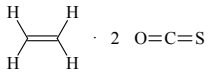
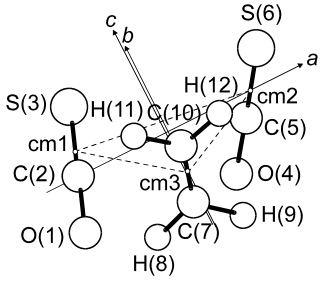
513 **$C_4H_4O_2S_2$** **Ethene – carbonyl sulfide (1/2)** **C_1**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0 [a])	Å	θ_0 [a])	deg
cm1... cm2	3.852(9)	cm1... cm2...cm3	60.53(50)
cm2...cm3	3.648(15)	S(6)–cm2...cm1	117.7(16)
		S(3)–cm1...cm3	108.0(27)
		C(10)–cm3...cm2	87.3(17)
		S(6)–cm2...cm1...cm3 [b])	–93.0(36)
		S(3)–cm1...cm3...cm2 [b])	–62.6(23)
		C(10)–cm3...cm2...cm1 [b])	–97.0(27)
		H(11)–C(10)–cm3...cm2 [b])	130.0(10)

The moments of inertia were fitted to a structure in which the plane of the ethene is roughly parallel to a plane formed by the OCS monomers aligned with parallel dipoles. The transitions were split into doublets separated by 30-100 kHz by a tunneling motion in the complex. Isotopic studies indicated that this motion involved rotation of the ethene in its molecular plane.



[a]) cm1, cm2 and cm3 denote the centers of mass of O(1)C(2)S(3), O(4)C(5)S(6) and ethene, respectively.
[b]) Dihedral angle.

Peebles, R.A., Peebles, S.A., Kuczkowski, R.L.: J. Mol. Struct. **612** (2002) 261.