

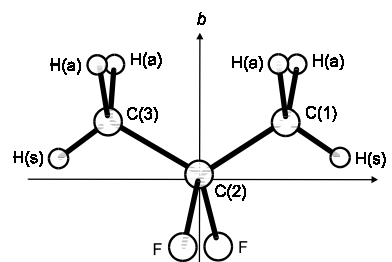
1250  
ED, MW

**C<sub>3</sub>H<sub>6</sub>F<sub>2</sub>**

**2,2-Difluoropropane**

**C<sub>2v</sub>**  
**H<sub>3</sub>C–CF<sub>2</sub>–CH<sub>3</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H	1.102(4)	C–C–C	115.3(4)
C–F	1.370(2)	F–C–F	106.2(4)
C–C	1.512(3)	H–C–H	108.0(12)
		tilt (CH <sub>3</sub> ) <sup>b)</sup>	2.9(21)



Local C<sub>3v</sub> symmetry was assumed for the CH<sub>3</sub> groups.

The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> The CH<sub>3</sub> group is tilted toward the CF<sub>2</sub> group.

Mack, H.-G., Dakkouri, M., Oberhammer, H.: J. Phys. Chem. **95** (1991) 3136.

MW

$r_0$	Å	$\theta_0$	deg
C–C	1.517(1)	C–C–C	115.5(1)
C–F	1.370(1)	C–C–F	108.7(1)
C–H	1.087(7)	F–C–F	106.1(1)
C...C	2.567	C–C–H	109.4(4)

$r_s$	Å	$\theta_s$	deg
C–H(s)	1.100(7)	H(s)–C–H(a)	109.6(3)
C–H(a)	1.092(7)	H(a)–C–H(a)	109.7(7)
C...C	2.561		

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
H(s)	2.1300	0.1795	0.00
H(a)	1.3214	1.5053	±0.8931
C(1)	1.2805	0.8779	0.00

<sup>a)</sup> Fixed.

Takeo, H., Sugie, M., Matsumura, C.: J. Mol. Struct. **352/353** (1995) 267.

See also:

Nanaie, H., Guirgis, G.A., Durig, J.R.: Spectrochim. Acta A **49** (1993) 2039.