

1471
ED, MW

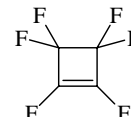
C₄F₆

Hexafluorocyclobutene

C_{2v}

	r_g [Å] ^{a)}	r_α^0 [Å] ^{a)}	θ_α	deg ^{a)}
C–F ^{b)}	1.336(4)	1.332(4)	C(1)=C(2)–F	135.1(7)
Δ (C–F) ^{c)}	0.033(13)	0.034(13)	F–C–F	107.6(5)
C(1)=C(2)	1.328(24)	1.325(24)	C(1)=C(2)–C(3) ^{e)}	94.9(5)
C–C ^{b)}	1.530(3)	1.528(3)	C(2)–C(3)–C(4) ^{e)}	85.1(5)
Δ (C–C) ^{d)}	0.082(11)	0.082(11)	C(4)–C(3)–F ^{e)}	114.7(3)
C(1)–F ^{e)}	1.314(10)	1.309(10)	C(2)–C(3)–F ^{e)}	116.8(4)
C(3)–F ^{e)}	1.347(4)	1.344(4)	C(4)–C(1)–F ^{e)}	130.0(11)
C(2)–C(3) ^{e)}	1.503(5)	1.500(5)	ϕ ^{f)}	2.4(6)
C(3)–C(4) ^{e)}	1.585(8)	1.582(8)		

The ED data from [1] were reanalyzed using the rotational constants from the literature as structural constraints. The nozzle was at 19...20 °C.



^{a)} Twice the estimated standard errors.

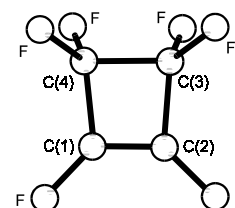
^{b)} Average value.

^{c)} Δ (C–F) = [C(3)–F] – [C(1)–F].

^{d)} Δ (C–C) = [C(3)–C(4)] – [C(2)–C(3)].

^{e)} Dependent parameter.

^{f)} Angle between the vectors bisecting the C–C–C and F–C–F bond angles. The positive value indicates the CF₂ groups are tipped toward each other.



Hedberg, L., Hedberg, K.: J. Phys. Chem. **97** (1993) 10349.

[1] Császár, A., Hedberg, K.: J. Phys. Chem. **94** (1990) 3525.

MW

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1)=C(2)	1.333(6)	C(1)=C(2)–F	135(1)
C(1)–F	1.31(2)	F–C–F	106(1)
C(3)–F	1.358 ^{b)}	C(1)=C(2)–C(3)	94.3(2)
C(2)–C(3)	1.478(6)	C(2)–C(3)–C(4)	85.7(2)
C(3)–C(4)	1.552(6)	C(4)–C(3)–F	115(1)
		C(2)–C(3)–F	117.0(3)
		X–C(4)–C(3) ^{c)}	135.6(3)

^{a)} Not all uncertainties were estimated in the original paper.

^{b)} Assumed.

^{c)} X is a point on the bisector of the F–C–F angle.

Xu, L.-W., Klausner, M.E., Andrews, A.M., Kuczkowski, R.L.: J. Phys. Chem. **97** (1993) 10346.