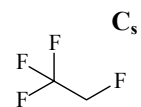


217
MW, IR

 $\text{C}_2\text{H}_2\text{F}_4$

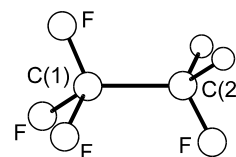
1,1,1,2-Tetrafluoroethane



r_0	\AA		θ_0	deg	
	fit 1	fit 2		fit 1	fit 2
C–C	1.514(6)	1.505(4)	C(2)–C(1)–F(<i>anti</i>)	109.8(2)	111.21(1)
C(1)–F	1.338 ^{a)}	1.338 ^{a)}	C(2)–C(1)–F(<i>gauche</i>)	111.21(2)	111.21(1)
C(2)–F	1.392 ^{a)}	1.392 ^{a)}	C(1)–C(2)–F	108.4(6)	108.5(3)
C–H	1.095 ^{a)}	1.095 ^{a)}	tilt(CF ₃) ^{b)}	0 ^{a)}	1.9(1) ^{c)}
			C–C–H	112.8 ^{a)}	112.8 ^{a)}

^{a)} Assumed.

^{b)} Tilt angle between the C_3 axis of the CF₃ group and the C–C bond direction.

^{c)} Away from C(2)–F bond.

 Xu, L.-H., Andrews, A.M., Cavanagh, R.R., Fraser, G.T., Irikura, K.K., Lovas, F.J., Grabow, J.-U., Stahl, W., Crawford, M.K., Smalley, R.J.: J. Phys. Chem. A **101** (1997) 2288.

 Replaces [II/25B\(3, 604\)](#), MW