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Synthesis and characterization of enantiopure planar–chiral phosphorus-linked diferrocenes

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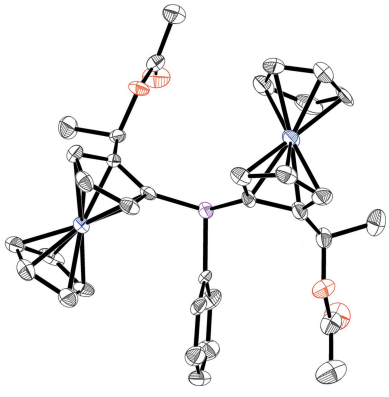
In the course of an ongoing synthetic project on cyclic diferrocenylphosphines, we obtained a group of planar–chiral diferrocenyl compounds useful as precursors for subsequent cyclization. Here we report the crystal structures of two symmetric compounds $[(Fc^{A})_2(Ph)P]$, one of which contains four stereogenic centres (two C chiral and two planar chiral centres), *i.e.* 1,1′-(phenylphosphanediyl)bis{(2S_p)-2-[(1*R*)-1-(acetyloxy)ethyl]ferrocene}, $[Fe_2(C_5H_5)_2(C_{24}H_{25}O_4P)]$, and the other phosphine sulfide is a purely planar–chiral compound (two planar chiral centres), *i.e.* bis[(2S_p)–2-ethenylferrocen-1-yl]phenylphosphane sulfide, $[Fe_2(C_5H_5)_2(C_{20}H_{17}PS)]$. Owing to the stereocentres present, reactions performed on $[(Fc^{A})_2(Ph)P]$-type compounds strongly favour one ferrocene unit over the other due to diastereoselectivity. Furthermore, we present four related structures where the ferrocene units are not identical $[(Fc^{A})(Fc^{B})(Ph)P]$. These are {(2S_p)-2-[(1*R*)-1-(acetyloxy)ethyl]ferrocen-1-yl}[(2S_p)-2-ethenylferrocen-1-yl]phenyl-(*S*)-phosphine sulfide, $[Fe_2(C_5H_5)_2(C_{22}H_{21}O_2PS)]$, [(2$S_p$)-2-ethenylferrocen-1-yl]{(2S_p)-2-[(1*R*)-1-hydroxyethyl]ferrocen-1-yl}phenyl-(*S*)-phosphine sulfide, $[Fe_2(C_5H_5)_2(C_{20}H_{19}OPS)]$, {(2$S_p$)-2-[(1*R*)-1-(acetyloxy)ethyl]ferrocen-1-yl}{(2S_p)-2-[(1*R*)-1-hydroxyethyl]ferrocen-1-yl}phenyl-(*R*)-phosphine sulfide, $[Fe_2(C_5H_5)_2(C_{22}H_{23}O_3PS)]$, and {(2$S_p$)-2-[(1*R*)-1-benzylamino)ethyl]ferrocen-1-yl}[(2S_p)-2-ethenylferrocen-1-yl]phenyl-(*S*)-phosphine sulfide, $[Fe_2(C_5H_5)_2(C_{27}H_{26}NPS)]$. All of the structures are accessible in one step from known precursors.

1. Introduction

Metallocenes decorated with at least two different substituents on the same ring are planar–chiral (Schaarschmidt & Lang, 2013). They are useful as voluminous asymmetry-inducing groups in asymmetric transformations (Stepnicka, 2008). Even beyond academic research, disubstituted ferrocenes have been used in industrial asymmetric synthesis, for instance, in the hydrogenation of imines (Blaser *et al.*, 2007).

The potential of asymmetric induction may be improved by designing ligands including two planar–chiral ferrocene units. One example is the phosphorous-linked diferrocene Pigiphos (Barbaro & Togni, 1995), developed by the group of Togni. A multitude of ligands for transition-metal complexes have been synthesized and applied in asymmetric homogeneous catalysis [*e.g.* Rh^{I} in hydrosilylations (Hayashi *et al.*, 1974), Rh^{III} in acetalizations (Barbaro *et al.*, 1999), Pd^{II} in hydroaminations (Gischig & Togni, 2004, 2005), Ru^{II} in transfer hydrogenations (Barbaro *et al.*, 1997, 2003) and olefin cyclopropanations (Lee *et al.*, 1999), and Ni^{II} in hydroaminations (Fadini & Togni, 2004, 2007, 2008), hydrophosphinations (Sadow & Togni, 2005), Nazarov cyclizations (Walz & Togni, 2008) and dipolar cycloadditons (Milosevic & Togni, 2013)].



The performance of catalysts may be enhanced further by making the angle of the two ferrocene units rigid *via* ring closure, yielding a diferrocenyl (macro)cycle (Xiao *et al.*, 2002), possibly with inclusion of another (planar–chiral) ferrocene unit (Wang *et al.*, 2006). Stanphos (Broggini, 2003) is a *P,P*-ligand diferroceno ring and has been employed in asymmetric hydroalkoxylations (Barreiro *et al.*, 2012) and the hydroxylation of 1,3-ketoesters (Smith *et al.*, 2010).

In the course of the synthesis of cyclic diferrocene monophosphines with potential in asymmetric catalysis, we prepared compounds such as **6**–**9** (Fig. 1) potentially useful for a cyclization step. Their synthetic access starting from commercially available [1-(dimethylamino)ethyl]ferrocene (**1**) is outlined in Fig. 1. Beyond the desired cyclized products like **9a** (Honegger & Widhalm, 2019*b*), several side products were isolated and characterized.

2. Experimental

2.1. Synthesis and crystallization

2.1.1. Synthesis of 1,1-(phenylphosphanediyl)bis{(2*S*)-2-[(1*R*)-1-(acetyloxy)ethyl]ferrocene} (7). Diaminophosphine **2** (619 mg, 1.00 mmol; Barreiro *et al.*, 2012) was suspended in Ac_2O (1 ml) in a flame-dried Schlenk tube under argon. The suspension was degassed and stirred for 7 d at room temperature, then for 7 h at 100 °C. From the dark-red solution, Ac_2O was removed under reduced pressure and the residue was purified by column chromatography (SiO_2, 0–100% EtOAc in heptane) yielding diacetate **7** (yield 177 mg, 27%) as pale-red crystals upon removal of the solvent (m.p. 155–156 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62–7.56 (*m*, 2H), 7.37–7.30 (*m*, 3H), 6.20 (*dt*, *J* = 2.5, 6.4 Hz, 1H), 5.99 (*dt*, *J* = 2.9, 6.4 Hz, 1H), 4.52 (*m*, 1H), 4.45 (*m*, 1H), 4.43 (*pt*, *J* = 2.5 Hz, 1H), 4.35 (*m*, 1H), 4.34 (*m*, 1H), 4.30 (*m*, 1H), 4.04 (*s*, 5H), 3.72 (*s*, 5H), 2.11 (*s*, 3H), 1.96 (*d*, *J* = 6.4 Hz, 3H), 1.56 (*d*, *J* = 6.4 Hz, 3H), 1.32 (*s*, 3H). ^{31}P NMR: δ −44.57 (*s*). HRMS (*m*/*z* calculated for $C_{34}H_{35}Fe_2NaO_4P$) $[M + Na]^+$ 673.0869; found 673.0877.

2.1.2. Synthesis of monovinyl monoacetyl phosphine sulfide 8a, monovinyl monohydroxy phosphine sulfide 8b and monohydroxy monoacetyl phosphine sulfide 8c. Diamine phosphine sulfide **3** (653 mg, 1.00 mmol; Honegger & Widhalm, 2019*a*) was suspended in Ac_2O (1 ml) in a flame-dried Schlenk tube. The suspension was degassed and stirred under argon for 7 d at room temperature, then for 7 h at 100 °C until the starting material was completely consumed (thin-layer chromatography, TLC). Ac_2O was removed under reduced pressure and the residue was purified by column chromatography (SiO_2, 0–100% EtOAc in heptane), yielding several mixed fractions, as well as compounds **8a** (yield 135 mg, 22%), **8b** (yield 99 mg, 17%) and **8c** (yield 74 mg, 12%) as orange crystals upon removal of the solvent.

Analytical data for **8a**: m.p. 177–178 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.13 (*dd*, *J* = 17.7, 10.8 Hz, 1H), 7.77 (*dd*, *J* = 13.3, 7.4 Hz, 2H), 7.47–7.41 (*m*, 3H), 6.49 (*q*, *J* = 6.4 Hz, 1H), 5.46 (*dd*, *J* = 17.7, 1.7 Hz, 1H), 5.16 (*dd*, *J* = 10.8, 1.6 Hz, 1H), 4.84 (*m*, 1H), 4.59 (*m*, 1H), 4.36 (*s*, 5H), 4.30 (*m*, 1H), 4.28 (*m*, 1H), 4.14 (*s*, 5H), 3.78 (*m*, 1H), 3.54 (*m*, 1H), 1.57 (*d*, *J* = 6.5 Hz, 3H), 1.04 (*s*, 3H). ^{13}C{^{1}H} NMR: δ 169.39 (C_q), 135.44 (*d*, J_{CP} = 88.3 Hz, C_q), 134.47 (CH), 132.29 (*d*, J_{CP} = 10.5 Hz, CH), 130.77 (*d*, J_{CP} = 2.8 Hz, CH), 127.49 (*d*, J_{CP} = 12.2 Hz, CH), 111.38 (CH_2), 88.95 (*d*, J_{CP} = 12.1 Hz, C_q), 88.43 (*d*, J_{CP} = 12.0 Hz, C_q), 79.19 (*d*, J_{CP} = 95.2 Hz, C_q), 75.84 (*d*, J_{CP} = 11.4 Hz, CH), 75.03 (*d*, J_{CP} = 12.0 Hz, CH), 74.46 (*d*, J_{CP} = 95.1 Hz, C_q), 71.15 (CH), 70.94 (CH), 70.60 (*d*, J_{CP} = 9.0 Hz, CH), 69.88 (*d*, J_{CP} = 10.2 Hz, CH), 68.40 (*d*, J_{CP} = 10.3 Hz, CH), 68.14 (*d*, J_{CP} = 8.9 Hz, CH), 67.99 (CH), 20.03 (CH_3), 18.49 (CH_3). ^{31}P NMR: δ 39.14 (*s*). HRMS (*m*/*z* calculated for $C_{32}H_{31}Fe_2O_2PS$) $[M]^+$ 622.0481, found 622.0462; $[M + Na]^+$ 645.0379, found 645.0358; $[M + K]^+$ 661.0118, found 661.0104.

