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(*S*,*S*,*Rp*)-(+)-2-{1-[1-(2-Diphenylphosphinoferrocenyl)ethyl]pyrrolidin-2-yl}-propan-2-ol

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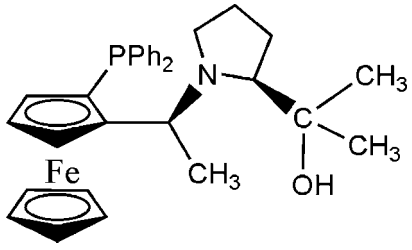
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.033; wR factor = 0.088; data-to-parameter ratio = 18.6.

The title compound, [Fe(C_5H_5)($C_{26}H_{31}$NOP)], contains one planar and two central chiral centers. It is of interest with respect to asymmetric catalysis. In the ferrocenyl moiety, the cyclopentadienyl (Cp) rings are twisted from the eclipsed conformation by 15.83° (average value). The two Cp rings make a dihedral angle of 5.24 (10)°. There are intramolecular O—H···N, C—H···P and C—H···π hydrogen bonds. The structure is packed by one prominent and other weak C—H···π contacts and hydrophobic interactions.

Related literature

For related literature, see: Dai *et al.* (2003); Togni (1996).



Experimental

Crystal data

[Fe(C_5H_5)($C_{26}H_{31}$NOP)]
M_r = 525.43
Orthorhombic, $P2_12_12_1$
a = 10.1102 (4) Å
b = 13.6587 (5) Å
c = 19.4363 (8) Å
V = 2684.00 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 293 (2) K
0.31 × 0.25 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.825, T_{max} = 0.898
16205 measured reflections
6152 independent reflections
5154 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 0.92
6152 reflections
330 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 2685 Friedel pairs
Flack parameter: 0.022 (12)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	2.53	2.844 (2)	104
C11—H11···P1	0.98	2.86	3.371 (2)	114
C16—H16···P1	0.98	2.87	3.778 (2)	154

Table 2
Selected torsion angles (°).

C1—*Cg*3—*Cg*4—C7	16.63	C4—*Cg*3—*Cg*4—C10	15.63
C2—*Cg*3—*Cg*4—C8	15.99	C5—*Cg*3—*Cg*4—C6	15.80
C3—*Cg*3—*Cg*4—C9	15.20		

*Cg*3 is the centroid of the Cp ring system C1–C5, *Cg*4 is the centroid of the Cp ring system C6–C10.

Table 3
X—H···*Cg* (π-ring) interaction geometry (Å, °).

X—H···*Cg*	X—H	H···*Cg*	X···*Cg*	X—H···*Cg*
C1—H1···*Cg*6	0.98	2.95	3.66 (3)	131
C30—H30···*Cg*3$^{(i)}$	0.98	2.96	3.864 (3)	165

*Cg*6 is the centroid of the π-ring system C26–C31. *Cg*3 is the centroid of the Cp ring system C1–C5. Symmetry code: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2031).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m2499-m2500 [**doi:10.1107/S160053680704305X**]

(*S*,*S*,*Rp*)-(+)-2-{1-[1-(2-Diphenylphosphinoferrocenyl)ethyl]pyrrolidin-2-yl}propan-2-ol

J.-T. Liu, Y.-J. Mao, R.-M. Xi and W.-L. Dong

Comment

The application of ferrocenyl ligands possessing planar chirality in asymmetric catalysis has received considerable interest (Dai *et al.*, 2003). Ferrocenyl ligands with planar and central chirality have shown efficiency as ligands for catalytic asymmetric synthesis both in research and industrial processes (Togni, 1996). The molecule of the title compound contains one planar and two central chiral centers (I) (Scheme 1).

The X-ray structure analysis of the title compound (Figure 2) proves the absolute configuration shown in Scheme 1. The diastereomeric ferrocenyl ligand (I) was prepared from enantiopure (*S, Rp*)-1-(2-diphenylphosphinoferrocenyl)ethyl acetate by replacement of the acetoxy group by (*S*)-2-(pyrrolidine-2-yl)propane-2-ol with retention of the configuration on the α-carbon atom.

In the ferrocenyl moiety, the cyclopentadienyl (Cp) rings are twisted from the eclipsed conformation·The values of the torsion angles defined with C atoms of Cp rings in opposite position and ring centroids (C– *Cg*3- *Cg*4- C) are in the range 15.20- 16.63° (Table 1)·The rings are nearly parallel with dihedral angle of 5.24°between the two best planes.

The pyrrolidine ring adopts an envelope conformation. The methylene group is inclined to the atoms defining the planar part of the five member ring by 40.71° or 38.36°.

The structure has intramolecular hydrogen bonds such as O1—H1A···N1, C11—H11···P1 and C16—H16···P1 (Table 2). Furthermore, there is one intramoleculear C—H···π contact C1—H1···*Cg*6 with distances C1···*Cg*6 3.66 (3) Å, angle around H1 131 °, and *Cg*6 is the centroid (centre of gravity) of the π-ring system C26 to C31 (Table 3).

The intermolecular C–H···π contact which connects molecules is C30—H30···*Cg*3 with distances C30···*Cg*3 3.864 (3) Å, angle around H30 165 °. The symmetry operation of the intermolecular contact for *Cg*3 is (−1/2 + *x*, 1/2 − *y*, 1 − *z*), which represents a 2_1 axis helical chain as shown in Table 3 and Fig. 3.

Experimental

(*S*)- 2-(pyrrolidine-2-yl)propane-2-ol(0.645 g, 5 mmol) and (*S, Rp*)-1-(2-diphenylphosphinoferrocenyl)ethyl acetate(0.228 g, 0.5 mmol) were dissolved in methanol(3 mL) and the reaction mixture was gently refluxed in an oil bath heated to 347–352 K under N_2-atmosphere for 7 h (Fig. 1). The solvent was evaporated *in vacuo* and the residue was purified by chromatography on Al_2O_3-column with ethyl acetate–petroleum ether(1:20) as eluent. The title compound (0.234 g, 89%) was obtained as a yellow solid, mp 439.7- 440.2 K. Crystals suitable for X-ray diffraction analysis were grown from cyclohexane- DCM (20:1) solution at 277 K. Spectroscopic analysis: ^{1}H NMR (300 MHz, $CDCl_3$, TMS p.p.m.): d 0.607 (s, 3H), 0.750 (m, 1H), 0.938(m, 1H), 1.119(s, 3H), 1.135(m, 1H), 1.283(m, 1H), 1.639(d, 3H), 2.584(m, 2H), 2.734(m, 1H), 3.833(s, 5H), 4.208(m, 1H), 4.211(m, 1H), 4.439(m, 1H), 4.512(m, 1H), 7.218–7.767(m, 10H).

