

Structure Data of Free Polyatomic Molecules

 101
MW

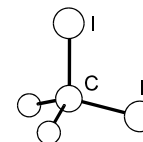
 CH_2I_2
Diiodomethane
Methylene iodide

 C_{2v}
 CH_2I_2

r_0	\AA^a	θ_0	deg^a
C–I	2.135(3)	I–C–I	113.90(30)
C–H	1.066(15)	H–C–H	111.6(24)
r_{av}^b	\AA^a	θ_{av}^b	deg^a
C–I	2.1364(6)	I–C–I	113.83(5)
C–H	1.078(2)	H–C–H	113.3(3)

Atom	$a_0 [\text{\AA}]$	$b_0 [\text{\AA}]$	$c_0 [\text{\AA}]$
I	± 1.7896	-0.0654	0.0
C	0.0	1.0988	0.0
H	0.0	1.6981	± 0.8822

^{a)} Three times the estimated standard errors.

^{b)} The authors call r^* structure.

 Kisiel, Z., Pszczółkowski, L., Favero, L.B., Caminati, W.: J. Mol. Spectrosc. **189** (1998) 283.