Analytical data for **8b**: m.p. 205–206 °C (decomposition). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (*dd*, *J* = 17.6, 10.8 Hz, 1H), 7.87–7.81 (*m*, 2H), 7.51–7.42 (*m*, 3H), 5.49 (*dd*, *J* = 17.6, 1.6 Hz, 1H), 5.23–5.17 (*m*, 1H), 5.20 (*dd*, *J* = 10.8, 1.7 Hz, 1H), 4.88 (*m*, 1H), 4.49 (*m*, 1H), 4.34 (*s*, 5H), 4.33 (*m*, 1H), 4.24 (*m*, 1H), 4.17 (*s*, 5H), 3.77 (*m*, 1H), 3.71 (*m*, 1H), 2.41 (*d*, *J* = 5.3 Hz, 1H), 1.26 (*d*, *J* = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR: δ 135.30 (*d*, J_{CP} = 87.1 Hz, C_q), 134.25 (CH), 132.10 (*d*, J_{CP} = 10.3 Hz, CH), 131.38 (*d*, J_{CP} = 2.8 Hz, CH), 127.96 (*d*, J_{CP} = 12.1 Hz, CH), 111.74 (CH_2), 94.90 (*d*, J_{CP} = 12.3 Hz, C_q), 88.43 (*d*, J_{CP} = 11.8 Hz, C_q), 78.56 (*d*, J_{CP} = 95.4 Hz, C_q), 75.05 (*d*, J_{CP} = 12.0 Hz, CH), 74.97 (*d*, J_{CP} = 12.6 Hz, CH), 73.48 (*d*, J_{CP} = 96.0 Hz, C_q), 71.22 (CH), 71.00 (*d*, J_{CP} = 9.7 Hz, CH), 70.72 (CH), 70.10 (*d*, J_{CP} = 10.4 Hz, CH), 68.38 (*d*, J_{CP} = 9.1 Hz, CH), 68.04 (*d*, J_{CP} = 10.5 Hz, CH), 64.38 (CH), 21.91 (CH_3). ^{31}P NMR: δ 40.52 (*s*). HRMS (*m*/*z* calculated for $C_{30}H_{29}Fe_2OPS$) $[M]^+$ 580.0376, found 580.0360; $[M + Na]^+$ 603.0273, found 603.0273; $[M + K]^+$ 619.0013, found 619.0018.

Analytical data for **8c**: m.p. 174–175 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20–8.14 (*m*, 2H), 7.57–7.54 (*m*, 3H), 6.60 (*q*, *J* = 6.3 Hz, 1H), 4.93 (*m*, 1H), 4.67 (*m*, 2H), 4.49 (*m*, 1H), 4.38 (*m*, 1H), 4.34 (*m*, 1H), 4.11 (*s*, 5H), 4.10 (*s*, 5H), 1.90 (*s*, 3H), 1.83 (*d*, *J* = 6.3 Hz, 3H), 1.63 (*m*, 1H), 1.43 (*dd*, *J* = 19.2, 6.4 Hz, 1H), 1.40 (*d*, *J* = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR: δ 169.70 (C_q), 135.42 (*d*, J_{CP} = 87.3 Hz, C_q), 132.21 (*d*, J_{CP} = 10.5 Hz, CH), 131.47 (*d*, J_{CP} = 2.9 Hz, CH), 127.88 (*d*, J_{CP} = 12.2 Hz, CH), 93.49 (*d*, J_{CP} = 11.8 Hz, C_q), 93.47 (*d*, J_{CP} = 13.5 Hz, C_q), 75.85 (*d*, J_{CP} = 13.4 Hz, CH), 74.53 (C_q), 73.91 (C_q), 71.53 (*d*, J_{CP} = 9.3 Hz, CH), 70.93 (CH), 70.60 (*d*, J_{CP} = 60.4 Hz, CH), 70.58 (CH), 70.27 (*d*, J_{CP} = 9.3 Hz, CH), 69.48 (*d*, J_{CP} = 10.1 Hz, CH), 68.87 (CH), 68.56 (*d*, J_{CP} = 10.9 Hz, CH), 64.20 (CH), 22.37 (CH_3), 22.23 (CH_3), 21.80 (CH_3). ^{31}P NMR: δ 39.12 (*s*). HRMS (*m*/*z* calculated for $C_{32}H_{33}Fe_2O_3PS$) $[M]^+$ 640.0587, found 640.0566; $[M + Na]^+$ 663.0485, found 663.0463.

2.1.3. Catalytic experiments: asymmetric allylic alkylation (Widhalm *et al.*, 1996). In a flame-dried Schlenk tube, the diferrocene ligand (0.010 mmol, 1 mol%) and $[Pd(allyl)Cl]_2$ (1.8 mg, 0.005 mmol, 0.5 mol%) were dissolved in degassed DCM (1 ml) in that order under argon. The yellow solution was stirred for 20 min while it turned orange. To the solution, freshly distilled 1,3-diphenylallyl acetate (252 mg, 1.00 mmol), dimethyl malonate (0.340 ml, 3.00 mmol, 3 equiv.), bis(trimethylsilyl)acetamide (0.740 ml, 3.00 mmol, 3 equiv.) and a

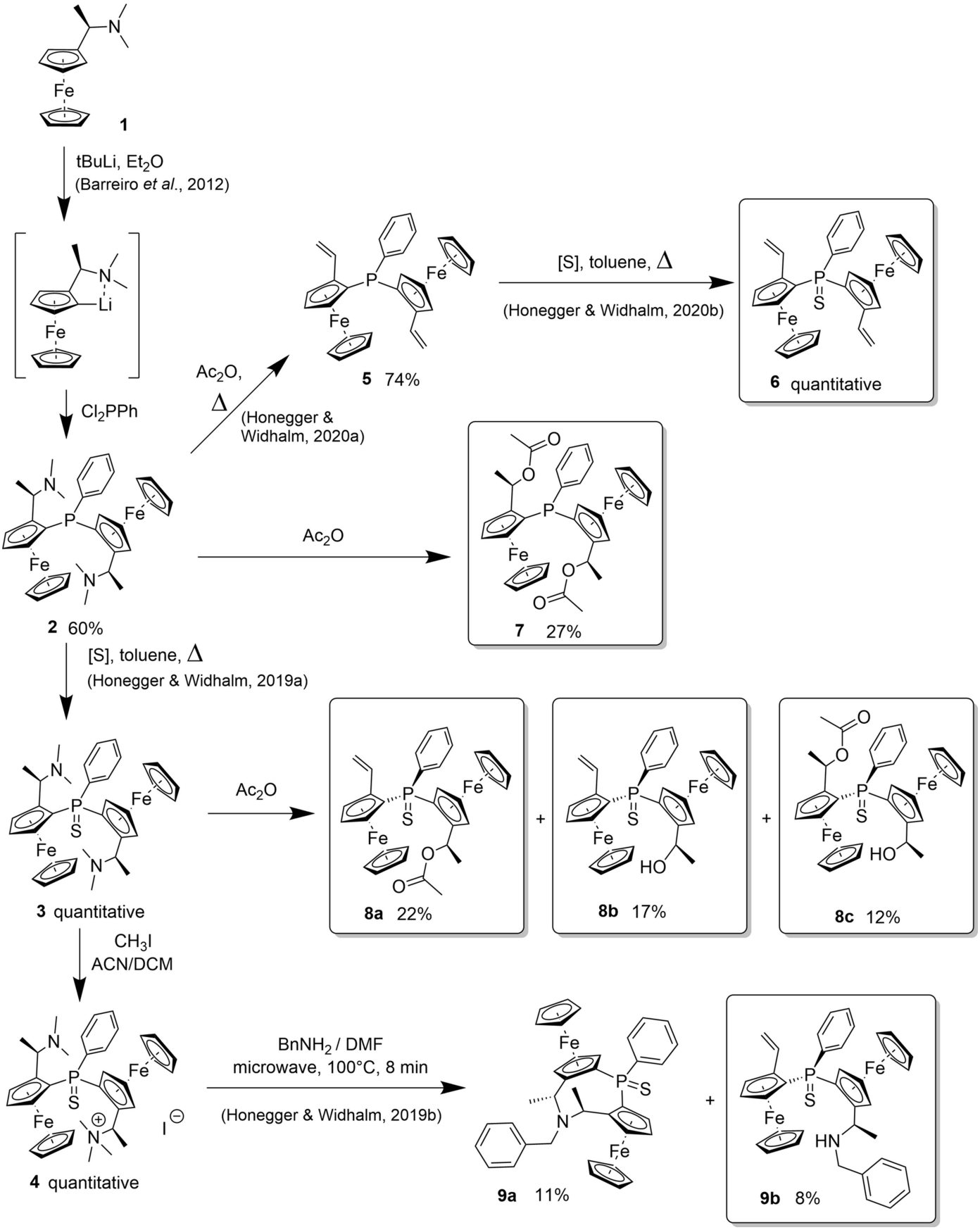


Figure 1
Synthetic route towards the crystallized phosphorous-linked diferrocenes **6**, **7**, **8a**, **8b**, **8c** and **9b**.