Refinement

All H atoms were placed in geometrically calculated positions(C—H = 0.93–0.98 Å and O—H = 0.82 Å) and refined using a riding model, their isotropic displacement parameters were set to 1.2 times (1.5 times for CH_3 groups) the equivalent displacement parameter of their parent atoms.

The pyrrolidine ring shows positional disorder of atom C14. The flipping of H atoms at C13 and C15 were also considered in the refinement. The final site occupatio ratio of the related atoms was 0.6:0.4.

The absolute configuration of the structure of the crystal could be determined reliably; the Flack parameter (Flack, 1983) was refined using 2685 Friedel opposite reflections.

Figures

Fig. 1. Reaction scheme.

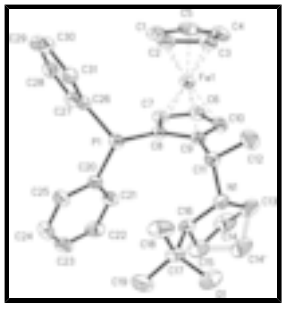


Fig. 2. The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level and H atoms omitted.

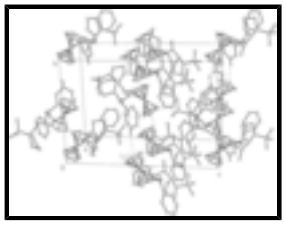


Fig. 3. View of the structure along the *a* axis. H atoms were omitted for clarity except those which were involved with *X*—H···*Cg*(π-ring) interactions.

(*S*,*S*,*R*p)-(+)-2-{1-[1-(2-diphenylphosphino ferrocenyl)ethyl]pyrrolidin-2-yl}propan-2-ol

Crystal data

$[Fe(C_5H_5)(C_{26}H_{31}NOP)]$	D_x = 1.300 Mg m^{-3}
M_r = 525.43	Melting point: 440.0 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.1102 (4) Å	Cell parameters from 5318 reflections
b = 13.6587 (5) Å	θ = 2.3–26.6º
c = 19.4363 (8) Å	μ = 0.65 mm^{-1}
V = 2684.00 (18) Å^3	T = 293 (2) K
Z = 4	Prism, yellow

F_{000} = 1112	0.31 × 0.25 × 0.17 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	6152 independent reflections
Radiation source: fine-focus sealed tube	5154 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -13 \rightarrow 12$
T_{min} = 0.825, T_{max} = 0.898	$k = -17 \rightarrow 16$
16205 measured reflections	$l = -24 \rightarrow 25$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.088	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.92	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
6152 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
330 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack, 1983
Secondary atom site location: difference Fourier map	Flack parameter: 0.022 (12)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.3621 (3)	0.4260 (2)	0.54550 (16)	0.0660 (8)	
H1	0.2659	0.4298	0.5514	0.079*	
C2	0.4284 (3)	0.38314 (16)	0.49015 (16)	0.0586 (7)	

H2	0.3865	0.3525	0.4501	0.070*
C3	0.5653 (3)	0.39228 (16)	0.50107 (16)	0.0561 (6)
H3	0.6352	0.3689	0.4703	0.067*
C4	0.5839 (3)	0.44111 (18)	0.56433 (14)	0.0610 (7)
H4	0.6692	0.4574	0.5853	0.073*
C5	0.4588 (3)	0.4623 (2)	0.59210 (14)	0.0711 (8)
H5	0.4414	0.4952	0.6360	0.085*
C6	0.4875 (3)	0.67342 (16)	0.52054 (11)	0.0493 (6)
H6	0.4975	0.7021	0.5665	0.059*
C7	0.3657 (2)	0.65036 (14)	0.48780 (11)	0.0425 (5)
H7	0.2772	0.6605	0.5071	0.051*
C8	0.3952 (2)	0.60983 (14)	0.42156 (10)	0.0353 (4)
C9	0.5380 (2)	0.60872 (15)	0.41390 (10)	0.0387 (4)
C10	0.5916 (2)	0.64693 (16)	0.47607 (12)	0.0470 (5)
H10	0.6860	0.6536	0.4864	0.056*
C11	0.6132 (2)	0.58181 (15)	0.34878 (11)	0.0422 (5)
H11	0.5540	0.5409	0.3211	0.051*
C12	0.7380 (3)	0.5216 (2)	0.36188 (15)	0.0698 (8)
H12A	0.7786	0.5051	0.3187	0.105*
H12B	0.7151	0.4626	0.3860	0.105*
H12C	0.7988	0.5591	0.3892	0.105*
C16	0.5389 (2)	0.71609 (15)	0.27045 (12)	0.0436 (5)
H16	0.4559	0.6966	0.2926	0.052*
C17	0.5344 (3)	0.68590 (18)	0.19393 (12)	0.0514 (6)
C18	0.5072 (4)	0.57731 (19)	0.18663 (13)	0.0742 (9)
H18A	0.4985	0.5611	0.1388	0.111*
H18B	0.4267	0.5612	0.2103	0.111*
H18C	0.5791	0.5408	0.2062	0.111*
C19	0.4297 (3)	0.7435 (3)	0.15570 (15)	0.0805 (9)
H19A	0.4543	0.8114	0.1545	0.121*
H19B	0.3463	0.7367	0.1788	0.121*
H19C	0.4221	0.7190	0.1096	0.121*
C20	0.1972 (2)	0.66731 (17)	0.32383 (11)	0.0423 (5)
C21	0.2223 (3)	0.76359 (18)	0.34252 (13)	0.0503 (6)
H21	0.2799	0.7767	0.3786	0.060*
C22	0.1622 (3)	0.8404 (2)	0.30780 (15)	0.0649 (8)
H22	0.1803	0.9047	0.3206	0.078*
C23	0.0764 (3)	0.8222 (3)	0.25479 (16)	0.0727 (9)
H23	0.0369	0.8742	0.2317	0.087*
C24	0.0487 (3)	0.7287 (3)	0.23584 (17)	0.0799 (9)
H24	−0.0101	0.7165	0.2001	0.096*
C25	0.1085 (3)	0.6517 (2)	0.27006 (14)	0.0647 (7)
H25	0.0890	0.5879	0.2568	0.078*
C26	0.1488 (2)	0.50485 (16)	0.41030 (11)	0.0426 (5)
C27	0.0678 (2)	0.55690 (18)	0.45498 (12)	0.0496 (5)
H27	0.0759	0.6246	0.4582	0.060*
C28	−0.0248 (2)	0.5084 (2)	0.49475 (13)	0.0632 (6)
H28	−0.0771	0.5436	0.5254	0.076*
C29	−0.0403 (3)	0.4090 (2)	0.48939 (15)	0.0693 (8)

