

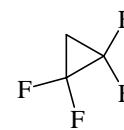
1064
MW

C₃H₂F₄

1,1,2,2-Tetrafluorocyclopropane

C_{2v}

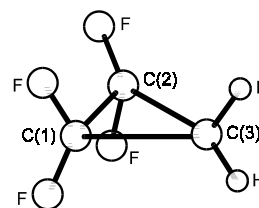
r_0	Å	θ_0	deg
C(1)–C(2)	1.474(1)	F–C(1,2)–F	110.0(3)
C(1)–C(3)	1.497(5)	H–C(3)–H	118.1(2)
C(1)–F	1.343(2)	C(1)–C(2)–F(p) ^{a)}	150.0(1)
C(3)–H	1.087(2)	C(3)–C(1,2)–F(p) ^{a)}	149.5(1)
F...F (gem)	2.200(1)		
F...F (vic)	2.808(1)		



r_s	Å	θ_s	deg
C(1)–C(2)	1.471(1)	F–C(1,2)–F	109.9(4)
C(1)–C(3)	1.497(10)	H–C(3)–H	118.0(4)
C(1)–F	1.344(4)	C(1)–C(2)–F(p) ^{a)}	150.1(1)
C(3)–H	1.088(5)	C(3)–C(1,2)–F(p) ^{a)}	149.4(1)
F...F (gem)	2.200(1)		
F...F (vic)	2.809(3)		

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1,2)	±0.7368	0.00	0.0872
C(3)	0.00	0.00	1.3907
H	0.00	±0.9324	1.9496
F	±1.4041	±1.1001	–0.2988

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1,2)	±0.7355	0.00	0.0860
C(3)	0.00	0.00	1.3896
H	0.00	±0.9323	1.9498
F	±1.4043	±1.1001	–0.2991



^{a)} F(p) denotes the projection of the fluorine atom in the cyclopropyl ring plane.

Beauchamp, R.N., Gillies, C.W., Craig, N.C.: J. Am. Chem. Soc. **109** (1987) 1696.