Table 1
Experimental details.

	6	**7**	**8a**
Crystal data			
Chemical formula	$[Fe_2(C_5H_5)_2(C_{20}H_{17}PS)]$	$[Fe_2(C_5H_5)_2(C_{24}H_{25}O_4P)]$	$[Fe_2(C_5H_5)_2(C_{22}H_{21}O_2PS)]$
M_r	562.24	650.29	622.30
Crystal system, space group	Monoclinic, $P2_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	130	130	100
a, b, c (Å)	8.4709 (7), 14.1401 (11), 21.0310 (17)	7.631 (2), 10.877 (2), 36.025 (8)	7.4923 (3), 12.0133 (4), 31.758 (1)
α, β, γ (°)	90, 91.880 (3), 90	90, 90, 90	90, 90, 90
V (Å^3)	2517.7 (4)	2990.2 (12)	2858.45 (17)
Z	4	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.32	1.06	1.17
Crystal size (mm)	0.28 × 0.25 × 0.13	0.15 × 0.08 × 0.06	0.21 × 0.14 × 0.05
Data collection			
Diffractometer	Bruker X8 APEXII	Bruker X8 APEXII	Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.620, 0.746	0.562, 0.745	0.607, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35484, 14468, 13352	46099, 5441, 4085	52739, 8330, 7214
R_{int}	0.038	0.150	0.062
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.708	0.602	0.704
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.071, 1.03	0.065, 0.122, 1.04	0.032, 0.062, 1.04
No. of reflections	14468	5441	8330
No. of parameters	613	374	345
No. of restraints	1	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.37	0.94, −0.43	0.34, −0.34
Absolute structure	Flack x determined using 5751 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 1235 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack x determined using 2809 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.019 (5)	−0.02 (2)	−0.007 (5)

	8b	**8c**	**9b**
Crystal data			
Chemical formula	$[Fe_2(C_5H_5)_2(C_{20}H_{19}OPS)]$	$[Fe_2(C_5H_5)_2(C_{22}H_{23}O_3PS)]$	$[Fe_2(C_5H_5)_2(C_{27}H_{26}NPS)]$
M_r	580.26	640.31	669.40
Crystal system, space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Temperature (K)	130	130	130
a, b, c (Å)	7.5285 (3), 17.6463 (7), 39.3333 (15)	7.8204 (11), 17.835 (3), 20.394 (2)	12.3578 (9), 14.4342 (10), 17.4796 (15)
α, β, γ (°)	90, 90, 90	90, 90, 90	90, 90, 90
V (Å^3)	5225.4 (4)	2844.5 (7)	3117.9 (4)
Z	8	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.27	1.18	1.08
Crystal size (mm)	0.25 × 0.2 × 0.17	0.1 × 0.06 × 0.01	0.22 × 0.11 × 0.09
Data collection			
Diffractometer	Bruker X8 APEXII	Bruker X8 APEXII	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.650, 0.746	0.568, 0.745	0.486, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38763, 14944, 11780	35430, 5258, 3417	38997, 9160, 7062
R_{int}	0.045	0.167	0.075
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.606	0.706
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.137, 1.04	0.054, 0.093, 1.02	0.040, 0.091, 0.98
No. of reflections	14944	5258	9160
No. of parameters	635	356	384
No. of restraints	1	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement

Table 1 (continued)

	8b	8c	9b
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.08, −1.80	0.42, −0.41	0.43, −0.35
Absolute structure	Flack *x* determined using 4140 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack *x* determined using 1051 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)	Flack *x* determined using 2549 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.010 (7)	0.00 (2)	−0.016 (10)

Computer programs: *APEX2* (Bruker, 2009), *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2009, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

catalytic amount of potassium acetate were added in that order. The reaction mixture was degassed once and stirred for 48 h at room temperature until the catalytic conversion was complete. To the solution, Et_2O (15 ml) was added. The organic layer was washed twice with saturated aqueous NH_4Cl solution, dried over Na_2SO_4 and the solvent removed under reduced pressure. The residue was dried, dissolved in DCM (2 ml) and filtered through SiO_2. The enantiomeric excess (e.e.) was detected *via* chiral high-performance liquid chromatography (HPLC; Chiralcel OD-H, 2% isopropanol in *n*-heptane).

2.2. Melting points

The melting points were measured on a Reichelt Thermovar Kofler apparatus and are uncorrected.

2.3. Chiral high-performance liquid chromatography (HPLC)

HPLC analysis was performed on an Agilent Technologies 1200 series system using a Chiralcel OD-H chiral column.

2.4. NMR spectroscopy

Routine NMR spectra were recorded on a 400 MHz Bruker AVIII 400 spectrometer operating at 400.27 (^{1}H), 100.66 (^{13}C) and 162.04 MHz (^{31}P) with an autosampler. The ^{1}H and ^{13}C{^{1}H} NMR spectra used for substance characterization were recorded either on a 600 MHz Bruker AVIII 600 spectrometer operating at 600.25 (^{1}H) and 150.95 MHz (^{13}C) or on a Bruker AVIII 700 spectrometer operating at 700.40 (^{1}H) and 176.13 MHz (^{13}C). ^{13}C NMR spectra were recorded in J-modulated mode. NMR chemical shifts are referenced to nondeuterated $CHCl_3$ residual shifts at 7.26 ppm for ^{1}H NMR and to $CDCl_3$ at 77.00 ppm for ^{13}C NMR. Coupling patterns in the ^{1}H and ^{13}C NMR spectra are denoted using standard abbreviations: *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet), *m* (multiplet) and *p* (pseudo). For the ^{13}C NMR spectra, carbon resonances were identified as C_q, CH, CH_2 and CH_3.

2.5. High-resolution mass spectroscopy (HRMS)

HRMS were recorded by a Bruker Maxis ESI oa-RTOF mass spectrometer equipped with a quadrupole analyzer ion guide.

2.6. Preparative column chromatography

Preparative column chromatography was carried out on an Biotage Isolera One automated flash chromatography instrument using self-packed columns containing either SiO_2 (Macherey–Nagel silica gel 60M, particle size 40–63 µm) or Al_2O_3 (Merck aluminium oxide 90 standardized, activation grade II–III).

2.7. X-ray diffractometry

X-ray diffraction was performed on a Bruker X8 APEXII diffractometer, a Bruker D8 Venture diffractometer and a Bruker APEXII CCD diffractometer, all with Mo *Kα* radiation.

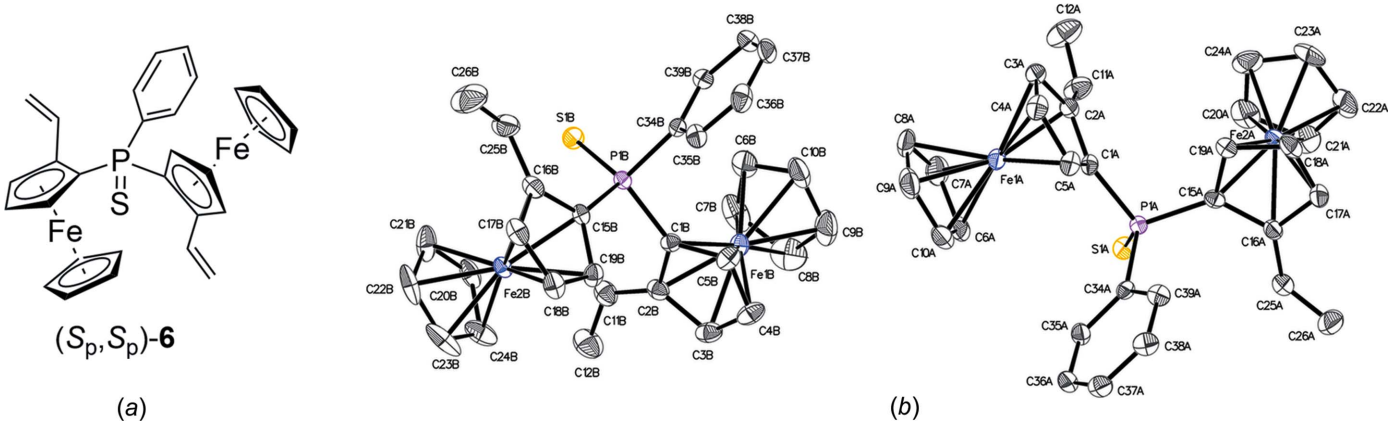


Figure 2
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of divinyl **6**. The ellipsoid probability level of this figure and all subsequent figures is 50%.

2.8. Refinement

The structures were solved by direct methods and refined using full-matrix least-squares techniques. Non-H atoms were refined with anisotropic displacement parameters. H atoms were inserted at calculated positions and refined using a riding model. C—H bond lengths in the aromatic and olefin bond systems were constrained at 0.950 Å, aliphatic CH_2 groups at 0.990 Å and aliphatic CH_3 groups at 0.980 Å. The default values of *SHELXL* (Sheldrick, 2008) were used for the riding-atom model. Fixed U_{iso} values of 1.2 times were used for all C(H) and C(H,H) groups, and fixed U_{iso} values of 1.5 times were used for all C(H,H,H) and O(H) groups. Details for each compound are summarized in the CIF file under the keyword '_refine_special_details'.

The position of the acidic atom H1*B* at **8b** was stabilized using a length-fixing restraint. Several reflections, primarily inner ones, have been omitted to avoid wrong interpretations.

The amine H atom of compound **9b** was refined taking account of the two possible configurations of the N atom. The choice was stable and in agreement with the position of available electron density.

Crystal data, data collection and structure refinement details are summarized in Table 1.

