metal-organic papers

Dicarbonyl(η^5-cyclopentadienyl)iodoiron(II)

Matthias Zeller, Evelyn Lazich and Allen D. Hunter*

Department of Chemistry, Youngstown State University, One University Plaza, Youngstown, OH 44555, USA

Correspondence e-mail: adhunter@ysu.edu

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.005 Å
R factor = 0.026
wR factor = 0.059
Data-to-parameter ratio = 18.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, [Fe(C_5H_5)I(CO)$_2$], there are two independent molecules in the asymmetric unit. They exhibit a three-legged-piano-stool geometry.
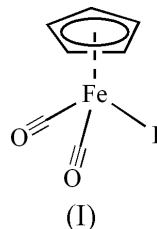
Comment

The title compound, (I), is a widely used and easily prepared precursor for a variety of organometallic iron complexes. While some similar complexes with substituted Cp rings have been structurally characterized (McArdle *et al.*, 1999; Akita *et al.*, 1996; and others), the structure of the parent compound with a simple Cp ring has not yet been reported.

(I)

There are two independent molecules in the asymmetric unit. They exhibit the expected three-legged-piano-stool geometry (Fig. 1). The bond distances and bond angles for the two molecules are essentially identical (Table 1). The OC—Fe—I angles are 89.18 (8)–91.41 (8)° and the OC—Fe—CO angles are slightly larger [93.95 (12) and 93.83 (12)°]. The iodo substituent exhibits a nearly staggered conformation with respect to the Cp ring, the I1—Fe1$\cdots$Cg1—C11 and I2—
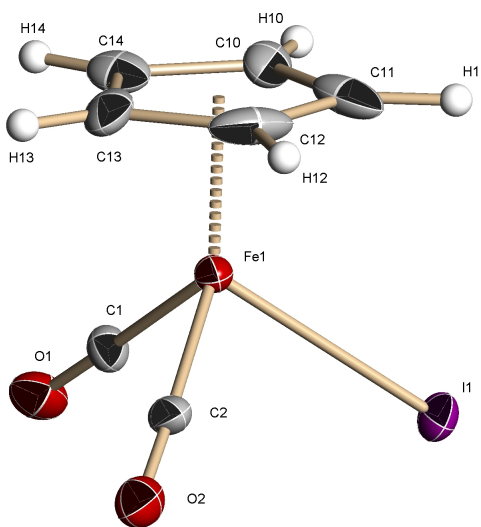
Figure 1
Structure of one of the two independent molecules in (I), showing 30% probability displacement ellipsoids.

Fe2···$Cg2$—C21 torsion angles being 15.9 and 17.5°, respectively, where $Cg1$ and $Cg2$ are the centroids of the Cp rings. The distances between the metal and the ring centroid are 1.717 (20) and 1.725 (20) Å. All bond length and angles are in agreement with values reported for similar complexes.

Experimental

The title complex, (I), was prepared as described by Hunter (2003). X-ray quality crystals were grown from a toluene–decane mixture.

Crystal data

[Fe(C$_5$H$_5$)I(CO)$_2$]	$D_x = 2.374$ Mg m^{-3}
$M_r = 303.86$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6438
$a = 13.1442$ (7) Å	reflections
$b = 10.2568$ (6) Å	$\theta = 2.5$–28.3°
$c = 12.8680$ (7) Å	$\mu = 5.35$ mm^{-1}
$\beta = 101.502$ (1)°	$T = 100$ (2) K
$V = 1699.99$ (16) Å^3	Block, red
$Z = 8$	$0.22 \times 0.17 \times 0.17$ mm

Data collection

Bruker SMART APEX CCD diffractometer	4207 independent reflections
	4077 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.025$
Absorption correction: multi-scan (SADABS in SAINT-Plus; Bruker, 1997–1999)	$\theta_{max} = 28.3°$
	$h = -17 \rightarrow 17$
	$k = -13 \rightarrow 13$
$T_{min} = 0.295$, $T_{max} = 0.400$	$l = -17 \rightarrow 17$
17 192 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.6662P]$
$R[F^2 > 2\sigma(F^2)] = 0.026$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.059$	
$S = 1.32$	$(\Delta/\sigma)_{max} = 0.001$
4207 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
229 parameters	$\Delta\rho_{min} = -0.69$ e Å^{-3}
Only coordinates of H atoms refined	

Table 1
Selected geometric parameters (Å, °).

C3—Fe2	1.777 (3)	Fe1—C2	1.780 (3)
I2—Fe2	2.6082 (4)	Fe1—C1	1.783 (3)
I1—Fe1	2.6063 (4)	Fe2—C4	1.785 (3)
C2—Fe1—C1	93.95 (12)	C3—Fe2—C4	93.83 (12)
C2—Fe1—I1	91.41 (8)	C3—Fe2—I2	90.55 (9)
C1—Fe1—I1	89.41 (9)	C4—Fe2—I2	89.18 (8)

All H atoms were positioned from difference Fourier maps, and refined with U_{iso}(H) values defined as $1.2U_{eq}$(parent atom). The C—H bond lengths are 0.87 (4)–1.00 (4) Å. The s.u. values of the cell parameters were derived by the software, giving values that are unreasonably small (Herbstein, 2000).

Data collection: SMART (Bruker, 1997–2000); cell refinement: SAINT-Plus (Bruker, 1997–1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXL97; software used to prepare material for publication: SHELXL97.

References

Akita, M., Terada, M., Tanaka, M. & Morooka, Y. (1996). *J. Organomet. Chem.* **510**, 255–261.
Bruker (1997–2000). *SMART*. Version 5.625 for WNT/2000. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1997–1999). *SAINT-Plus*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Herbstein, F. H. (2000). *Acta Cryst.* B**56**, 547–557.
Hunter, A. D. (2003). *Inorganic Experiments*, 2nd ed., edited by J. D. Woolins, pp. 214–221. Weinheim, Germany: Wiley-VCH.
McArdle, P., O'Neill, L. & Cunningham, D. (1999). *Inorg. Chim. Acta*, **291**, 252–257.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.