H29	−0.1017	0.3767	0.5168	0.083*	
C30	0.0356 (3)	0.3577 (2)	0.44329 (15)	0.0668 (8)	
H30	0.0231	0.2906	0.4384	0.080*	
C31	0.1301 (3)	0.40437 (18)	0.40422 (13)	0.0530 (6)	
H31	0.1817	0.3685	0.3736	0.064*	
Fe1	0.47849 (3)	0.528215 (19)	0.498686 (16)	0.04009 (9)	
N1	0.6497 (2)	0.66738 (15)	0.30560 (10)	0.0468 (5)	
P1	0.28173 (6)	0.55894 (4)	0.35818 (3)	0.03890 (13)	
O1	0.6585 (2)	0.70818 (16)	0.16220 (11)	0.0733 (6)	
H1A	0.7172	0.6760	0.1805	0.110*	
C13	0.7295 (3)	0.7435 (2)	0.34085 (17)	0.0690 (9)	0.606 (5)
H13A	0.8057	0.7618	0.3134	0.083*	0.606 (5)
H13B	0.7596	0.7208	0.3855	0.083*	0.606 (5)
C14	0.6346 (6)	0.8288 (3)	0.3484 (3)	0.0771 (17)	0.606 (5)
H14A	0.5756	0.8195	0.3872	0.092*	0.606 (5)
H14B	0.6818	0.8901	0.3540	0.092*	0.606 (5)
C15	0.5603 (3)	0.82650 (19)	0.28158 (16)	0.0694 (8)	0.606 (5)
H15A	0.6120	0.8549	0.2446	0.083*	0.606 (5)
H15B	0.4767	0.8610	0.2852	0.083*	0.606 (5)
C13'	0.7295 (3)	0.7435 (2)	0.34085 (17)	0.0690 (9)	0.394 (5)
H13C	0.8223	0.7255	0.3415	0.083*	0.394 (5)
H13D	0.6995	0.7527	0.3878	0.083*	0.394 (5)
C14'	0.7082 (10)	0.8361 (6)	0.2987 (5)	0.084 (3)	0.394 (5)
H14C	0.7622	0.8365	0.2575	0.101*	0.394 (5)
H14D	0.7262	0.8946	0.3254	0.101*	0.394 (5)
C15'	0.5603 (3)	0.82650 (19)	0.28158 (16)	0.0694 (8)	0.394 (5)
H15C	0.5385	0.8630	0.2403	0.083*	0.394 (5)
H15D	0.5063	0.8503	0.3193	0.083*	0.394 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0695 (17)	0.0564 (17)	0.0721 (19)	−0.0025 (14)	0.0044 (15)	0.0300 (14)
C2	0.0778 (16)	0.0351 (11)	0.0628 (17)	−0.0028 (11)	−0.0135 (14)	0.0124 (12)
C3	0.0721 (15)	0.0395 (11)	0.0567 (14)	0.0100 (10)	−0.0116 (15)	0.0056 (13)
C4	0.0739 (17)	0.0536 (15)	0.0556 (15)	0.0058 (14)	−0.0211 (13)	0.0114 (12)
C5	0.108 (2)	0.0671 (18)	0.0387 (13)	0.0085 (17)	0.0035 (14)	0.0204 (12)
C6	0.0722 (16)	0.0385 (11)	0.0372 (11)	−0.0027 (11)	−0.0073 (10)	−0.0052 (8)
C7	0.0571 (13)	0.0330 (10)	0.0374 (12)	0.0051 (9)	−0.0019 (9)	−0.0019 (8)
C8	0.0447 (11)	0.0285 (10)	0.0327 (10)	0.0026 (8)	−0.0033 (8)	0.0026 (8)
C9	0.0459 (12)	0.0325 (10)	0.0375 (10)	−0.0015 (9)	−0.0036 (9)	0.0022 (8)
C10	0.0512 (13)	0.0432 (12)	0.0466 (12)	−0.0040 (10)	−0.0085 (10)	0.0017 (9)
C11	0.0443 (11)	0.0427 (12)	0.0396 (11)	0.0020 (9)	0.0002 (9)	0.0017 (9)
C12	0.0602 (15)	0.083 (2)	0.0659 (17)	0.0234 (15)	0.0025 (13)	0.0093 (16)
C16	0.0506 (12)	0.0369 (11)	0.0432 (11)	−0.0014 (10)	0.0082 (10)	0.0040 (9)
C17	0.0657 (15)	0.0491 (13)	0.0394 (12)	−0.0024 (12)	0.0078 (11)	0.0079 (10)
C18	0.128 (3)	0.0558 (16)	0.0388 (13)	−0.0158 (18)	0.0062 (16)	−0.0057 (11)
C19	0.092 (2)	0.095 (2)	0.0543 (18)	0.0138 (19)	−0.0033 (16)	0.0224 (16)

C20	0.0432 (12)	0.0457 (13)	0.0379 (11)	0.0022 (10)	0.0021 (9)	0.0077 (9)
C21	0.0545 (14)	0.0512 (14)	0.0451 (14)	0.0096 (13)	0.0017 (11)	0.0048 (10)
C22	0.0781 (19)	0.0485 (16)	0.0680 (18)	0.0153 (15)	0.0144 (15)	0.0100 (13)
C23	0.0628 (17)	0.084 (2)	0.0714 (19)	0.0225 (16)	0.0024 (15)	0.0325 (17)
C24	0.0631 (18)	0.102 (3)	0.075 (2)	0.0004 (18)	−0.0233 (15)	0.0265 (19)
C25	0.0667 (17)	0.0670 (17)	0.0603 (16)	−0.0095 (14)	−0.0186 (13)	0.0135 (13)
C26	0.0482 (12)	0.0403 (12)	0.0393 (11)	−0.0042 (9)	−0.0071 (9)	0.0060 (9)
C27	0.0477 (12)	0.0504 (13)	0.0507 (13)	0.0014 (11)	−0.0006 (10)	0.0061 (11)
C28	0.0494 (12)	0.0930 (19)	0.0472 (13)	0.0017 (13)	0.0017 (12)	0.0107 (14)
C29	0.0616 (16)	0.0818 (19)	0.0646 (18)	−0.0210 (14)	−0.0123 (14)	0.0327 (16)
C30	0.0746 (18)	0.0529 (15)	0.0729 (18)	−0.0203 (15)	−0.0180 (16)	0.0186 (13)
C31	0.0616 (15)	0.0445 (13)	0.0528 (14)	−0.0085 (12)	−0.0131 (12)	0.0020 (11)
Fe1	0.05131 (17)	0.03507 (15)	0.03388 (15)	0.00183 (12)	−0.00484 (15)	0.00278 (13)
N1	0.0480 (11)	0.0493 (12)	0.0430 (10)	−0.0080 (9)	0.0028 (8)	0.0024 (9)
P1	0.0447 (3)	0.0374 (3)	0.0345 (3)	−0.0005 (2)	−0.0015 (2)	−0.0021 (2)
O1	0.0793 (13)	0.0776 (14)	0.0631 (13)	−0.0072 (11)	0.0299 (11)	0.0018 (10)
C13	0.0708 (19)	0.075 (2)	0.0614 (19)	−0.0344 (18)	−0.0015 (14)	0.0037 (14)
C14	0.110 (4)	0.050 (3)	0.071 (3)	−0.029 (3)	0.005 (3)	−0.013 (2)
C15	0.093 (2)	0.0421 (14)	0.0734 (19)	−0.0022 (15)	0.0080 (16)	−0.0028 (13)
C13'	0.0708 (19)	0.075 (2)	0.0614 (19)	−0.0344 (18)	−0.0015 (14)	0.0037 (14)
C14'	0.098 (6)	0.070 (5)	0.083 (6)	−0.045 (5)	0.003 (5)	−0.003 (4)
C15'	0.093 (2)	0.0421 (14)	0.0734 (19)	−0.0022 (15)	0.0080 (16)	−0.0028 (13)

