

1012
MW

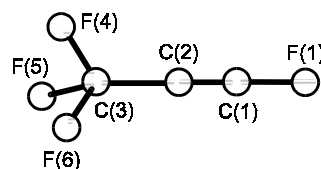
C₃F₄

1,3,3,3-Tetrafluoropropyne

C_{3v}
FC≡C–CF₃

r_{av}	Å	θ_{av}	deg
C(1)≡C(2)	1.2016(19)	F–C–F	108.02(20)
C(2)–C(3)	1.4566(34)		
C(1)–F	1.2737(44)		
C(3)–F	1.3387(20)		

Atom	a_{av} [Å]	b_{av} [Å]	c_{av} [Å]
F(1)	–3.0669	0.0	0.0
C(1)	–1.7932	0.0	0.0
C(2)	–0.5916	0.0	0.0
C(3)	0.8650	0.0	0.0
F(4)	1.3423	1.2507	0.0
F(5,6)	1.3423	0.6254	±1.0831



Shrinkage corrections ^a):

Species	δr (C–F)	δr (C–C)	δr (C≡C)	δr (C(1)–F)
CF ₃ C≡CF	–	–	–	–
¹³ CF ₃ C≡CF	–0.00013	–0.00008	–	–
CF ₃ ¹³ C≡CF	0.00001	0.00001	0.00004	–
CF ₃ C≡ ¹³ CF	–	–0.00001	0.00005	–0.00001

^a) Assumed; corrections are $r_z(\text{isotope}) - r_z(\text{parent})$.

Cox, A.P., Ellis, M.C., Summers, T.D., Sheridan, J.: J. Chem. Soc., Faraday Trans. **88** (1992) 1079.