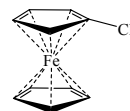


885
MW $C_{10}H_9ClFe$

Chloroferrocene

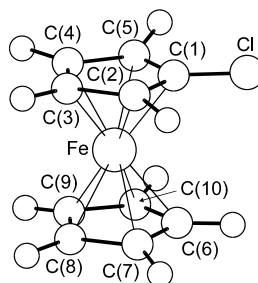
 C_s

r_0	Å	θ_0	deg
C(1)–Cl	1.721(12)	C(5)–C(1)–C(2)	109.4(14)
C(1)–C(2)	1.425(13)	C(1)–C(2)–C(3)	107.0(9)
C(2)–C(3)	1.433(12)	C(2)–C(3)–C(4)	108.3(6)
C(3)–C(4)	1.427(17)	C(10)–C(6)–C(7)	108 ^{a)}
Fe–C(1)	2.017(10)	C(6)–C(7)–C(8)	108 ^{a)}
Fe–C(2)	2.041(8)	C(7)–C(8)–C(9)	108 ^{a)}
Fe–C(3)	2.042(10)	C–Cl bent ^{b)}	2.7(6)
C(6)–C(7)	1.432(5)	tilt(C_5H_4) ^{c)}	1.43(8)
C(7)–C(8)	1.432(5)		
C(8)–C(9)	1.432(5)		
Fe–C(6)	2.048(5)		
Fe–C(7)	2.048(5)		
Fe–C(8)	2.048(5)		



r_s	Å ^{d)}	θ_s	deg ^{d)}
C(1)–Cl	1.726(5)	C(5)–C(1)–C(2)	109.1(3)
C(1)–C(2)	1.422(3)	C(1)–C(2)–C(3)	107.1(3)
C(2)–C(3)	1.420(4)	C(2)–C(3)–C(4)	108.3(3)
C(3)–C(4)	1.424(3)	C(10)–C(6)–C(7)	107.6(3)
Fe–C(1)	2.012(3)	C(6)–C(7)–C(8)	108.3(3)
Fe–C(2)	2.039(4)	C(7)–C(8)–C(9)	107.9(3)
Fe–C(3)	2.050(7)	C–Cl bent ^{b)}	4.1(5)
C(6)–C(7)	1.427(2)	tilt(C_5H_4) ^{c)}	2.2(4)
C(7)–C(8)	1.430(2)		
C(8)–C(9)	1.425(3)		
Fe–C(6)	2.040(7)		
Fe–C(7)	2.048(5)		
Fe–C(8)	2.055(5)		

Atom	x_0 [Å] ^{e)}	y_0 [Å] ^{e)}	z_0 [Å] ^{e)}
Fe	0.0	0.0	0.0
C(6)	1.218	0.0	1.646
C(7)	0.376	1.158	1.646
C(8)	–0.985	0.716	1.646
C(9)	–0.985	–0.716	1.646
C(10)	0.376	–1.158	1.646
H(6)	2.292	0.0	1.725
H(7)	0.709	2.183	1.725
H(8)	–1.857	1.349	1.725
H(9)	–1.857	–1.349	1.725
H(10)	0.709	–2.183	1.725
C(1)	1.226	0.0	–1.602
C(2)	0.403	1.163	–1.628
C(3)	–0.957	0.714	–1.657
C(4)	–0.957	–0.714	–1.657
C(5)	0.403	–1.163	–1.628
Cl	2.947	0.0	–1.643
H(2)	0.755	2.181	–1.707
H(3)	–1.821	1.357	–1.736
H(4)	–1.821	–1.357	–1.736
H(5)	0.755	–2.181	–1.707



Structure Data of Free Polyatomic Molecules

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
Fe	0.477(0.477) ^{f)}	0.200(0.193) ^{f)}	0.011(0.061) ^{f)}
C(6)	1.012	1.772	0.101i ^{g)}
C(7)	1.542	1.118	1.152
C(8)	2.391	0.055	0.712
C(1)	1.531	0.250	0.040
C(2)	1.039	0.914	1.158
C(3)	0.227	1.990	0.712
Cl	2.636	1.073	0.007i ^{g)}

The carbon atoms of the two cyclopentadienyl ligands are eclipsed, similar to normal ferrocene. The average Fe–C distance is 2.042(9) Å, and the estimated displacement of C–H bonds out of the planes of the carbon atoms is 4(2)° away from the metal atom.

^{a)} Assumed.

^{b)} The bent angle of C–Cl from the plane of carbon atoms.

^{c)} The tilt angle of the substituted C₅H₄Cl ligand with respect to the unsubstituted C₅H₅ ligand.

^{d)} Estimated standard errors.

^{e)} A Cartesian coordinate system: the origin is taken to be at the Fe atom, *z* is perpendicular to the unsubstituted C₅H₅ ligand plane, and *x* is in the plane containing the Cl, C(1), and Fe atoms.

^{f)} Values in parentheses are obtained from the combination of ⁵⁶Fe–⁵⁷Fe, while others from the ⁵⁶Fe–⁵⁴Fe.

^{g)} Imaginary value.

Drouin, B.J., Dannemiller, J.J., Kukolich, S.G.: J. Chem. Phys. **112** (2000) 747.