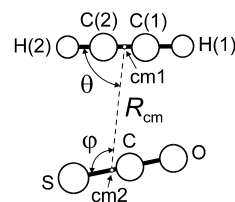


349  
MW $C_3H_2OS$ **Ethyne – carbonyl sulfide (1/1)**  
(weakly bound complex) $C_s$  (parallel form)  
(effective symmetry class)  
(large-amplitude motion)  
 $HC\equiv CH \cdot OCS$ 

$r_0$	$\text{\AA}$	$\theta_0$	deg
$R_{cm}$	3.6062(13)	$\theta^a$	84.5(78)
		$\varphi^a$	106.7(9)

Atom	$a_0 [\text{\AA}]$	$b_0 [\text{\AA}]$
H(1)	2.89644	1.22515
C(1)	2.63408	0.19710
C(2)	2.33661	-0.96855
H(2)	2.07425	-1.99660
cm1 <sup>b)</sup>	2.48535	-0.38572
cm2 <sup>c)</sup>	-1.07823	0.16733
S	-1.52652	-0.76999
O	-0.35243	1.68489
C	-0.85124	0.64194



The observed rotational constants are consistent with a nearly parallel arrangement of the monomer subunits.

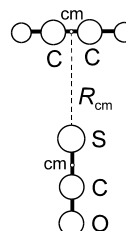
<sup>a)</sup> See figure for the definition.

<sup>b)</sup> Center of mass of ethyne.

<sup>c)</sup> Center of mass of carbonyl sulfide.

Peebles, S.A., Kuczkowski, R.L.: J. Phys. Chem. A **103** (1999) 3884.

$r_0$	$\text{\AA}$
$R_{cm}$	4.622(2)

 $C_{2v}$  (T-shaped form)

The complex has the OCS monomer interacting with the triple bond of the ethyne monomer through the S atom. The effects of nuclear spin statistics on the relative intensities of the transitions confirm the  $C_{2v}$  symmetry of the complex. A semi-empirical model and *ab initio* calculations suggest that this second isomer is less stable than the near-parallel isomer.

Peebles, S.A., Kuczkowski, R.L.: Chem. Phys. Lett. **312** (1999) 357.