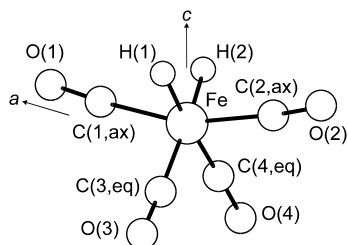


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MW**C₄H₂FeO₄****Tetracarbonyldihydroiron****C_{2v}**
H₂Fe(CO)₄

r_0	Å	θ_0	deg
Fe–H	1.576(64)	H–Fe–H	88.0(28)
Fe–C(1)	1.815(54)	C(3)–Fe–C(4)	99.4(43)
Fe–C(3)	1.818(65)	C(1)–Fe–C(2)	154.2(42)
C(1)≡O(1)	1.123(80)	Fe–C(3)≡O(3)	177.8(68) ^{a)}
C(3)≡O(3)	1.141(74)	Fe–C(1)≡O(1)	172.5(56) ^{a)}

r_s	Å	θ_s	deg ^{b)}
Fe–H	1.590(4)	H–Fe–H	86.7(20)
Fe–C(1)	1.798(17)	C(3)–Fe–C(4)	99.7(20)
Fe–C(3)	1.815(30)	C(1)–Fe–C(2)	152.7(20)

Atom	a_0 [Å]	b_0 [Å]	c_0 [Å]
C(1)	1.769	0.0	0.705
C(2)	–1.769	0.0	0.705
O(1)	2.821	0.0	1.097
O(2)	–2.821	0.0	1.097
C(3)	0.0	1.387	–0.877
C(4)	0.0	–1.387	–0.877
O(3)	0.0	2.285	–1.580
O(4)	0.0	–2.285	–1.580
H(1)	0.0	1.094	1.433
H(2)	0.0	–1.094	1.433
Fe	0.0	0.0	0.299



All of the analyses show that the H atoms are separated by about 2.2 Å, and this indicates that the complex is clearly a “classical dihydride” rather than an η^2 –“dihydrogen” complex. The DFT analysis of the anharmonicity in the Fe–H symmetric stretching potential is shown to support the observed deuterium isotope effects observed for the hydrogen atom coordinates. The anharmonicity effects are larger for the Fe–H stretching coordinate than for the H–Fe–H interbond angle. The r_0 (Fe–D) bond lengths were observed to be 0.05(4) Å shorter than the r_0 (Fe–H) bond lengths.

^{a)} All of the carbonyl groups are bent toward the hydrogen atoms.

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

Drouin, B.J., Kukolich, S.G.: J. Am. Chem. Soc. **120** (1998) 6774.

[II/25C \(3, 1509\)](#)