

1505  
MW

**C<sub>4</sub>H<sub>2</sub>F<sub>4</sub>**

**3,3,4,4-Tetrafluorocyclobutene**

**C<sub>2v</sub>**

$r_0$	Å	$\theta_0$	deg
C(1)=C(2)	1.348(3)	C=C-C	93.6(1)
C(1)-C(3)	1.502(3)	C-C-C	86.4(2)
C(3)-C(4)	1.536(3)	C(3)-C(4)-X <sup>a)</sup>	136.3(5)
C-F	1.358(2)	F-C-F	106.2(2)
C-H	1.079(1)	C-C-H	132.1(2)

$r_s$	Å <sup>b)</sup>	$\theta_s$	deg <sup>b)</sup>
C(1)=C(2)	1.350(3)	C=C-C	93.7(1)
C(1)-C(3)	1.500(3)	C-C-C	86.3(2)
C(3)-C(4)	1.542(3)	C(3)-C(4)-X <sup>a)</sup>	136.2(3)
C-F	1.357(2)	F-C-F	106.2(2)
C-H	1.080(1)	C-C-H	132.2(5)

Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
C(1,2)	±0.6750	0.0	-1.5165
C(3,4)	±0.7708	0.0	-0.0197
H	±1.4281	0.0	-2.2913
F	±1.3569	±1.0856	0.5460

<sup>a)</sup> X is a point on the bisector of the F-C-F angle.

<sup>b)</sup> Uncertainties were not all estimated in the original paper.

Andrews, A.M., Maruca, S.L., Hillig, K.W., Kuczkowski, R.L., Craig, N.C.: J. Phys. Chem. **95** (1991) 7714.

