

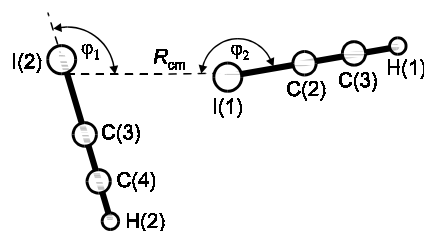
1510  
IR

$C_4H_2I_2$

**Iodoacetylene dimer**  
(weakly bound complex)

$C_s$   
(effective symmetry class)  
 $IC\equiv CH \cdot IC\equiv CH$

$r_0$	$\text{\AA}$	$\theta_0$	deg
$R_{cm}$	4.44(2) <sup>a)</sup>	$\varphi_1$	108.9
I(1)...C(3)	3.763	$\varphi_2$	161.68
I...I	4.201		



Considering the smallness of the inertial defect, the molecule can be assumed to be planar. The distance between the center of masses of the monomers can be easily deduced from the  $C_0$  rotational constant of the dimer, assuming that the structure of the two monomers is unchanged on complex formation. The exact shape of the dimer is more problematic. Two different antiparallel structures ( $C_{2h}$  symmetry) are compatible with the  $A_0$ ,  $B_0$ , and  $C_0$  rotational constants but both give an iodine-iodine contact distance smaller than the sum of covalent van der Waals radii. Moreover, with both structures, the intensity ratio of the  $A$  and  $B$  components in the hybrid IR band would be significantly smaller than the observed ratio. For all these reasons, the authors favor a nearly T-shaped structure, with the I atom of one monomer pointing towards one of the C atoms (the iodine-bound one) of the other monomer. We give here just one of the possible set of structural values, so no uncertainty estimates can be readily made.

<sup>a)</sup> Uncertainty was not given in the original paper.

Kerstel, E.R.T., Lehmann, K.K., Mentel, T. F., Scoles, G., Timmermans, J.H.: J. Mol. Spectrosc. **162** (1993) 342.