

1099  
MW

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

**3,3,3-Trifluoro-1-propene**

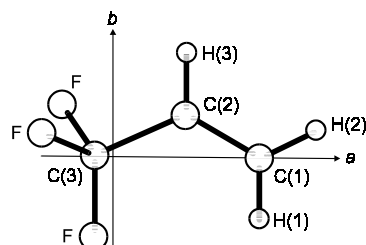
**C<sub>s</sub>**  
H<sub>2</sub>C=CH-CF<sub>3</sub>

$r_0$	Å	$\theta_0$	deg
C–C	1.489(2)	F–C–F	106.8(3)
C=C	1.312(10)	C=C–C	124.8(4)
C–H(1)	1.085(11)	C=C–H(1)	120.6(10)
C–H(2)	1.092(9)	C=C–H(2)	122.8(10)
C–H(3)	1.109(3)	C=C–H(3)	121.2(10)
C–F	1.345 <sup>a)</sup>	tilt (CF <sub>3</sub> ) <sup>b)</sup>	1.0(8)

Atom	$a_s$ [Å]	$b_s$ [Å]
C(2)	1.0655	0.6605
H(1)	2.2022	–1.0868
H(2)	3.1732	0.4899
H(3)	1.0499	1.7699

<sup>a)</sup> Assumed.

<sup>b)</sup> Tilt angle of CF<sub>3</sub> relative to C–C, the positive sign meaning away from the vinyl group.



Saito, S., Makino, F.: Bull. Chem. Soc. Jpn. **47** (1974) 1863.

ED, MW

**C<sub>s</sub> assumed**

$r_g$	Å <sup>a)</sup>	$\theta_{av}$	deg <sup>a)</sup>
C(2)–C(3)	1.495(6)	C(2)–C(3)–F	112.0(2)
C(1)=C(2)	1.318(8)	C(1)=C(2)–C(3)	125.8(11)
C(1)–H	1.100(18)	C(2)=C(1)–H	111.3(40)
C(3)–F	1.347(3)		

One of the C–F bonds is eclipsed with respect to the double bond.  
The measurements were made at room temperature.

<sup>a)</sup> Estimated error limits.

<sup>b)</sup> Assumed.

Tokue, I., Fukuyama, T., Kuchitsu, K.: J. Mol. Struct. **17** (1973) 207.