Geometric parameters (Å, °)

C1—C2	1.397 (4)	C18—H18A	0.96
C1—C5	1.422 (4)	C18—H18B	0.96
C1—Fe1	2.040 (3)	C18—H18C	0.96
C1—H1	0.98	C19—H19A	0.96
C2—C3	1.405 (4)	C19—H19B	0.96
C2—Fe1	2.052 (2)	C19—H19C	0.96
C2—H2	0.98	C20—C21	1.388 (3)
C3—C4	1.411 (4)	C20—C25	1.393 (3)
C3—Fe1	2.054 (2)	C20—P1	1.835 (2)
C3—H3	0.98	C21—C22	1.388 (4)
C4—C5	1.405 (4)	C21—H21	0.93
C4—Fe1	2.044 (2)	C22—C23	1.370 (4)
C4—H4	0.98	C22—H22	0.93
C5—Fe1	2.037 (2)	C23—C24	1.358 (5)
C5—H5	0.98	C23—H23	0.93
C6—C10	1.409 (3)	C24—C25	1.383 (4)
C6—C7	1.421 (3)	C24—H24	0.93
C6—Fe1	2.030 (2)	C25—H25	0.93
C6—H6	0.98	C26—C27	1.389 (3)
C7—C8	1.433 (3)	C26—C31	1.390 (3)
C7—Fe1	2.032 (2)	C26—P1	1.838 (2)
C7—H7	0.98	C27—C28	1.383 (3)
C8—C9	1.451 (3)	C27—H27	0.93
C8—P1	1.821 (2)	C28—C29	1.370 (4)

C8—Fe1	2.0491 (19)	C28—H28	0.93
C9—C10	1.424 (3)	C29—C30	1.373 (4)
C9—C11	1.522 (3)	C29—H29	0.93
C9—Fe1	2.070 (2)	C30—C31	1.377 (4)
C10—Fe1	2.032 (2)	C30—H30	0.93
C10—H10	0.98	C31—H31	0.93
C11—N1	1.485 (3)	N1—C13	1.485 (3)
C11—C12	1.528 (3)	O1—H1A	0.82
C11—H11	0.98	C13—C14	1.517 (6)
C12—H12A	0.96	C13—H13A	0.97
C12—H12B	0.96	C13—H13B	0.97
C12—H12C	0.96	C14—C15	1.500 (6)
C16—N1	1.471 (3)	C14—H14A	0.97
C16—C15	1.539 (3)	C14—H14B	0.97
C16—C17	1.544 (3)	C15—H15A	0.97
C16—H16	0.98	C15—H15B	0.97
C17—O1	1.430 (3)	C14'—H14C	0.97
C17—C19	1.514 (4)	C14'—H14D	0.97
C17—C18	1.515 (3)		
C2—C1—C5	107.8 (3)	C23—C22—C21	120.4 (3)
C2—C1—Fe1	70.51 (15)	C23—C22—H22	119.8
C5—C1—Fe1	69.46 (15)	C21—C22—H22	119.8
C2—C1—H1	126.1	C24—C23—C22	120.3 (3)
C5—C1—H1	126.1	C24—C23—H23	119.8
Fe1—C1—H1	126.1	C22—C23—H23	119.8
C1—C2—C3	108.6 (3)	C23—C24—C25	119.6 (3)
C1—C2—Fe1	69.57 (15)	C23—C24—H24	120.2
C3—C2—Fe1	70.07 (13)	C25—C24—H24	120.2
C1—C2—H2	125.7	C24—C25—C20	121.7 (3)
C3—C2—H2	125.7	C24—C25—H25	119.2
Fe1—C2—H2	125.7	C20—C25—H25	119.2
C2—C3—C4	107.7 (3)	C27—C26—C31	118.6 (2)
C2—C3—Fe1	69.90 (13)	C27—C26—P1	124.74 (17)
C4—C3—Fe1	69.47 (14)	C31—C26—P1	116.7 (2)
C2—C3—H3	126.1	C28—C27—C26	120.2 (2)
C4—C3—H3	126.1	C28—C27—H27	119.9
Fe1—C3—H3	126.1	C26—C27—H27	119.9
C5—C4—C3	108.2 (3)	C29—C28—C27	120.6 (3)
C5—C4—Fe1	69.57 (15)	C29—C28—H28	119.7
C3—C4—Fe1	70.24 (13)	C27—C28—H28	119.7
C5—C4—H4	125.9	C28—C29—C30	119.5 (3)
C3—C4—H4	125.9	C28—C29—H29	120.2
Fe1—C4—H4	125.9	C30—C29—H29	120.2
C4—C5—C1	107.6 (3)	C29—C30—C31	120.7 (3)
C4—C5—Fe1	70.15 (15)	C29—C30—H30	119.6
C1—C5—Fe1	69.71 (14)	C31—C30—H30	119.6
C4—C5—H5	126.2	C30—C31—C26	120.3 (3)
C1—C5—H5	126.2	C30—C31—H31	119.9
Fe1—C5—H5	126.2	C26—C31—H31	119.9

