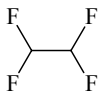
218 **$C_2H_2F_4$** **1,1,2,2-Tetrafluoroethane** **C_2** (*gauche*)

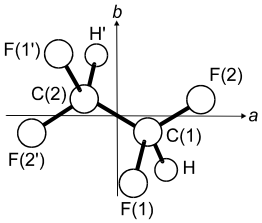
MW



r_0, r_s [a])	Å
C–H	1.104(4)
C–C	1.508(4)
C–F(1)	1.348(5)
C–F(2)	1.359(4)

θ_0, θ_s [a])	deg
C–C–H	112.4(3)
C–C–F(1)	110.1(3)
C–C–F(2)	109.1(4)
F–C–F	108.7 [b])
H–C–C–H [c])	65.2(7)
H–C–C–F(1) [c])	173.4(68)
H–C–C–F(2) [c])	54.2(7)

Atom	a [Å] [d])	b [Å] [d])	c [Å] [d])
C(1)	0.6826	–0.3200	–0.3801
C(2)	–0.6826	0.3200	–0.3801
H	0.8299	–0.9963	–1.2406
H'	–0.8299	0.9963	–1.2406
F(1)	0.8660	–1.0179	0.7581
F(2)	1.6292	0.6527	–0.4522
F(1')	–0.8660	1.0179	0.7581
F(2')	–1.6292	–0.6527	–0.4522



Gauche is the high-energy conformer, whereas the low-energy conformer, the *anti* form, is nonpolar and cannot be studied by MW.

[a]) The C and H Cartesian coordinates were constrained to the r_s values.
[b]) Assumed.
[c]) Dihedral angle.
[d]) The C and H coordinates are single- and double-substitution r_s values. The F coordinates are derived from mixed r_s, r_0 structure fitting.

Maté, B., Walker, A.H., Suenram, R.D., Craig, N.C.: J. Phys. Chem. A **104** (2000) 9489.

IR

C_{2h} (*anti*)

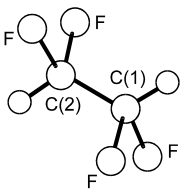
r_0	Å [a])
C–H	1.091(7)
C–C	1.504(7)
C–F	1.360(7)

θ_0	deg [a])
C–C–H	113.1(6)
C–C–F	108.7(6)
F–C–F	107.3(6)
F–C–C–F	63.5(12)

r_s [b])	Å [c])
C–H	1.087(5)
C–C	1.511(4)
C–F	1.359(7)

θ_s	deg [c])
C–C–H	112.9(3)
C–C–F	108.5(6)
F–C–F	107.4(6)
F–C–C–F	63.6(12)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C	±0.67390	0.0	±0.34124
H	±0.59852	0.0	±1.42577
F [b])	±1.36527	±1.09534	∓0.06966



[a]) Uncertainties were not estimated in the original paper.
[b]) The C and H Cartesian coordinates were constrained to the r_s values, while the F coordinates were fitted.
[c]) Costain uncertainties.

Craig, N.C., Oertel, C.M., Oertel, D.C., Lock, M.: J. Phys. Chem. A **105** (2001) 6008.
II/25B(**3**, 605)