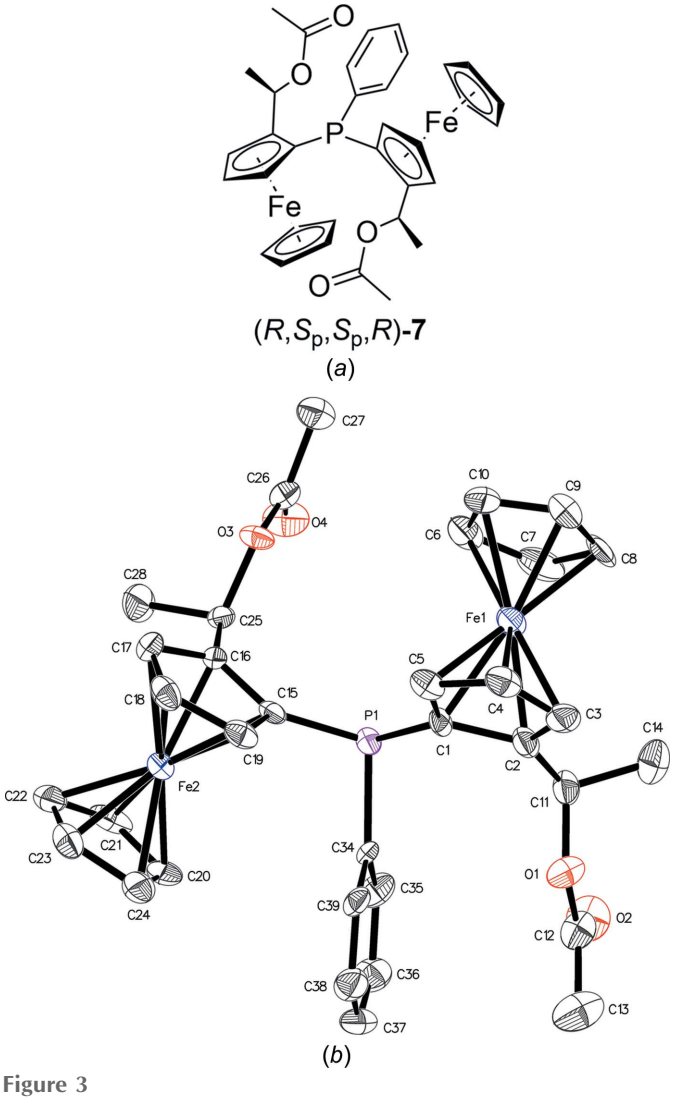


Figure 3
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of diacetate **7**.

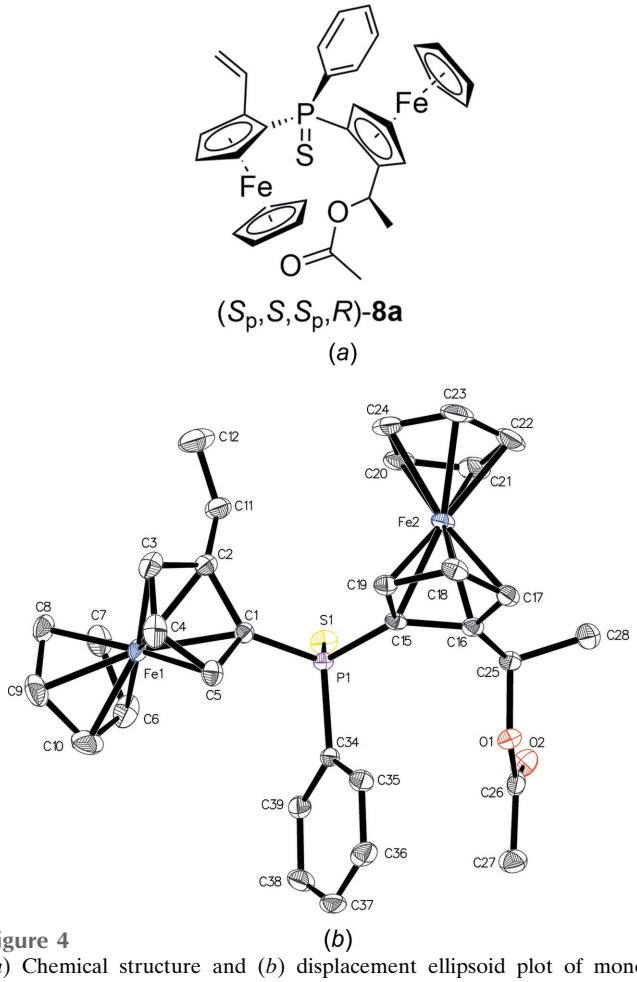


Figure 4
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of monoacetate **8a**.

3. Results and discussion

The syntheses carried out in the framework of this study are summarized in Fig. 1. The structure of the central diferrocene precursor **2** has been deposited previously (Steiner & Pioda, 1999) in the Cambridge Structural Database (Groom *et al.*, 2016). First, we eliminated the dimethylamine groups of **2** to obtain divinyl structure (S_p,S_p)-**5** by heating in acetic anhydride according to Honegger & Widhalm (2020). The sensitive phosphine was then protected by reaction with elemental sulfur to quantitatively produce divinylphosphine sulfide (S_p,S_p)-**6**, shown in Fig. 2 (Honegger *et al.*, 2020). The substance was readily isolated as orange crystals upon removal of the solvent. Cyclization attempts of **6** *via* ring-closing metathesis (RCM) failed, possibly due to the separation of the vinyl C atoms, steric strain in the product or interference of the Grubbs catalyst with the phosphine sulfide. However, Lewis acid-catalyzed hydrovinylation afforded the desired all-carbon backbone (Honegger & Widhalm, 2020).

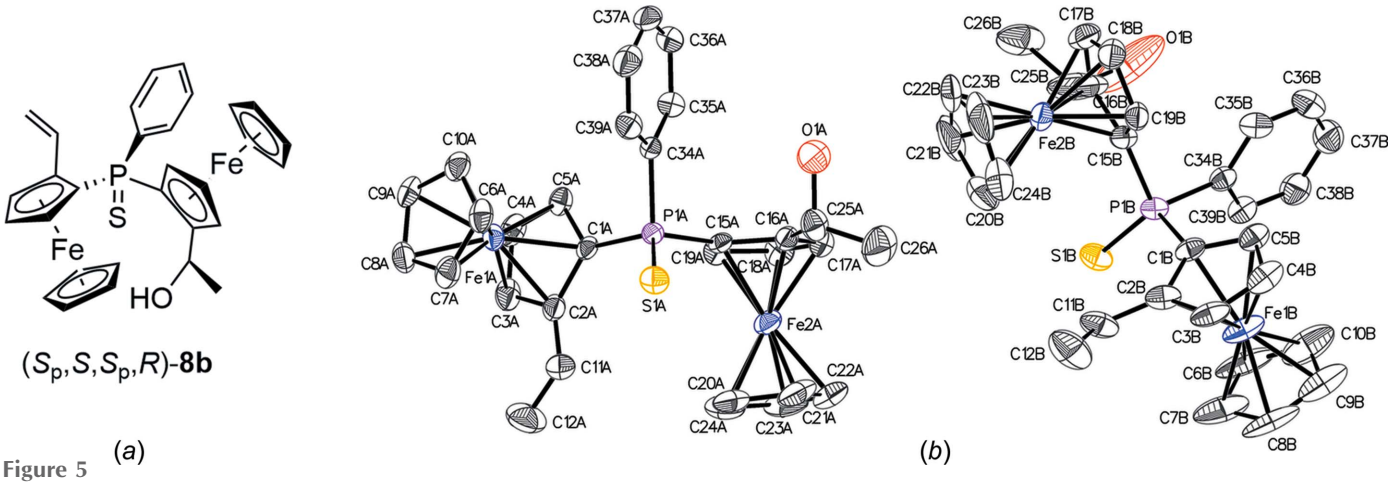


Figure 5
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of monohydroxide **8b**.

For an alternative approach, we replaced the diamino groups with more capable leaving groups in order to close the ring with bidentate nucleophiles. In one of these attempts, we replaced the amines by acetate groups using acetic anhydride. The resulting diacetate (R,S_p,S_p,R)-**7** crystallized upon removal of the solvent (Fig. 3). Alternatively, the reactive phosphino group was protected by reaction with elemental sulfur to yield phosphine sulfide (R,S_p,S_p,R)-**3** (Honegger & Widhalm, 2019*a*). In contrast to the unprotected phosphine, we could not obtain the diacetate from derivative (R,S_p,S_p,R)-**3**, but from the reaction mixture, three compounds, namely, (S_p,S,S_p,R)-**8a** (Fig. 4), (S_p,S,S_p,R)-**8b** (Fig. 5) and (R,S_p,R,S_p,R)-**8c** (Fig. 6) with acetate, hydroxy or vinyl side groups instead, could be isolated, indicating that the substitution was followed by elimination or cleavage of the acetyl group.

Alternatively, an attempt was made to convert the diamine (R,S_p,S_p,R)-**3** into a diammonium salt, yet only monomethiodide **4** was obtained in quantitative yield. Bridging with benzylamine afforded ring-closed **9a** along with the mono-eliminated crystalline side product (S_p,S,S_p,R)-**9b** (Fig. 7), both in poor yield (12 and 13%, respectively) (Honegger & Widhalm, 2019*b*).

