225.