C10—C6—C7	108.38 (19)	C6—Fe1—C7	40.96 (9)
C10—C6—Fe1	69.78 (13)	C6—Fe1—C10	40.58 (10)
C7—C6—Fe1	69.57 (12)	C7—Fe1—C10	68.77 (9)
C10—C6—H6	125.8	C6—Fe1—C5	104.48 (11)
C7—C6—H6	125.8	C7—Fe1—C5	113.65 (11)
Fe1—C6—H6	125.8	C10—Fe1—C5	126.93 (12)
C6—C7—C8	107.9 (2)	C6—Fe1—C1	126.94 (12)
C6—C7—Fe1	69.47 (12)	C7—Fe1—C1	106.53 (11)
C8—C7—Fe1	70.10 (11)	C10—Fe1—C1	165.25 (11)
C6—C7—H7	126.0	C5—Fe1—C1	40.82 (12)
C8—C7—H7	126.0	C6—Fe1—C4	114.49 (10)
Fe1—C7—H7	126.0	C7—Fe1—C4	146.66 (10)
C7—C8—C9	107.64 (18)	C10—Fe1—C4	107.83 (11)
C7—C8—P1	128.64 (17)	C5—Fe1—C4	40.28 (12)
C9—C8—P1	123.58 (15)	C1—Fe1—C4	67.92 (12)
C7—C8—Fe1	68.79 (11)	C6—Fe1—C8	68.91 (8)
C9—C8—Fe1	70.17 (11)	C7—Fe1—C8	41.10 (8)
P1—C8—Fe1	123.09 (10)	C10—Fe1—C8	68.83 (9)
C10—C9—C8	106.72 (19)	C5—Fe1—C8	148.50 (11)
C10—C9—C11	127.2 (2)	C1—Fe1—C8	117.48 (10)
C8—C9—C11	125.81 (18)	C4—Fe1—C8	170.91 (10)
C10—C9—Fe1	68.26 (12)	C6—Fe1—C2	166.26 (11)
C8—C9—Fe1	68.59 (11)	C7—Fe1—C2	130.26 (10)
C11—C9—Fe1	132.76 (14)	C10—Fe1—C2	153.11 (11)
C6—C10—C9	109.3 (2)	C5—Fe1—C2	67.72 (12)
C6—C10—Fe1	69.64 (13)	C1—Fe1—C2	39.92 (12)
C9—C10—Fe1	71.15 (12)	C4—Fe1—C2	67.48 (11)
C6—C10—H10	125.3	C8—Fe1—C2	111.40 (10)
C9—C10—H10	125.3	C6—Fe1—C3	149.21 (10)
Fe1—C10—H10	125.3	C7—Fe1—C3	169.83 (9)
N1—C11—C9	113.82 (17)	C10—Fe1—C3	119.07 (11)
N1—C11—C12	108.2 (2)	C5—Fe1—C3	67.78 (12)
C9—C11—C12	113.85 (19)	C1—Fe1—C3	67.54 (12)
N1—C11—H11	106.8	C4—Fe1—C3	40.29 (11)
C9—C11—H11	106.8	C8—Fe1—C3	133.14 (10)
C12—C11—H11	106.8	C2—Fe1—C3	40.03 (11)
C11—C12—H12A	109.5	C6—Fe1—C9	68.57 (9)
C11—C12—H12B	109.5	C7—Fe1—C9	69.14 (9)
H12A—C12—H12B	109.5	C10—Fe1—C9	40.59 (8)
C11—C12—H12C	109.5	C5—Fe1—C9	166.64 (11)
H12A—C12—H12C	109.5	C1—Fe1—C9	152.38 (11)
H12B—C12—H12C	109.5	C4—Fe1—C9	130.89 (11)
N1—C16—C15	105.7 (2)	C8—Fe1—C9	41.25 (8)
N1—C16—C17	110.43 (19)	C2—Fe1—C9	121.35 (10)
C15—C16—C17	113.7 (2)	C3—Fe1—C9	111.96 (10)
N1—C16—H16	109.0	C16—N1—C13	108.1 (2)
C15—C16—H16	109.0	C16—N1—C11	115.44 (18)
C17—C16—H16	109.0	C13—N1—C11	115.2 (2)
O1—C17—C19	106.9 (2)	C8—P1—C20	103.40 (10)

O1—C17—C18	109.1 (2)	C8—P1—C26	103.96 (10)
C19—C17—C18	109.6 (3)	C20—P1—C26	100.60 (10)
O1—C17—C16	109.4 (2)	C17—O1—H1A	109.5
C19—C17—C16	110.8 (2)	N1—C13—C14	103.8 (3)
C18—C17—C16	110.91 (18)	N1—C13—H13A	111.0
C17—C18—H18A	109.5	C14—C13—H13A	111.0
C17—C18—H18B	109.5	N1—C13—H13B	111.0
H18A—C18—H18B	109.5	C14—C13—H13B	111.0
C17—C18—H18C	109.5	H13A—C13—H13B	109.0
H18A—C18—H18C	109.5	C15—C14—C13	102.5 (3)
H18B—C18—H18C	109.5	C15—C14—H14A	111.3
C17—C19—H19A	109.5	C13—C14—H14A	111.3
C17—C19—H19B	109.5	C15—C14—H14B	111.3
H19A—C19—H19B	109.5	C13—C14—H14B	111.3
C17—C19—H19C	109.5	H14A—C14—H14B	109.2
H19A—C19—H19C	109.5	C14—C15—C16	102.3 (3)
H19B—C19—H19C	109.5	C14—C15—H15A	111.3
C21—C20—C25	117.3 (2)	C16—C15—H15A	111.3
C21—C20—P1	125.72 (19)	C14—C15—H15B	111.3
C25—C20—P1	116.70 (19)	C16—C15—H15B	111.3
C20—C21—C22	120.6 (3)	H15A—C15—H15B	109.2
C20—C21—H21	119.7	H14C—C14'—H14D	109.4
C22—C21—H21	119.7		
C5—C1—C2—C3	−0.3 (3)	C2—C1—Fe1—C10	−156.8 (4)
Fe1—C1—C2—C3	59.38 (17)	C5—C1—Fe1—C10	−38.1 (5)
C5—C1—C2—Fe1	−59.68 (18)	C2—C1—Fe1—C5	−118.7 (2)
C1—C2—C3—C4	0.3 (3)	C2—C1—Fe1—C4	−80.83 (17)
Fe1—C2—C3—C4	59.40 (17)	C5—C1—Fe1—C4	37.83 (17)
C1—C2—C3—Fe1	−59.08 (17)	C2—C1—Fe1—C8	91.11 (17)
C2—C3—C4—C5	−0.2 (3)	C5—C1—Fe1—C8	−150.23 (16)
Fe1—C3—C4—C5	59.45 (18)	C5—C1—Fe1—C2	118.7 (2)
C2—C3—C4—Fe1	−59.67 (17)	C2—C1—Fe1—C3	−37.14 (17)
C3—C4—C5—C1	0.0 (3)	C5—C1—Fe1—C3	81.52 (19)
Fe1—C4—C5—C1	59.90 (17)	C2—C1—Fe1—C9	57.6 (3)
C3—C4—C5—Fe1	−59.86 (18)	C5—C1—Fe1—C9	176.3 (2)
C2—C1—C5—C4	0.2 (3)	C5—C4—Fe1—C6	83.5 (2)
Fe1—C1—C5—C4	−60.18 (18)	C3—C4—Fe1—C6	−157.28 (16)
C2—C1—C5—Fe1	60.34 (17)	C5—C4—Fe1—C7	48.3 (3)
C10—C6—C7—C8	−0.6 (2)	C3—C4—Fe1—C7	167.53 (17)
Fe1—C6—C7—C8	−59.79 (14)	C5—C4—Fe1—C10	126.63 (18)
C10—C6—C7—Fe1	59.18 (15)	C3—C4—Fe1—C10	−114.19 (17)
C6—C7—C8—C9	−0.3 (2)	C3—C4—Fe1—C5	119.2 (3)
Fe1—C7—C8—C9	−59.65 (14)	C5—C4—Fe1—C1	−38.33 (18)
C6—C7—C8—P1	175.47 (15)	C3—C4—Fe1—C1	80.85 (19)
Fe1—C7—C8—P1	116.08 (16)	C5—C4—Fe1—C2	−81.6 (2)
C6—C7—C8—Fe1	59.39 (15)	C3—C4—Fe1—C2	37.55 (18)
C7—C8—C9—C10	1.0 (2)	C5—C4—Fe1—C3	−119.2 (3)
P1—C8—C9—C10	−174.98 (14)	C5—C4—Fe1—C9	165.67 (17)
Fe1—C8—C9—C10	−57.78 (14)	C3—C4—Fe1—C9	−75.1 (2)

