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μ-Diphenylphosphido-μ-hydrido-bis[carbonyl-(η^5-cyclopentadienyl)iron(II)]

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The title compound, $[Fe_2(C_5H_5)_2(C_{12}H_{10}P)H(CO)_2]$, features near symmetric hydride and phosphide bridges. The two carbonyl/cyclopentadienyl groups are in *trans* positions. One of the cyclopentadienyl rings is disordered over two positions, with occupancies of 0.65 and 0.35.

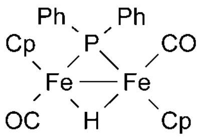
Key indicators

Single-crystal X-ray study
T = 198 K
Mean σ(C–C) = 0.002 Å
R factor = 0.017
wR factor = 0.045
Data-to-parameter ratio = 14.8

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

Comment

While dinuclear iron hydride complexes are a well known class of compounds, crystallographically characterized examples of the neutral monohydrido complexes are rare. The only examples are $(\mu_2\text{-CNMe}_2)(\mu_2\text{-H})Fe_2Cp_2(CO)_2$, (II) (Albano *et al.*, 2000), and $(\mu_2\text{-PPh}_2)(\mu_2\text{-H})(\mu_2\text{-dppm})Fe_2Cp_2$, (III) (dppm = $Ph_2P\text{-}CH_2\text{-}PPh_2$; Raubenheimer *et al.*, 1992).



(I)

The title compound, (I), features near symmetric hydride and phosphide bridges, with bond distances 1.66 (2) (Fe1—H1), 1.62 (2) (Fe2—H1), 2.1836 (4) (Fe1—P1) and 2.1940 (4) Å (Fe2—P2). The Fe—H distances are similar to those found in compounds (II) [1.59 (2) and 1.63 (2) Å] and

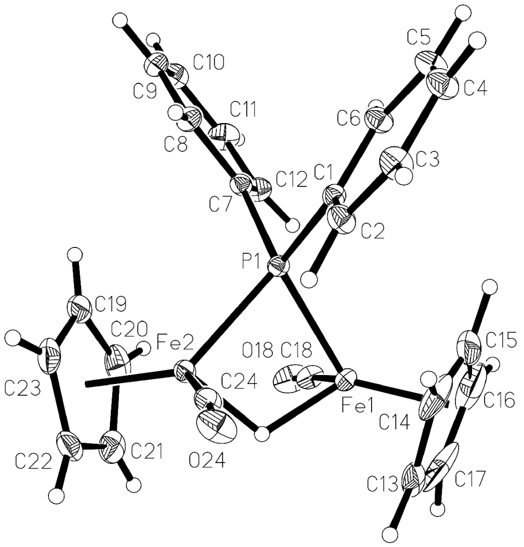


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 30% probability level. Only the major component of the disordered cyclopentadienyl ring is shown. H atoms, including the bridging H1 species, are shown as spheres of arbitrary radii.

(III) [1.68 (2) and 1.78 (2) Å]. The Fe—Fe distance [2.7098 (3) Å] is slightly shorter than in compound (III) [2.787 (1) Å], but significantly longer than in compound (II) [2.5877 (9) Å]; the latter difference is most likely due to the smaller C atom in the carbyne bridge. Compound (I) contains a planar four-membered heterocycle [atoms H1, Fe1, Fe2 and P1] and the cyclopentadienyl and carbonyl groups are in a *trans* geometry, respectively, with a C18—Fe1—Fe2—C24 torsion angle of 166.78 (7)°. This is in contrast to compounds (II) and (III), where a *cis* arrangement is observed, in compound (III) necessitated by the bridging dppm group. One of the cyclopentadienyl rings in complex (I) is disordered over two positions, with occupancies of 0.65 (C13–C17) and 0.35 (C13*A*–C17*A*), respectively.

Experimental

The title compound was prepared according to the literature procedure of Hayter (1963).

Crystal data

$[Fe_2(C_5H_5)_2(C_{12}H_{10}P)H(CO)_2]$
$M_r = 484.08$
Orthorhombic, $P2_12_12_1$
$a = 10.2945$ (5) Å
$b = 12.5071$ (6) Å
$c = 15.9110$ (8) Å
$V = 2048.61$ (17) Å^3
$Z = 4$
$D_x = 1.570$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6155 reflections
$\theta = 2.4$–28.6°
$\mu = 1.51$ mm^{-1}
$T = 198$ (2) K
Prism, dark red
0.48 × 0.35 × 0.30 mm

Data collection

Bruker SMART1000/*P*4 diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.561$, $T_{max} = 0.635$
14 556 measured reflections
4609 independent reflections
4506 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$
$h = -12 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.045$
$S = 1.05$
4609 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0186P)^2 + 0.1562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983), 1955 Friedel pairs
Flack parameter = −0.002 (8)

H atoms were placed in calculated positions, with C—H distances fixed at 0.95 Å and $U_{iso} = 1.2U_{eq}$ of the carrier C atom. Atom H1 was found in a Fourier difference map and refined with an isotropic displacement parameter.

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SAINT* (Bruker, 1997–1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1977*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Albano, V. G., Busetto, L., Monari, M. & Zanotti, V. (2000). *J. Organomet. Chem.* **606**, 163–168.

Bruker (1997–1999). *SMART* (Version 5.054) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Hayter, R. G. (1963). *J. Am. Chem. Soc.* **85**, 3120–3124.

Raubenheimer, H. G., Scott, F., Cronje, S. & vanRooyen, P. H. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1859–1863.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

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