

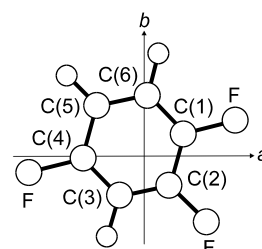
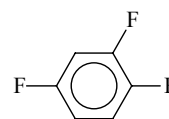
698
MW $\text{C}_6\text{H}_3\text{F}_3$

1,2,4-Trifluorobenzene

 C_s

r_s	\AA^a	θ_s	deg^a
C(1)–C(2)	1.378(2)	C(1)–C(2)–C(3)	121.81(20)
C(2)–C(3)	1.369(2)	C(2)–C(3)–C(4)	117.83(50)
C(3)–C(4)	1.378(5)	C(3)–C(4)–C(5)	122.35(50)
C(4)–C(5)	1.404(5)	C(4)–C(5)–C(6)	118.56(50)
C(5)–C(6)	1.365(2)	C(5)–C(6)–C(1)	119.93(20)
C(6)–C(1)	1.409(2)	C(6)–C(1)–C(2)	119.50(20)

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$
C(1)	1.0854	0.5771
C(2)	0.6690	−0.7365
C(3)	−0.6584	−1.0731
C(4)	−1.5817	−0.05 ^{b)}
C(5)	−1.2045	1.3027
C(6)	0.1258	1.6093

^{a)} Uncertainties were not estimated in the original paper.^{b)} The value directly obtained from Kraitchman's equation is imaginary, and the coordinate was chosen to be −0.05 Å.Jochims, E., Mäder, H., Stahl, W.: J. Mol. Spectrosc. **180** (1996) 116.[II/25D \(3, 2134\)](#)