C7—C8—C9—C11	−173.17 (18)	C7—C8—Fe1—C6	−37.91 (14)
P1—C8—C9—C11	10.8 (3)	C9—C8—Fe1—C6	81.13 (14)
Fe1—C8—C9—C11	128.0 (2)	P1—C8—Fe1—C6	−161.04 (15)
C7—C8—C9—Fe1	58.79 (14)	C9—C8—Fe1—C7	119.05 (18)
P1—C8—C9—Fe1	−117.21 (15)	P1—C8—Fe1—C7	−123.13 (19)
C7—C6—C10—C9	1.3 (2)	C7—C8—Fe1—C10	−81.56 (14)
Fe1—C6—C10—C9	60.32 (15)	C9—C8—Fe1—C10	37.49 (13)
C7—C6—C10—Fe1	−59.04 (15)	P1—C8—Fe1—C10	155.31 (16)
C8—C9—C10—C6	−1.4 (2)	C7—C8—Fe1—C5	45.4 (2)
C11—C9—C10—C6	172.7 (2)	C9—C8—Fe1—C5	164.4 (2)
Fe1—C9—C10—C6	−59.39 (16)	P1—C8—Fe1—C5	−77.7 (2)
C8—C9—C10—Fe1	57.98 (14)	C7—C8—Fe1—C1	83.78 (16)
C11—C9—C10—Fe1	−127.9 (2)	C9—C8—Fe1—C1	−157.17 (14)
C10—C9—C11—N1	−78.3 (3)	P1—C8—Fe1—C1	−39.34 (18)
C8—C9—C11—N1	94.7 (3)	C7—C8—Fe1—C2	127.34 (14)
Fe1—C9—C11—N1	−172.24 (16)	C9—C8—Fe1—C2	−113.61 (15)
C10—C9—C11—C12	46.4 (3)	P1—C8—Fe1—C2	4.21 (17)
C8—C9—C11—C12	−140.6 (2)	C7—C8—Fe1—C3	167.89 (14)
Fe1—C9—C11—C12	−47.5 (3)	C9—C8—Fe1—C3	−73.06 (17)
N1—C16—C17—O1	−56.6 (2)	P1—C8—Fe1—C3	44.76 (19)
C15—C16—C17—O1	62.1 (3)	C7—C8—Fe1—C9	−119.05 (18)
N1—C16—C17—C19	−174.2 (2)	P1—C8—Fe1—C9	117.82 (18)
C15—C16—C17—C19	−55.6 (3)	C1—C2—Fe1—C6	−19.1 (5)
N1—C16—C17—C18	63.9 (3)	C3—C2—Fe1—C6	−138.9 (4)
C15—C16—C17—C18	−177.5 (3)	C1—C2—Fe1—C7	−64.5 (2)
C25—C20—C21—C22	−1.0 (4)	C3—C2—Fe1—C7	175.71 (17)
P1—C20—C21—C22	173.03 (19)	C1—C2—Fe1—C10	167.2 (2)
C20—C21—C22—C23	0.4 (4)	C3—C2—Fe1—C10	47.3 (3)
C21—C22—C23—C24	0.3 (5)	C1—C2—Fe1—C5	38.31 (17)
C22—C23—C24—C25	−0.5 (5)	C3—C2—Fe1—C5	−81.5 (2)
C23—C24—C25—C20	−0.1 (5)	C3—C2—Fe1—C1	−119.8 (3)
C21—C20—C25—C24	0.8 (4)	C1—C2—Fe1—C4	82.04 (18)
P1—C20—C25—C24	−173.7 (2)	C3—C2—Fe1—C4	−37.79 (19)
C31—C26—C27—C28	3.0 (3)	C1—C2—Fe1—C8	−107.69 (16)
P1—C26—C27—C28	−176.45 (18)	C3—C2—Fe1—C8	132.48 (18)
C26—C27—C28—C29	−1.7 (4)	C1—C2—Fe1—C3	119.8 (3)
C27—C28—C29—C30	−1.0 (4)	C1—C2—Fe1—C9	−152.71 (16)
C28—C29—C30—C31	2.3 (4)	C3—C2—Fe1—C9	87.5 (2)
C29—C30—C31—C26	−0.9 (4)	C2—C3—Fe1—C6	162.26 (19)
C27—C26—C31—C30	−1.8 (3)	C4—C3—Fe1—C6	43.3 (3)
P1—C26—C31—C30	177.75 (18)	C2—C3—Fe1—C7	−18.9 (7)
C10—C6—Fe1—C7	−119.72 (19)	C4—C3—Fe1—C7	−137.8 (6)
C7—C6—Fe1—C10	119.72 (19)	C2—C3—Fe1—C10	−157.63 (18)
C10—C6—Fe1—C5	130.73 (16)	C4—C3—Fe1—C10	83.46 (19)
C7—C6—Fe1—C5	−109.55 (16)	C2—C3—Fe1—C5	81.3 (2)
C10—C6—Fe1—C1	169.13 (15)	C4—C3—Fe1—C5	−37.57 (19)
C7—C6—Fe1—C1	−71.15 (17)	C2—C3—Fe1—C1	37.04 (19)
C10—C6—Fe1—C4	89.16 (16)	C4—C3—Fe1—C1	−81.87 (19)
C7—C6—Fe1—C4	−151.11 (15)	C2—C3—Fe1—C4	118.9 (3)

