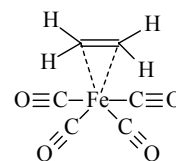


701
MW $\text{C}_6\text{H}_4\text{FeO}_4$ Tetracarbonyl(η^2 -ethene)iron C_{2v}

r_0	Å
Fe–C(1,2)	2.117(14)
Fe–C(ax)	1.815(2)
Fe–C(eq)	1.806(9)
C(1)=C(2)	1.419(7)
C(ax)≡O(ax)	1.142(3)
C(eq)≡O(eq)	1.145(3)
Fe–M ^a)	1.995(16)
[H]–M ^b)	0.217(2)
C–H	1.072(4)

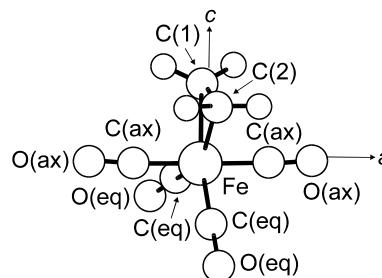
θ_0	deg
C(1)–Fe–C(2)	39.2(5)
C(ax)–Fe–C(ax)	175.1(22)
C(eq)–Fe–C(eq)	111.7(9)
Fe–C(ax)≡O(ax)	179.8(29)
Fe–C(eq)≡O(eq)	179.5(7)
C=C–H	120.6(5)
H–C–H	113.7(6)
Fe–C=C–H ^c)	103.6(9)



r_s	Å
Fe–C(1,2)	2.105(17)
Fe–C(ax)	1.811(1)
Fe–C(eq)	1.808(10)
C(1)=C(2)	1.412(3)
C(ax)≡O(ax)	1.145(2)
C(eq)≡O(eq)	1.147(2)
Fe–M ^a)	1.983(17)
[H]–M ^b)	0.219(3)
C–H	1.073(2)

θ_s	deg
C(1)–Fe–C(2)	39.2(3)
C(ax)–Fe–C(ax)	176.8(13)
C(eq)–Fe–C(eq)	111.4(9)
Fe–C(ax)≡O(ax)	178.2(12)
Fe–C(eq)≡O(eq)	179.4(5)
C=C–H	120.7(1)
H–C–H	113.3(2)
Fe–C=C–H ^c)	103.7(10)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
Fe	0.0	0.0	0.073
C(ax)	±1.814	0.0	0.148
O(ax)	±2.954	0.0	0.205
C(eq)	0.0	±1.496	–0.942
O(eq)	0.0	±2.448	–1.576
C(1,2)	0.0	±0.709	2.067
H	±0.897	±1.254	2.2835



The ethylene ligand exhibits significant structural changes upon complexation to iron, primarily an increase in the C–C bond length with movement of the hydrogen atoms away from the metal center. The plane of the hydrogen atoms is displaced 0.217(2) Å above the ethylene carbon atoms, along the c axis.

^a) M denotes the center of the C=C bond.

^b) [H] denotes the plane made by the ethylene hydrogen atoms.

^c) Dihedral angle.

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[II/25D \(3, 2168\)](#)