In the symmetric diferrocenes (S_p,S_p)-**6** and (S_p,S_p)-**7**, the ferrocene subunits are identical. Fig. 8 shows a system developed to distinguish them into an *re*-site and an *si*-site. Taking divinyl compound (S_p,S_p)-**6** as an example, both ferrocene units are planar–chiral (S_p). The P atom in compound (S_p,S_p)-**6** is prochiral; if any of the two vinylferrocene groups are modified, the ferrocene substituents become distinguishable and the P atom thus a chiral centre. Fig. 9 shows a hypothetical Markovnikov regioselective addition of HNu to divinyl (S_p,S_p)-**6**, Nu standing for a generalized nucleophile. Depending on whether HNu is added to the *re*-site or *si*-site vinyl group, the P atom becomes an (*S*)- or (*R*)-chiral centre, respectively. The two possible products are diastereomers since the reaction turns the P-atom centre from prochiral to centre-chiral. In addition, this reaction introduces a new chiral centre, but in a diastereoselective fashion since one of the two sites is blocked by the other ring of the ferrocenyl unit (Marquarding *et al.*, 1970). The two possible products are diastereomers, differing only in the resulting configuration of

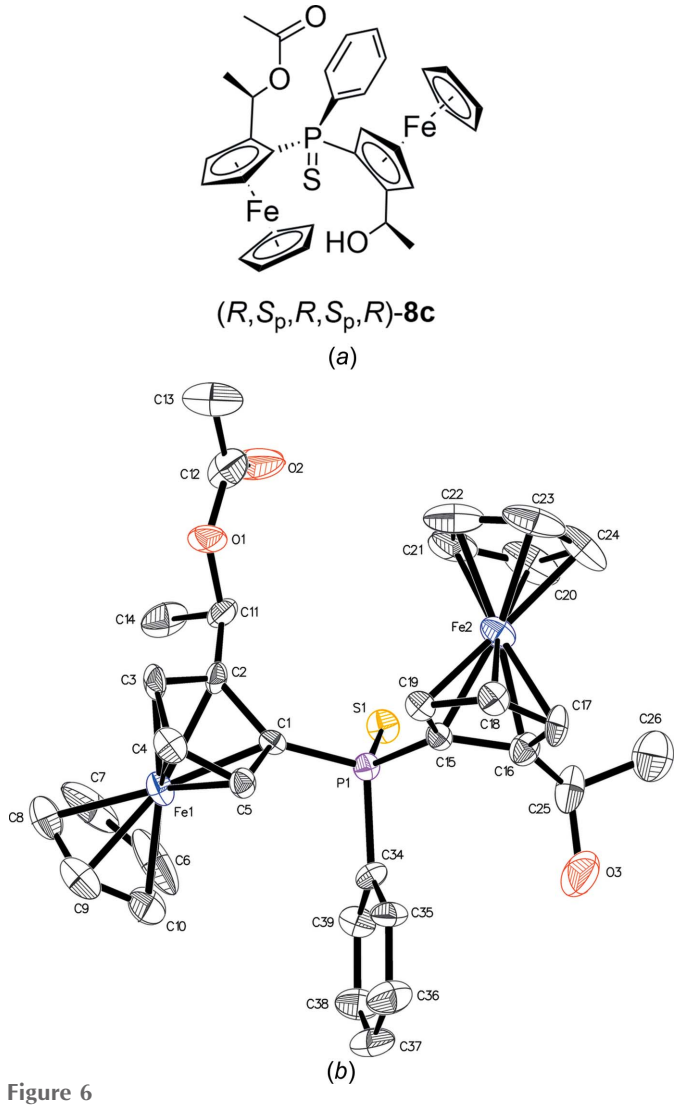


Figure 6
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of monoacetatemonohydroxide **8c**.

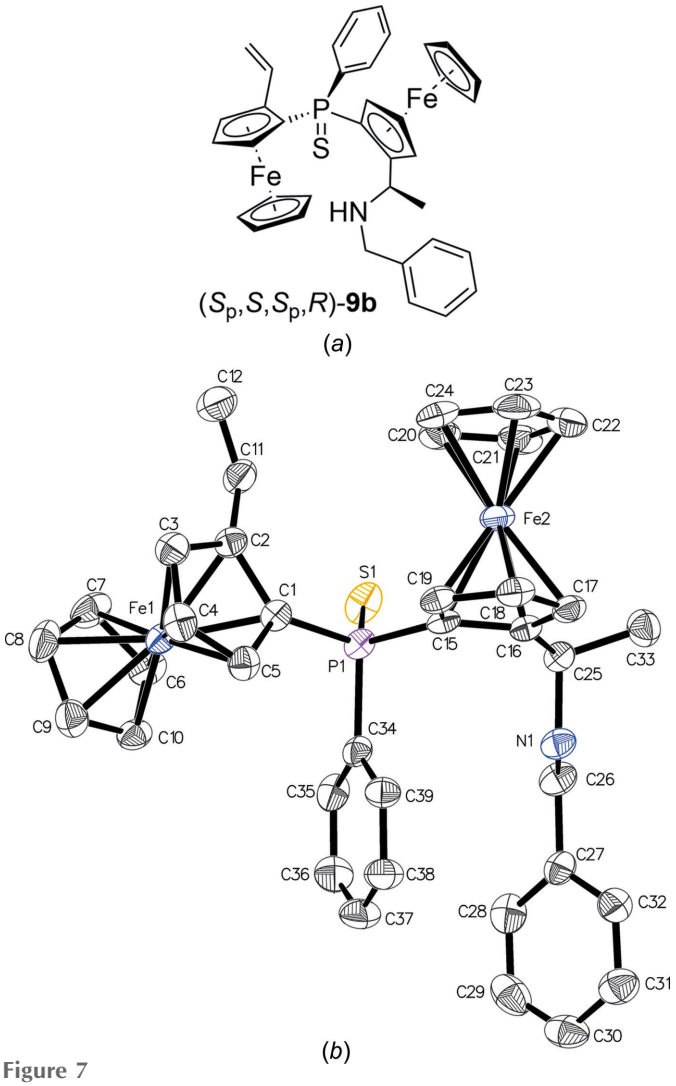


Figure 7
(*a*) Chemical structure and (*b*) displacement ellipsoid plot of benzylamine **9b**.

the P atom (epimers). In the compounds presented in this article, we know the configuration at the (S_p)-disubstituted ferrocene will be selectively (*R*), since the approach of the nucleophile from the (*S*)-site is blocked by the other cyclopentadienyl (Cp) ring (Marquarding *et al.*, 1970). Fig. 9 illustrates this by rotating the two possible products by 180° for better comparison with the other product; again, only the configuration of the P atom differs. We only observed the formation of one of the two possible diastereomers, hence the reaction proceeds diastereoselectively, as was observed for different reactions throughout this study. Typically, the *re*-site of the symmetrical (S_p,S_p)-precursors was more reactive.

Thus, the vinylferrocene groups are diastereotopic and their respective NMR shifts can be distinguished despite their apparent equality in connectivity when neglecting stereochemical aspects. In fact, protons attached to the inner vinyl protons in (S_p,S_p)-**6** differ so greatly in chemical shift that one of the two is found at a higher field than even aromatic protons (δ = 8.1 ppm; Honegger *et al.*, 2020).

The preferred conformation of ferrocenyl units with both Cp rings is a perpendicular arrangement, with the reactive *re*-ferrocene closer to the small sulfur residue and the less reactive *si*-ferrocene shielded by the bulkier phenyl group.

For the asymmetric diferrocene compounds (S_p,*S*,S_p,*R*)-**8a**, (S_p,*S*,S_p,*R*)-**8b** and (S_p,*S*,S_p,*R*)-**9b**, the ferrocenyl at the smaller sulfur group bears the more bulky substituent (acetate, hydroxy and benzyl), while the other ferrocenyl unit at the larger phenyl ring is substituted with a sterically less demanding vinyl group. Only hydroxyacetate (S_p,*R*,S_p,*R*)-**8c** shows the opposite preference. The preferred geometry might be mainly controlled by subtle inter- and intramolecular steric interactions as no π–π interactions could be detected. The protic H atoms in compounds **8b**, **8c** (O—H group) and **9b** (N—H group) form intramolecular hydrogen bonds with the π-system of the P-substituted phenyl group.

Since we obtained the sufficiently stable compound (S_p,S_p)-**6** in large enough quantities, we tested its asymmetry-inducing performance as a ligand in an *in-situ* formed Pd^{II} complex used for asymmetric allylic alkylation according to Widhalm *et al.* (1996). This purely planar–chiral compound achieved an enantiomeric excess of 35%, which is less than what we found for previously known (*R*,S_p,S_p,*R*)-**2** (57%). Regardless, the coordination structure of (S_p,S_p)-**6** and Pd^{II} remains an interesting question since neither phosphine (S_p,S_p)-**5** nor its phosphine oxide analog were able to activate Pd^{II}. We could not isolate the catalytically active Pd^{II} complex to study its structure, but we speculate that the phosphine sulfide might act as an electron donor to form a dative bond in transition-metal catalysts.

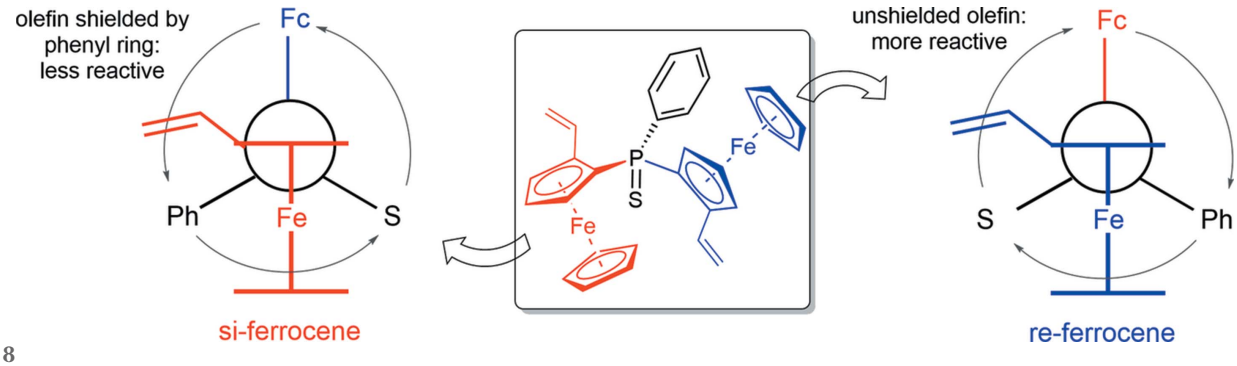


Figure 8
The *re*/*si* nomenclature for diferrocenes developed in the framework of this study to distinguish between the two ferrocenyl subunits.

