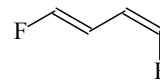


508
MW $C_4H_4F_2$ *(E,Z)*-1,4-Difluoro-1,3-butadiene C_s 

$r_s, r_0^a)$	$\text{\AA}^b)$	$\theta_s, \theta_0^a)$	$\text{deg}^b)$
C(1)=C(2)	1.349(11)	C(1)=C(2)-C(3)	120.1(8)
C(2)-C(3)	1.439(18)	C(2)-C(3)=C(4)	123.1(8)
C(3)=C(4)	1.345(2)	C(2)=C(1)-H(1)	127.4(11)
C(1)-H(1)	1.083(4)	C(1)=C(2)-H(2)	119.0 ^{c)}
C(2)-H(2)	1.082 ^{c)}	C(2)-C(3)-H(3)	116.0 ^{c)}
C(3)-H(3)	1.083 ^{c)}	C(3)=C(4)-H(4)	126.4(3)
C(4)-H(4)	1.092(2)	C(2)=C(1)-F(1)	121.3(11)
C(1)-F(1)	1.347(3)	C(3)=C(4)-F(4)	121.2(2)
C(4)-F(4)	1.347(3)	H(1)-C(1)-F(1)	111.3(2)
		C(3)-C(2)-H(2)	120.9(7)
		C(4)=C(3)-H(3)	120.9(8)
		H(4)-C(4)-F(4)	112.3(1)

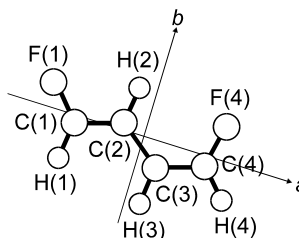
r_0	$\text{\AA}^d)$	θ_0	$\text{deg}^d)$
C(1)=C(2)	1.334(10)	C(1)=C(2)-C(3)	123.5(20)
C(2)-C(3)	1.411(20)	C(2)-C(3)=C(4)	124.5(10)
C(3)=C(4)	1.345(5)	C(2)=C(1)-H(1)	125.3(20)
C(1)-H(1)	1.081(5)	C(1)=C(2)-H(2)	119.0 ^{c)}
C(2)-H(2)	1.082 ^{c)}	C(2)-C(3)-H(3)	116.0 ^{c)}
C(3)-H(3)	1.083 ^{c)}	C(3)=C(4)-H(4)	126.4(5)
C(4)-H(4)	1.091(5)	C(2)=C(1)-F(1)	123.1(20)
C(1)-F(1)	1.351(5)	C(3)=C(4)-F(4)	121.2(5)
C(4)-F(4)	1.348(5)	H(1)-C(1)-F(1)	111.6(5)
		C(3)-C(2)-H(2)	117.5(20)
		C(4)=C(3)-H(3)	119.5(10)
		H(4)-C(4)-F(4)	112.4(5)

^{a)} r_s parameter set supplemented
in part by r_0 set.

^{b)} Uncertainties were estimated
by Costain's procedure.

^{c)} Assumed or dependent.

^{d)} Uncertainties were not estimated
in the original paper.



Craig, N.C., Oertel, C.M., Oertel, D.C., Tubergen, M.J., Lavrich, R.J., Chaka, A.M.:
J. Phys. Chem. A **106** (2002) 4230.