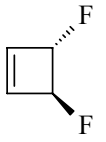
509 **$C_4H_4F_2$** ***trans*-3,4-Difluorocyclobutene** **C_2**

MW



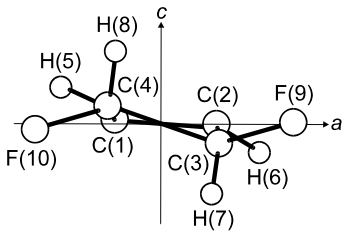
r_s/r_0	Å [a])
C(1)=C(2)	1.349(4)
C(1)–C(4)	1.503(9)
C(3)–C(4)	1.534(4)
C(1)–H(5)	1.081(3)
C(3)–H(7)	1.102(5)
C(3)–F(9)	1.398(6)

θ_s/θ_0	deg [a])
C(1)=C(2)–C(3)	93.3(2)
C(2)–C(3)–C(4)	86.2(5)
C(2)=C(1)–H(5)	134.4(2)
C(4)–C(1)–H(5)	132.3(3)
C(2)–C(3)–H(3)	117.8(5)
C(4)–C(3)–H(7)	112.6(4)
C(2)–C(3)–F(9)	115.9(4)
C(4)–C(3)–F(9)	115.6(5)
H(7)–C(3)–F(9)	107.7(6)
C(1)=C(2)–C(3)–C(4) [b])	–7.5(107)
C(4)–C(1)=C(2)–C(3) [b])	7.6(95)
C(2)–C(3)–C(4)–C(1) [b])	6.7(96)
H(5)–C(1)=C(2)–H(6) [b])	5.4(84)

r_0	Å [c])
C(1)=C(2)	1.351(5)
C(1)–C(4)	1.495(10)
C(3)–C(4)	1.538(5)
C(1)–H(5)	1.080(5)
C(3)–H(7)	1.104(5)
C(3)–F(9)	1.400(10)

θ_0	deg [c])
C(1)=C(2)–C(3)	93.3(5)
C(2)–C(3)–C(4)	86.2(5)
C(2)=C(1)–H(5)	134.4(5)
C(4)–C(1)–H(5)	132.3(5)
C(2)–C(3)–H(3)	118.3(10)
C(4)–C(3)–H(7)	112.6(5)
C(2)–C(3)–F(9)	116.2(5)
C(4)–C(3)–F(9)	115.5(5)
H(7)–C(3)–F(9)	107.2(10)
C(1)=C(2)–C(3)–C(4) [b])	–7.5(150)
C(4)–C(1)=C(2)–C(3) [b])	7.7(150)
C(2)–C(3)–C(4)–C(1) [b])	6.8(150)
H(5)–C(1)=C(2)–H(6) [b])	5.5(150)

Consistent with C_2 symmetry of the molecule, the ring is slightly puckered, and the C–F bonds are roughly equatorial.



[a]) A mixed set of r_s and r_0 structural parameters, more reliable than r_0.
[b]) Dihedral angle.
[c]) Uncertainties were not estimated in the original paper.

Craig, N.C., McCarty, L.V., Lingenfelter, P.T., Osmani, A.S., Rathore, O., Tubergen, M.J., Kuczkowski, R.L.: J. Phys. Chem. A **106** (2002) 6637.