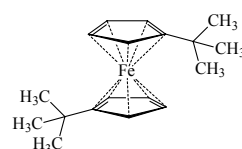


**940**      **C<sub>18</sub>H<sub>26</sub>Fe**ED, DFT  
calculations**1,1'-Bis(1,1-dimethylethyl)ferrocene**1,1'-Di-*t*-butylferrocene**C<sub>2</sub> assumed**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
Fe...C(ring)	2.069(1)	Fe...C(r)–C(t)	131.6(3)
C–C <sup>b)</sup>	1.481(1)	C–C(r)–C(t)	112.3(3)
C–H <sup>b)</sup>	1.111(3)	Fe...C(ring)–H	124.2(15)
Fe...X <sup>c)</sup>	1.671(1)	C–C–H	109.6(11)
C(ring)–C(ring) <sup>b)</sup>	1.434(1)	twist(ring) <sup>d)</sup>	97.7(4)
C(r)–C(t)	1.518(2)	twist( <i>t</i> -butyl) <sup>e)</sup>	165.2(5)
C(t)–C(m) <sup>b)</sup>	1.538(2)	twist(methyl) <sup>f)</sup>	63(3)
C(ring)–H <sup>b)</sup>	1.105(3)	$\gamma^g$	5.5 <sup>h)</sup>
C(m)–H <sup>b)</sup>	1.118(3)		

According to a molecular mechanics calculation, the molecule exists as a mixture of two C<sub>2</sub> conformers with essentially eclipsed ring-ring structure and with different angles between the two *t*-butyl groups, *ca.* 72° and 144°. However, it was impossible to distinguish them by the ED analysis. Each of the two rings was assumed to have local C<sub>5v</sub> symmetry, with the iron atom lying on the C<sub>5</sub> axis. Each methyl group and each *t*-butyl group were assumed to have local C<sub>3v</sub> and C<sub>3</sub> 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.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> Average value.

<sup>c)</sup> X is the center of the ring.

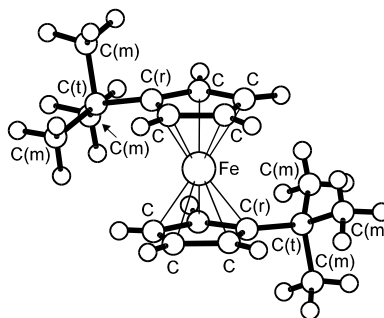
<sup>d)</sup> Angle between the two *t*-butyl groups, zero degree when the C(r)–C(t) bonds eclipse each other.

<sup>e)</sup> Twist angle of the *t*-butyl group, *i.e.*, C(m)–C(t)–C(r)...Fe torsional angle; zero degree for the eclipsed position.

<sup>f)</sup> Twist angle of the methyl group, *i.e.*, H–C(m)–C(t)–C(r) torsional angle; zero degree for the eclipsed position.

<sup>g)</sup> Angle between the C(r)–C(t) bond and the ring plane, bent toward the Fe atom.

<sup>h)</sup> 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.