C10—C6—Fe1—C8	−81.68 (14)	C2—C3—Fe1—C8	−70.2 (2)
C7—C6—Fe1—C8	38.04 (13)	C4—C3—Fe1—C8	170.86 (16)
C10—C6—Fe1—C2	−175.6 (4)	C4—C3—Fe1—C2	−118.9 (3)
C7—C6—Fe1—C2	−55.9 (5)	C2—C3—Fe1—C9	−113.08 (19)
C10—C6—Fe1—C3	60.0 (3)	C4—C3—Fe1—C9	128.01 (17)
C10—C6—Fe1—C9	−37.27 (13)	C10—C9—Fe1—C6	37.26 (14)
C7—C6—Fe1—C9	82.45 (14)	C8—C9—Fe1—C6	−82.02 (14)
C8—C7—Fe1—C6	119.02 (19)	C11—C9—Fe1—C6	158.4 (2)
C6—C7—Fe1—C10	−37.30 (14)	C10—C9—Fe1—C7	81.32 (14)
C8—C7—Fe1—C10	81.72 (13)	C8—C9—Fe1—C7	−37.96 (12)
C6—C7—Fe1—C5	84.94 (17)	C11—C9—Fe1—C7	−157.5 (2)
C8—C7—Fe1—C5	−156.04 (15)	C8—C9—Fe1—C10	−119.28 (18)
C6—C7—Fe1—C1	127.91 (15)	C11—C9—Fe1—C10	121.2 (3)
C8—C7—Fe1—C1	−113.07 (15)	C10—C9—Fe1—C5	−23.4 (5)
C6—C7—Fe1—C4	53.1 (2)	C8—C9—Fe1—C5	−142.6 (4)
C8—C7—Fe1—C4	172.13 (18)	C11—C9—Fe1—C5	97.8 (5)
C6—C7—Fe1—C8	−119.02 (19)	C10—C9—Fe1—C1	167.2 (2)
C6—C7—Fe1—C2	165.06 (15)	C8—C9—Fe1—C1	47.9 (3)
C8—C7—Fe1—C2	−75.92 (17)	C11—C9—Fe1—C1	−71.6 (3)
C8—C7—Fe1—C3	−60.1 (7)	C10—C9—Fe1—C4	−67.17 (17)
C6—C7—Fe1—C9	−80.93 (14)	C8—C9—Fe1—C4	173.55 (13)
C8—C7—Fe1—C9	38.08 (12)	C11—C9—Fe1—C4	54.0 (2)
C9—C10—Fe1—C6	−119.96 (19)	C10—C9—Fe1—C8	119.28 (18)
C6—C10—Fe1—C7	37.65 (13)	C11—C9—Fe1—C8	−119.6 (3)
C9—C10—Fe1—C7	−82.32 (13)	C10—C9—Fe1—C2	−153.39 (14)
C6—C10—Fe1—C5	−66.62 (19)	C8—C9—Fe1—C2	87.33 (15)
C9—C10—Fe1—C5	173.42 (15)	C11—C9—Fe1—C2	−32.2 (2)
C6—C10—Fe1—C1	−36.3 (5)	C10—C9—Fe1—C3	−109.54 (14)
C9—C10—Fe1—C1	−156.3 (4)	C8—C9—Fe1—C3	131.18 (13)
C6—C10—Fe1—C4	−107.09 (15)	C11—C9—Fe1—C3	11.6 (2)
C9—C10—Fe1—C4	132.95 (14)	C15—C16—N1—C13	3.9 (3)
C6—C10—Fe1—C8	81.89 (14)	C17—C16—N1—C13	127.2 (2)
C9—C10—Fe1—C8	−38.08 (12)	C15—C16—N1—C11	134.6 (2)
C6—C10—Fe1—C2	177.7 (2)	C17—C16—N1—C11	−102.1 (2)
C9—C10—Fe1—C2	57.7 (3)	C9—C11—N1—C16	−70.4 (2)
C6—C10—Fe1—C3	−149.53 (14)	C12—C11—N1—C16	161.9 (2)
C9—C10—Fe1—C3	90.51 (15)	C9—C11—N1—C13	56.8 (3)
C6—C10—Fe1—C9	119.96 (19)	C12—C11—N1—C13	−70.8 (3)
C4—C5—Fe1—C6	−110.95 (18)	C7—C8—P1—C20	72.69 (19)
C1—C5—Fe1—C6	130.59 (18)	C9—C8—P1—C20	−112.20 (18)
C4—C5—Fe1—C7	−153.36 (16)	Fe1—C8—P1—C20	160.86 (12)
C1—C5—Fe1—C7	88.17 (19)	C7—C8—P1—C26	−32.0 (2)
C4—C5—Fe1—C10	−72.9 (2)	C9—C8—P1—C26	143.08 (17)
C1—C5—Fe1—C10	168.66 (16)	Fe1—C8—P1—C26	56.14 (14)
C4—C5—Fe1—C1	118.5 (2)	C21—C20—P1—C8	2.0 (2)
C1—C5—Fe1—C4	−118.5 (2)	C25—C20—P1—C8	175.99 (19)
C4—C5—Fe1—C8	175.91 (16)	C21—C20—P1—C26	109.2 (2)
C1—C5—Fe1—C8	57.4 (3)	C25—C20—P1—C26	−76.7 (2)
C4—C5—Fe1—C2	80.98 (18)	C27—C26—P1—C8	61.2 (2)

C1—C5—Fe1—C2	−37.48 (17)	C31—C26—P1—C8	−118.32 (18)
C4—C5—Fe1—C3	37.58 (16)	C27—C26—P1—C20	−45.6 (2)
C1—C5—Fe1—C3	−80.89 (18)	C31—C26—P1—C20	134.86 (18)
C4—C5—Fe1—C9	−54.0 (5)	C16—N1—C13—C14	21.5 (3)
C1—C5—Fe1—C9	−172.5 (4)	C11—N1—C13—C14	−109.4 (3)
C2—C1—Fe1—C6	174.42 (15)	N1—C13—C14—C15	−38.8 (4)
C5—C1—Fe1—C6	−66.9 (2)	C13—C14—C15—C16	40.7 (4)
C2—C1—Fe1—C7	134.09 (15)	N1—C16—C15—C14	−27.9 (4)
C5—C1—Fe1—C7	−107.25 (18)	C17—C16—C15—C14	−149.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	2.53	2.844 (2)	104
C11—H11···P1	0.98	2.86	3.371 (2)	114
C16—H16···P1	0.98	2.87	3.778 (2)	154

