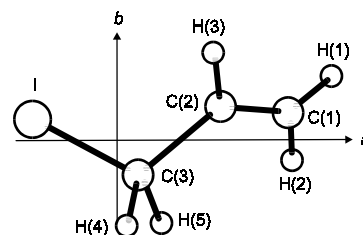


1211  $\text{C}_3\text{H}_5\text{I}$   
ED, MW

### 3-Iodo-1-propene

$\text{C}_1$  (*skew*)  
 $\text{H}_2\text{C}=\text{CH}-\text{CH}_2\text{I}$

$r_g$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
C–H	1.081(12)	C=C–C	123.0(11)
C=C	1.348(10)	C–C–I	111.7(12)
C–C	1.478(13)	C=C–H	120.0 <sup>b</sup>
C–I	2.186(8)	H–C(3)–H	109.5 <sup>b</sup>
		C(2)–C(3)–H	110.6(21)
		$\phi(\text{skew})^c$	110.6(23)



Only one conformer (*skew*) was observed.  
The nozzle temperature was 298 K.

<sup>a</sup>) Twice the estimated standard errors including a systematic error.

<sup>b</sup>) Assumed.

<sup>c</sup>) C(1)=C(2)–C(3)–I torsional angle;  $\phi = 0^\circ$  when C–I is eclipsed with respect to the C=C bond.

Hagen, K., Shen, Q., Stølevik, R.: J. Phys. Chem. **95** (1991) 8632.

MW

$r_0$	$\text{\AA}^a$	$\theta_0$	$\text{deg}^a$
C(1)=C(2)	1.354 <sup>b</sup>	C(1)=C(2)–C(3)	121.6 <sup>b</sup>
C(2)–C(3)	1.480 <sup>b</sup>	C(2)–C(3)–I	107.6(10)
C–I	2.189(10)	C(2)=C(1)–H	120.0 <sup>b</sup>
C(1,2)–H	1.080 <sup>b</sup>	H–C(3)–H	111.0 <sup>b</sup>
C(3)–H	1.095 <sup>b</sup>	H–C(1)–H	120.0 <sup>b</sup>
		C(2)–C(3)–H	107.0 <sup>b</sup>
		C(1)=C(2)–H	120.0 <sup>b</sup>
		$\phi(\text{C(1)=C(2)–C(3)–I})$	119.4(30)

<sup>a</sup>) Uncertainties were not estimated in the original paper.

<sup>b</sup>) Assumed.

Sasada, Y., Niide, Y., Takano, M., Satoh, T.: J. Mol. Spectrosc. **66** (1977) 421.