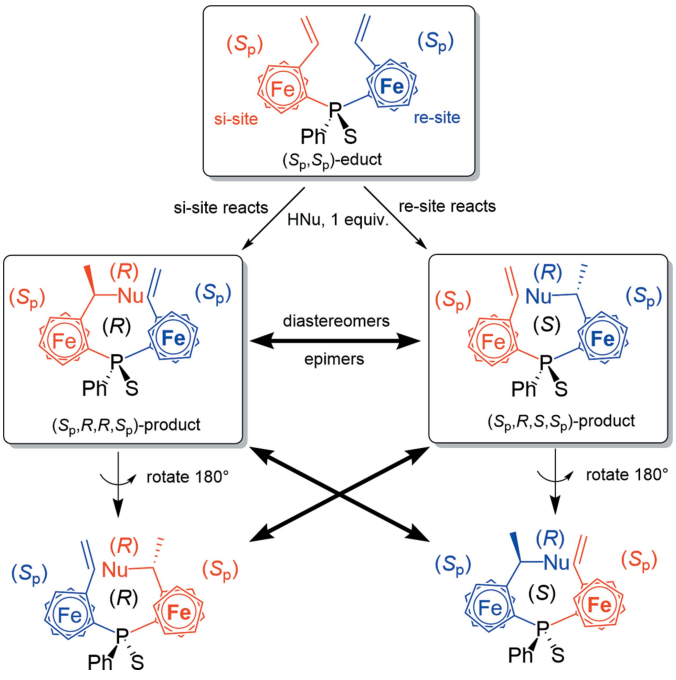


Figure 9
Hypothetical Markovnikov-selective addition of HNu to a symmetrical di(vinylferrocene), with Nu standing for an arbitrary nucleophile. The other Cp rings have been omitted for clarity and represented indirectly by the planar–chiral configuration (S_p).

4. Conclusion

We present the crystal structures of six homochiral phosphorous-linked diferrocenes. All the ferrocene units are planar–chiral (S_p) and five of the compounds include one or two centre-chiral C atoms (R) also. Interestingly, the molecules lack strong intermolecular interactions and exhibit no π-stacking, even though most of the C atoms are aromatic. Compounds **8b**, **8c** and **9b** include acidic H atoms (RO—H and R_2N—H) capable of forming hydrogen bridges with the π-electron systems of the phenyl ring.

Four of the presented compounds contain two differently substituted ferrocene units, [(Fc^A)(Fc^B)(Ph)P], while in the other two compounds, the two ferrocene compounds are equal, [(Fc^A)$_2$(Ph)P]. Due to the planar chirality of the ferrocene units, the linking P atom is prochiral and one of the two equal ferrocene units reacts far more readily with reagents than the other due to diastereoselectivity. This ability of selective chemical ferrocene subunit differentiation suggests the application of such diferrocenes in asymmetric organic chemistry, for instance, as ligands, catalysts and auxiliaries.

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supporting information

Acta Cryst. (2021). C**77**, 152-160 [https://doi.org/10.1107/S2053229621001996]

Synthesis and characterization of enantiopure planar–chiral phosphorus-linked diferrocenes

Philipp Honegger, Alexander Roller and Michael Widhalm

Computing details

Data collection: *APEX2* (Bruker, 2009) for (6), (7), (8b), (8c), (9b); *APEX3* (Bruker, 2016) for (8a). Cell refinement: *SAINT* (Bruker, 2009) for (6), (7), (8b), (8c), (9b); *SAINT* (Bruker, 2016) for (8a). Data reduction: *SAINT* (Bruker, 2009) for (6), (7), (8b), (8c), (9b); *SAINT* (Bruker, 2016) for (8a). For all structures, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Bis[(2S_p)-2-ethenylferrocen-1-yl]phenylphosphane sulfide (6)

Crystal data

$[Fe_2(C_5H_5)_2(C_{20}H_{17}PS)]$
M_r = 562.24
Monoclinic, $P2_1$
a = 8.4709 (7) Å
b = 14.1401 (11) Å
c = 21.0310 (17) Å
β = 91.880 (3)°
V = 2517.7 (4) Å^3
Z = 4
$F(000)$ = 1160
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9832 reflections
θ = 2.4–29.6°
μ = 1.32 mm^{-1}
T = 130 K
Block, clear brown
0.28 × 0.25 × 0.13 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: sealed xray tube, Incoatec IuS
Detector resolution: 8 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008
T_{min} = 0.620, T_{max} = 0.746
35484 measured reflections
14468 independent reflections
13352 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 30.2°, θ_{min} = 1.9°
h = −11→11
k = −18→19
l = −29→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.071
S = 1.03
14468 reflections
613 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 0.1684P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.42 e Å^{-3}

$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Absolute structure: Flack *x* determined using 5751 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.019 (5)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups 2.a Aromatic/amide H refined with riding coordinates: C3A(H3A), C4A(H4A), C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C9A(H9A), C10A(H10A), C11A(H11A), C17A(H17A), C18A(H18A), C19A(H19A), C20A(H20A), C21A(H21A), C22A(H22A), C23A(H23A), C24A(H24A), C25A(H25A), C35A(H35A), C36A(H36A), C37A(H37A), C38A(H38A), C39A(H39A), C3B(H3B), C4B(H4B), C5B(H5B), C6B(H6B), C7B(H7B), C8B(H8B), C9B(H9B), C10B(H10B), C11B(H11B), C17B(H17B), C18B(H18B), C19B(H19B), C20B(H20B), C21B(H21B), C22B(H22B), C23B(H23B), C24B(H24B), C25B(H25B), C35B(H35B), C36B(H36B), C37B(H37B), C38B(H38B), C39B(H39B) 2.b X=CH2 refined with riding coordinates: C12A(H12A,H12B), C26A(H26A,H26B), C12B(H12C,H12D), C26B(H26C,H26D)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1A	0.59127 (5)	0.38914 (3)	0.76817 (2)	0.01812 (9)
Fe2A	0.34181 (5)	0.28622 (3)	1.02977 (2)	0.02048 (10)
S1A	0.19010 (8)	0.24467 (5)	0.83624 (4)	0.02041 (15)
P1A	0.28675 (8)	0.35995 (5)	0.87163 (3)	0.01445 (14)
C1A	0.4891 (3)	0.3803 (2)	0.85297 (13)	0.0169 (5)
C2A	0.6190 (3)	0.3136 (2)	0.85085 (14)	0.0200 (6)
C3A	0.7578 (3)	0.3677 (2)	0.83929 (14)	0.0219 (6)
H3A	0.860707	0.342545	0.834320	0.026*
C4A	0.7172 (4)	0.4648 (2)	0.83646 (15)	0.0238 (6)
H4A	0.788282	0.515584	0.830075	0.029*
C5A	0.5525 (3)	0.4732 (2)	0.84477 (14)	0.0212 (6)
H5A	0.494171	0.530619	0.844890	0.025*
C6A	0.4324 (4)	0.3460 (3)	0.69950 (15)	0.0273 (7)
H6A	0.329694	0.321977	0.706505	0.033*
C7A	0.5717 (4)	0.2919 (3)	0.69722 (16)	0.0351 (8)
H7A	0.579373	0.225308	0.702281	0.042*
C8A	0.6980 (4)	0.3544 (3)	0.68606 (17)	0.0400 (9)
H8A	0.805586	0.336929	0.682343	0.048*
C9A	0.6370 (5)	0.4470 (3)	0.68138 (17)	0.0385 (9)
H9A	0.696106	0.502846	0.674043	0.046*
C10A	0.4714 (4)	0.4421 (3)	0.68958 (16)	0.0315 (8)
H10A	0.399862	0.493815	0.688593	0.038*
C11A	0.6117 (4)	0.2110 (2)	0.85674 (19)	0.0317 (8)
H11A	0.510176	0.182481	0.857177	0.038*
C12A	0.7362 (5)	0.1550 (3)	0.8615 (2)	0.0439 (10)
H12A	0.839555	0.181071	0.861221	0.053*
H12B	0.722528	0.088529	0.865200	0.053*