Selected torsion angles (°)

C1—*Cg*3—*Cg*4—C7	16.63	C4—*Cg*3—*Cg*4—C10	15.63
C2—*Cg*3—*Cg*4—C8	15.99	C5—*Cg*3—*Cg*4—C6	15.80
C3—*Cg*3—*Cg*4—C9	15.20		

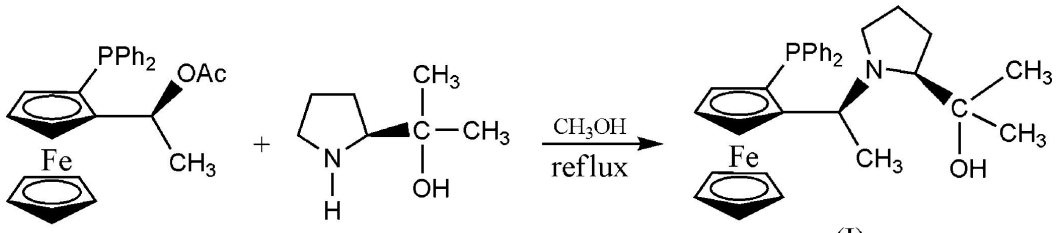
*Cg*3 is the centroid of the Cp ring system C1 to C5, *Cg*4 is the centroid of the Cp ring system C6 to C10.

X—H···Cg (π-ring) interaction geometry (Å, °)

X—H···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C1—H1···*Cg*6	0.98	2.95	3.66 (3)	131
C30—H30···*Cg*3$^{(i)}$	0.98	2.96	3.864 (3)	165

*Cg*6 is the centroid of the π-ring system C26 to C31. *Cg*3 is the centroid of the Cp ring system C1 to C5. Symmetry code: (i) −1/2 + *x*, 1/2 − *y*, 1 − *z*.

Fig. 1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OAc
Fe
CH3
+
CH3
C
CH3
N
H
OH
CH3OH
reflux
PPh2
N
CH3
C
CH3
Fe
CH3
OH

(I)

Fig. 2

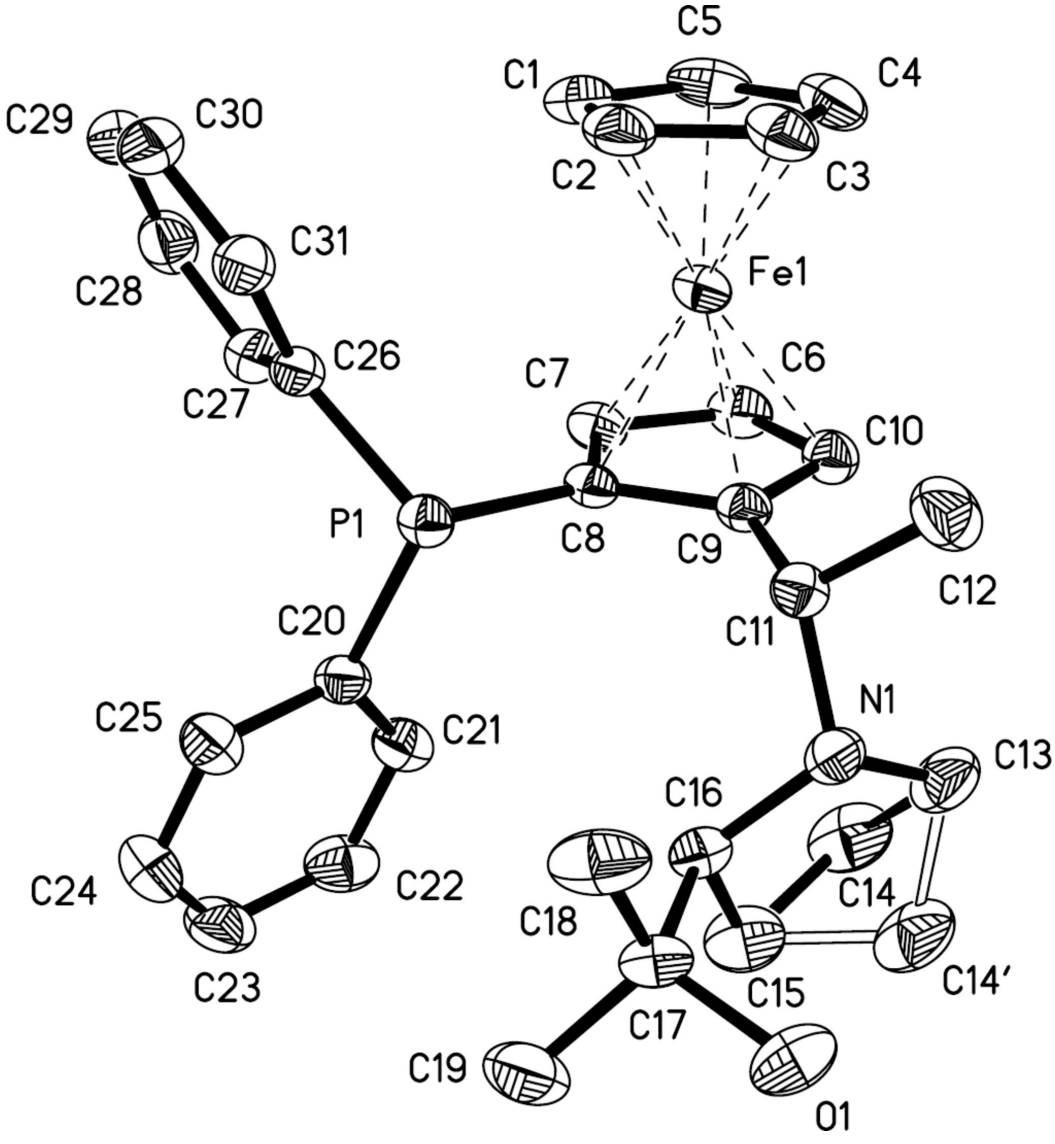
C5
C1
C4
C29
C30
C2
C3
C31
Fe1
C28
C26
C7
C6
C27
C10
P1
C8
C9
C12
C20
C11
N1
C25
C21
C13
C16
C24
C22
C14
C18
C14′
C15
C23
C17
C19
O1

Fig. 3