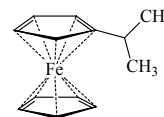


920 **C₁₃H₁₆Fe**ED, DFT
calculations**(1-Methylethyl)ferrocene**

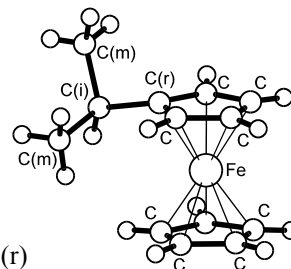
Isopropylferrocene

C₁

r_a	\AA^a	θ_a	deg^a
Fe...C(ring)	2.058(1)	Fe...C(r)–C(i)	126.2(7)
C–C ^{b)}	1.473(3)	C–C(r)–C(i)	111.9(7)
C–H ^{b)}	1.088(8)	Fe...C(ring)–H	123.2(8)
Fe...X ^{c)}	1.659(1)	C(i)–C(m)–H	110.3(9)
C(ring)–C(ring) ^{b)}	1.432(1)	C(r)–C(i)–H	107.1(9)
C(r)–C(i)	1.501(6)	C(m)–C(i)–C(m)	111.4(9)
C(i)–C(m) ^{b)}	1.525(6)	twist(ring) ^{d)}	1.5(8)
C(ring)–H ^{b)}	1.083(8)	H–C(i)–C(r)...Fe	–39.1(20)/172(7)
C(m)–H ^{b)}	1.092(8)	C(m)–C(i)–C(r)...Fe	77.9(20)/–71(7)
		twist(methyl) ^{e)}	45(4)
		$\gamma^f)$	0.0 ^{g)}

The molecule was found to exist as a mixture of two conformers with essentially eclipsed ring-ring structure and different H–C(i)–C(r)...Fe torsional angles (see table). However, it was impossible to determine the exact ratio of the two conformers. Each of the two rings was assumed to have local C_{5v} symmetry, with the iron atom lying on the C₅ axis. Each methyl group and isopropyl group were assumed to have local C_{3v} and C_s symmetry, respectively. Differences in the C–C and C–H bond lengths were loosely restrained to the values from B3PW91/6-31G* calculations.

The nozzle temperature was 450 K.



^{a)} Estimated standard errors.

^{b)} Average value.

^{c)} X is the center of the ring.

^{d)} Angle between the two HC(ring)Fe planes, zero degree when the H–C(ring) bonds eclipse each other.

^{e)} Twist angle of the methyl group, *i.e.*, H–C(m)–C(i)–C(r) torsional angle; zero degree for the eclipsed position.

^{f)} Angle between the C(r)–C(i) bond and the ring plane, bent toward the Fe atom.

^{g)} Dependent parameter.

Morrison, C.A., Bone, S.A., Rankin, D.W.H., Robertson, H.E., Parsons, S., Coxall, R.A., Fraser, S., Howell, J.A.S., Yates, P.C., Fey, N.: *Organometallics* **20** (2001) 2309.