C15A	0.2891 (3)	0.37435 (19)	0.95609 (13)	0.0165 (5)
C16A	0.1574 (3)	0.3685 (2)	0.99792 (14)	0.0199 (6)
C17A	0.2133 (4)	0.3990 (2)	1.05901 (15)	0.0251 (6)
H17A	0.152217	0.401675	1.096047	0.030*
C18A	0.3743 (4)	0.4249 (2)	1.05595 (15)	0.0253 (7)
H18A	0.439104	0.447892	1.090285	0.030*
C19A	0.4219 (4)	0.4105 (2)	0.99281 (14)	0.0200 (6)
H19A	0.524061	0.422635	0.977344	0.024*
C20A	0.3700 (5)	0.1500 (2)	0.99818 (19)	0.0363 (8)
H20A	0.354740	0.128376	0.955649	0.044*
C21A	0.2537 (5)	0.1534 (3)	1.0451 (2)	0.0370 (9)
H21A	0.146630	0.134393	1.039531	0.044*
C22A	0.3241 (5)	0.1897 (3)	1.10095 (19)	0.0392 (9)
H22A	0.272511	0.199723	1.139823	0.047*
C23A	0.4849 (5)	0.2092 (3)	1.08999 (19)	0.0387 (9)
H23A	0.560390	0.234164	1.119883	0.046*
C24A	0.5121 (5)	0.1842 (3)	1.0259 (2)	0.0384 (9)
H24A	0.609726	0.189669	1.005267	0.046*
C25A	−0.0024 (4)	0.3364 (3)	0.98061 (15)	0.0268 (7)
H25A	−0.015263	0.298115	0.943691	0.032*
C26A	−0.1297 (4)	0.3564 (3)	1.01206 (18)	0.0425 (10)
H26A	−0.121857	0.394507	1.049228	0.051*
H26B	−0.229525	0.332743	0.997623	0.051*
C34A	0.1858 (3)	0.4661 (2)	0.84285 (13)	0.0167 (5)
C35A	0.1176 (3)	0.4667 (2)	0.78168 (14)	0.0208 (6)
H35A	0.118585	0.411088	0.756380	0.025*
C36A	0.0481 (4)	0.5487 (2)	0.75779 (15)	0.0247 (6)
H36A	0.003166	0.549417	0.715804	0.030*
C37A	0.0440 (4)	0.6296 (2)	0.79492 (16)	0.0255 (7)
H37A	−0.002851	0.685774	0.778184	0.031*
C38A	0.1075 (4)	0.6288 (2)	0.85581 (16)	0.0258 (7)
H38A	0.102374	0.684046	0.881348	0.031*
C39A	0.1794 (4)	0.5473 (2)	0.88043 (16)	0.0221 (6)
H39A	0.223789	0.547136	0.922511	0.027*
Fe1B	0.53902 (5)	0.23164 (3)	0.47208 (2)	0.01884 (9)
Fe2B	0.80931 (5)	0.47524 (3)	0.26413 (2)	0.01774 (9)
S1B	0.95491 (9)	0.23114 (5)	0.36024 (3)	0.02119 (15)
P1B	0.85530 (8)	0.33963 (5)	0.40045 (3)	0.01426 (14)
C1B	0.6510 (3)	0.32641 (19)	0.41800 (14)	0.0164 (5)
C2B	0.5245 (3)	0.2811 (2)	0.38130 (14)	0.0217 (6)
C3B	0.3818 (4)	0.3004 (2)	0.41331 (16)	0.0266 (7)
H3B	0.279689	0.278405	0.400389	0.032*
C4B	0.4162 (4)	0.3570 (2)	0.46686 (18)	0.0277 (7)
H4B	0.341367	0.380487	0.495600	0.033*
C5B	0.5810 (4)	0.3730 (2)	0.47076 (16)	0.0234 (6)
H5B	0.635955	0.408555	0.502793	0.028*
C6B	0.6873 (5)	0.1251 (2)	0.50028 (17)	0.0333 (8)
H6B	0.793577	0.117307	0.488182	0.040*

C7B	0.5564 (6)	0.0883 (3)	0.46780 (19)	0.0437 (11)
H7B	0.555952	0.051390	0.430039	0.052*
C8B	0.4207 (5)	0.1171 (3)	0.5027 (2)	0.0516 (12)
H8B	0.313519	0.102389	0.492333	0.062*
C9B	0.4764 (5)	0.1711 (3)	0.5551 (2)	0.0450 (10)
H9B	0.412882	0.199608	0.586226	0.054*
C10B	0.6396 (5)	0.1755 (3)	0.55361 (17)	0.0375 (9)
H10B	0.707315	0.207273	0.583520	0.045*
C11B	0.5368 (4)	0.2225 (2)	0.32414 (15)	0.0276 (7)
H11B	0.637698	0.197376	0.315255	0.033*
C12B	0.4184 (5)	0.2019 (3)	0.28402 (19)	0.0410 (9)
H12C	0.315616	0.225699	0.291244	0.049*
H12D	0.436039	0.163360	0.247952	0.049*
C15B	0.8579 (3)	0.4497 (2)	0.35782 (13)	0.0167 (5)
C16B	0.9899 (4)	0.4966 (2)	0.32904 (15)	0.0225 (6)
C17B	0.9330 (4)	0.5848 (2)	0.30432 (15)	0.0246 (6)
H17B	0.994001	0.630332	0.282763	0.030*
C18B	0.7721 (4)	0.5929 (2)	0.31718 (15)	0.0261 (7)
H18B	0.706045	0.644825	0.305485	0.031*
C19B	0.7242 (4)	0.5117 (2)	0.35024 (15)	0.0215 (6)
H19B	0.621223	0.499955	0.364985	0.026*
C20B	0.7661 (4)	0.3503 (2)	0.21765 (15)	0.0277 (7)
H20B	0.763789	0.289255	0.236456	0.033*
C21B	0.9011 (5)	0.3958 (3)	0.19350 (17)	0.0379 (9)
H21B	1.004752	0.370180	0.193194	0.046*
C22B	0.8548 (6)	0.4862 (3)	0.16987 (16)	0.0424 (10)
H22B	0.921530	0.531793	0.151302	0.051*
C23B	0.6919 (6)	0.4954 (3)	0.17912 (18)	0.0454 (11)
H23B	0.628950	0.548636	0.167507	0.055*
C24B	0.6367 (5)	0.4115 (3)	0.20880 (18)	0.0370 (9)
H24B	0.531268	0.399269	0.220500	0.044*
C25B	1.1506 (4)	0.4595 (3)	0.32533 (19)	0.0378 (9)
H25B	1.167593	0.395397	0.337110	0.045*
C26B	1.2724 (5)	0.5077 (4)	0.3071 (3)	0.0589 (14)
H26C	1.260328	0.572105	0.294929	0.071*
H26D	1.373268	0.478476	0.305983	0.071*
C34B	0.9487 (3)	0.3666 (2)	0.47744 (13)	0.0173 (5)
C35B	0.9515 (4)	0.4587 (2)	0.50108 (15)	0.0235 (6)
H35B	0.911046	0.509103	0.475552	0.028*
C36B	1.0134 (4)	0.4770 (3)	0.56195 (16)	0.0297 (7)
H36B	1.013790	0.539678	0.578296	0.036*
C37B	1.0743 (4)	0.4036 (3)	0.59841 (15)	0.0321 (8)
H37B	1.116488	0.416100	0.639959	0.039*
C38B	1.0745 (4)	0.3125 (3)	0.57538 (15)	0.0300 (7)
H38B	1.117118	0.262545	0.600793	0.036*
C39B	1.0121 (4)	0.2941 (2)	0.51466 (14)	0.0232 (6)
H39B	1.012919	0.231342	0.498523	0.028*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1A	0.01786 (19)	0.0205 (2)	0.0162 (2)	−0.00154 (15)	0.00287 (15)	−0.00044 (16)
Fe2A	0.0217 (2)	0.0224 (2)	0.0172 (2)	0.00156 (17)	−0.00156 (16)	0.00518 (17)
S1A	0.0204 (3)	0.0172 (3)	0.0236 (4)	−0.0040 (3)	0.0002 (3)	−0.0031 (3)
P1A	0.0148 (3)	0.0146 (3)	0.0139 (3)	−0.0011 (2)	0.0003 (2)	0.0000 (3)
C1A	0.0163 (12)	0.0175 (13)	0.0168 (13)	−0.0025 (10)	0.0010 (10)	−0.0007 (11)
C2A	0.0179 (14)	0.0248 (15)	0.0174 (14)	−0.0017 (11)	0.0001 (11)	0.0028 (11)
C3A	0.0174 (13)	0.0282 (16)	0.0202 (15)	−0.0021 (12)	0.0015 (11)	0.0010 (12)
C4A	0.0226 (14)	0.0249 (15)	0.0240 (16)	−0.0087 (12)	0.0036 (12)	−0.0057 (13)
C5A	0.0221 (14)	0.0198 (13)	0.0219 (15)	−0.0039 (12)	0.0050 (11)	−0.0035 (12)
C6A	0.0272 (16)	0.0371 (18)	0.0175 (15)	−0.0047 (14)	−0.0011 (12)	−0.0032 (14)
C7A	0.0388 (19)	0.041 (2)	0.0251 (17)	0.0039 (16)	0.0015 (14)	−0.0160 (16)
C8A	0.0300 (18)	0.070 (3)	0.0203 (17)	0.0019 (18)	0.0075 (13)	−0.0093 (18)
C9A	0.037 (2)	0.057 (2)	0.0213 (17)	−0.0127 (18)	0.0047 (15)	0.0087 (17)
C10A	0.0304 (18)	0.043 (2)	0.0209 (16)	−0.0024 (15)	−0.0030 (13)	0.0068 (15)
C11A	0.0235 (16)	0.0253 (17)	0.047 (2)	0.0009 (12)	0.0064 (14)	0.0094 (15)
C12A	0.0326 (19)	0.0250 (18)	0.075 (3)	0.0052 (15)	0.0124 (19)	0.0104 (19)
C15A	0.0183 (12)	0.0147 (13)	0.0165 (13)	0.0004 (10)	−0.0005 (10)	0.0012 (11)
C16A	0.0218 (14)	0.0227 (14)	0.0153 (13)	0.0029 (11)	−0.0007 (10)	0.0014 (11)
C17A	0.0279 (16)	0.0308 (17)	0.0168 (14)	0.0054 (13)	0.0038 (12)	−0.0003 (13)
C18A	0.0315 (17)	0.0266 (15)	0.0174 (15)	0.0013 (13)	−0.0044 (13)	−0.0024 (12)
C19A	0.0205 (14)	0.0211 (14)	0.0183 (14)	−0.0009 (11)	−0.0025 (11)	0.0005 (11)
C20A	0.050 (2)	0.0211 (16)	0.038 (2)	0.0080 (15)	0.0013 (17)	0.0050 (15)
C21A	0.038 (2)	0.0249 (17)	0.048 (2)	−0.0015 (15)	0.0046 (17)	0.0132 (16)
C22A	0.052 (2)	0.0340 (19)	0.032 (2)	0.0101 (17)	0.0047 (17)	0.0196 (16)
C23A	0.042 (2)	0.037 (2)	0.037 (2)	0.0070 (16)	−0.0144 (17)	0.0147 (16)
C24A	0.0331 (18)	0.0302 (18)	0.052 (2)	0.0112 (15)	0.0042 (17)	0.0125 (17)
C25A	0.0216 (14)	0.0384 (18)	0.0204 (15)	0.0005 (13)	−0.0007 (12)	0.0009 (14)
C26A	0.0217 (16)	0.073 (3)	0.033 (2)	−0.0001 (18)	0.0025 (14)	−0.007 (2)
C34A	0.0143 (12)	0.0185 (13)	0.0173 (13)	−0.0009 (10)	0.0016 (10)	0.0018 (11)
C35A	0.0221 (14)	0.0244 (15)	0.0159 (14)	−0.0006 (12)	0.0014 (11)	0.0022 (12)
C36A	0.0238 (15)	0.0310 (16)	0.0193 (15)	0.0006 (13)	−0.0013 (12)	0.0072 (13)
C37A	0.0229 (15)	0.0218 (15)	0.0318 (18)	0.0021 (12)	0.0023 (13)	0.0099 (13)
C38A	0.0273 (16)	0.0191 (14)	0.0309 (18)	0.0016 (12)	0.0003 (13)	0.0012 (13)
C39A	0.0233 (15)	0.0199 (14)	0.0229 (15)	−0.0001 (11)	−0.0022 (12)	0.0001 (12)
Fe1B	0.0214 (2)	0.01669 (19)	0.0186 (2)	−0.00228 (16)	0.00382 (16)	0.00082 (17)
Fe2B	0.0239 (2)	0.01526 (19)	0.01395 (19)	0.00233 (16)	−0.00102 (15)	0.00088 (16)
S1B	0.0253 (3)	0.0184 (3)	0.0198 (4)	0.0053 (3)	0.0009 (3)	−0.0027 (3)
P1B	0.0159 (3)	0.0139 (3)	0.0129 (3)	0.0000 (2)	−0.0004 (3)	−0.0002 (3)
C1B	0.0156 (13)	0.0144 (12)	0.0192 (14)	0.0004 (10)	0.0002 (10)	0.0024 (11)
C2B	0.0211 (14)	0.0219 (14)	0.0217 (15)	−0.0046 (12)	−0.0023 (11)	0.0052 (12)
C3B	0.0180 (14)	0.0252 (16)	0.0364 (19)	−0.0037 (12)	−0.0020 (13)	0.0067 (14)
C4B	0.0197 (14)	0.0209 (15)	0.043 (2)	0.0014 (12)	0.0064 (13)	0.0007 (14)
C5B	0.0220 (14)	0.0176 (14)	0.0307 (17)	−0.0002 (11)	0.0045 (12)	−0.0038 (12)
C6B	0.046 (2)	0.0219 (15)	0.0324 (19)	0.0095 (15)	0.0063 (16)	0.0082 (14)
C7B	0.081 (3)	0.0175 (16)	0.032 (2)	−0.0041 (18)	−0.002 (2)	0.0038 (15)

