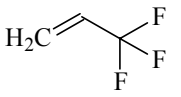
354 **$C_3H_3F_3$** **3,3,3-Trifluoro-1-propene** **C_s**

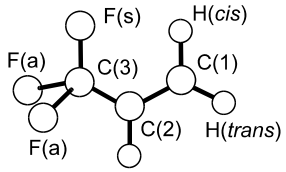
MW



r_0	Å	θ_0	deg
C(1)=C(2)	1.330(2)	C(1)=C(2)–C(3)	123.1(5)
C(2)–C(3)	1.490(2)	C(1)=C(2)–H	122.2(5)
C(2)–H	1.081(2)	C(2)=C(1)–H(*trans*) [a])	120.6(5)
C(1)–H(*trans*) [a])	1.080(2)	C(2)=C(1)–H(*cis*) [a])	120.7(5)
C(1)–H(*cis*) [a])	1.080(2)	C(2)–C(3)–F(s) [b])	113.5(5)
C(3)–F(s) [b])	1.340(2)	C(2)–C(3)–F(a) [b])	111.3(5)
C(3)–F(a) [b])	1.347(2)	F(a)–C(3)–F(a) [b])	106.6(5)

$r_{I\varepsilon}$	Å	$\theta_{I\varepsilon}$	deg
C(1)=C(2)	1.330(2)	C(1)=C(2)–C(3)	122.9(5)
C(2)–C(3)	1.488(2)	C(1)=C(2)–H	122.3(5)
C(2)–H	1.081(2)	C(2)=C(1)–H(*trans*) [a])	120.9(5)
C(1)–H(*trans*) [a])	1.081(2)	C(2)=C(1)–H(*cis*) [a])	120.5(5)
C(1)–H(*cis*) [a])	1.080(2)	C(2)–C(3)–F(s) [b])	113.2(5)
C(3)–F(s) [b])	1.336(2)	C(2)–C(3)–F(a) [b])	111.2(5)
C(3)–F(a) [b])	1.342(2)	F(a)–C(3)–F(a) [b])	106.9(5)

The CF_3 internal rotation barrier was determined to be 612(2) and 653.06(83) cm^{-1} by using the internal axis method and the ρ axis method, respectively.



[a]) H(*trans*) and H(*cis*) denote the hydrogen atoms bonded to C(1), which are *trans* and *cis* to the CF_3 group, respectively.

[b]) F(s) and F(a) denote the fluorine atoms located in plane and out of plane, respectively.

Alonso, J.L., Lesarri, A., López, J.C., Blanco, S., Kleiner, I., Demaison, J.: Mol. Phys. **91** (1997) 731.

Replaces II/25C (**3**, 1099), MW