C8B	0.045 (2)	0.038 (2)	0.071 (3)	−0.0213 (18)	−0.002 (2)	0.029 (2)
C9B	0.056 (3)	0.043 (2)	0.036 (2)	−0.0007 (19)	0.0186 (19)	0.0113 (19)
C10B	0.056 (2)	0.037 (2)	0.0202 (17)	0.0078 (17)	0.0025 (16)	0.0074 (15)
C11B	0.0306 (16)	0.0288 (16)	0.0232 (16)	−0.0076 (13)	−0.0019 (13)	0.0043 (13)
C12B	0.044 (2)	0.045 (2)	0.033 (2)	−0.0086 (17)	−0.0111 (17)	−0.0043 (17)
C15B	0.0200 (13)	0.0163 (13)	0.0139 (13)	−0.0007 (10)	0.0003 (10)	0.0004 (10)
C16B	0.0225 (14)	0.0239 (15)	0.0211 (15)	−0.0057 (12)	−0.0015 (12)	0.0048 (12)
C17B	0.0346 (17)	0.0190 (14)	0.0201 (15)	−0.0079 (13)	−0.0015 (13)	0.0026 (12)
C18B	0.0415 (19)	0.0151 (14)	0.0220 (16)	0.0049 (12)	0.0053 (14)	−0.0007 (12)
C19B	0.0260 (15)	0.0171 (13)	0.0215 (15)	0.0043 (11)	0.0052 (12)	0.0003 (12)
C20B	0.048 (2)	0.0199 (15)	0.0150 (14)	0.0001 (14)	−0.0025 (13)	−0.0033 (12)
C21B	0.062 (2)	0.0283 (18)	0.0248 (17)	0.0006 (17)	0.0159 (17)	−0.0055 (15)
C22B	0.083 (3)	0.0294 (19)	0.0151 (16)	−0.0097 (19)	0.0058 (17)	0.0034 (15)
C23B	0.080 (3)	0.0237 (18)	0.030 (2)	−0.0011 (18)	−0.028 (2)	0.0049 (15)
C24B	0.044 (2)	0.0324 (18)	0.0337 (19)	−0.0021 (15)	−0.0188 (17)	−0.0024 (15)
C25B	0.0209 (16)	0.049 (2)	0.044 (2)	0.0001 (15)	−0.0007 (15)	0.0204 (18)
C26B	0.026 (2)	0.069 (3)	0.082 (4)	−0.007 (2)	0.007 (2)	0.024 (3)
C34B	0.0149 (12)	0.0227 (14)	0.0143 (13)	−0.0003 (10)	0.0013 (10)	0.0002 (11)
C35B	0.0265 (15)	0.0237 (15)	0.0204 (15)	−0.0032 (12)	0.0009 (12)	−0.0008 (12)
C36B	0.0325 (17)	0.0344 (17)	0.0225 (16)	−0.0091 (15)	0.0035 (13)	−0.0099 (15)
C37B	0.0254 (16)	0.056 (2)	0.0148 (14)	−0.0070 (15)	0.0002 (12)	−0.0051 (15)
C38B	0.0273 (16)	0.044 (2)	0.0190 (16)	0.0052 (14)	−0.0014 (13)	0.0073 (15)
C39B	0.0212 (14)	0.0293 (16)	0.0189 (14)	0.0037 (12)	−0.0014 (11)	−0.0005 (13)

Geometric parameters (Å, º)

Fe1A—C1A	2.012 (3)	Fe1B—C1B	2.015 (3)
Fe1A—C2A	2.048 (3)	Fe1B—C2B	2.033 (3)
Fe1A—C3A	2.045 (3)	Fe1B—C3B	2.034 (3)
Fe1A—C4A	2.060 (3)	Fe1B—C4B	2.056 (3)
Fe1A—C5A	2.038 (3)	Fe1B—C5B	2.031 (3)
Fe1A—C6A	2.035 (3)	Fe1B—C6B	2.037 (3)
Fe1A—C7A	2.032 (3)	Fe1B—C7B	2.035 (4)
Fe1A—C8A	2.035 (4)	Fe1B—C8B	2.021 (4)
Fe1A—C9A	2.049 (4)	Fe1B—C9B	2.031 (4)
Fe1A—C10A	2.052 (3)	Fe1B—C10B	2.049 (4)
Fe2A—C15A	2.027 (3)	Fe2B—C15B	2.032 (3)
Fe2A—C16A	2.043 (3)	Fe2B—C16B	2.039 (3)
Fe2A—C17A	2.038 (3)	Fe2B—C17B	2.038 (3)
Fe2A—C18A	2.053 (3)	Fe2B—C18B	2.034 (3)
Fe2A—C19A	2.046 (3)	Fe2B—C19B	2.037 (3)
Fe2A—C20A	2.055 (4)	Fe2B—C20B	2.046 (3)
Fe2A—C21A	2.050 (4)	Fe2B—C21B	2.037 (3)
Fe2A—C22A	2.035 (3)	Fe2B—C22B	2.038 (4)
Fe2A—C23A	2.040 (3)	Fe2B—C23B	2.037 (3)
Fe2A—C24A	2.044 (4)	Fe2B—C24B	2.048 (3)
S1A—P1A	1.9600 (10)	S1B—P1B	1.9563 (10)
P1A—C1A	1.794 (3)	P1B—C1B	1.792 (3)

P1A—C15A	1.787 (3)	P1B—C15B	1.796 (3)
P1A—C34A	1.821 (3)	P1B—C34B	1.819 (3)
C1A—C2A	1.451 (4)	C1B—C2B	1.449 (4)
C1A—C5A	1.432 (4)	C1B—C5B	1.435 (4)
C2A—C3A	1.431 (4)	C2B—C3B	1.430 (4)
C2A—C11A	1.457 (4)	C2B—C11B	1.466 (5)
C3A—H3A	0.9500	C3B—H3B	0.9500
C3A—C4A	1.416 (5)	C3B—C4B	1.404 (5)
C4A—H4A	0.9500	C4B—H4B	0.9500
C4A—C5A	1.417 (4)	C4B—C5B	1.414 (4)
C5A—H5A	0.9500	C5B—H5B	0.9500
C6A—H6A	0.9500	C6B—H6B	0.9500
C6A—C7A	1.407 (5)	C6B—C7B	1.385 (6)
C6A—C10A	1.416 (5)	C6B—C10B	1.400 (5)
C7A—H7A	0.9500	C7B—H7B	0.9500
C7A—C8A	1.413 (6)	C7B—C8B	1.443 (6)
C8A—H8A	0.9500	C8B—H8B	0.9500
C8A—C9A	1.411 (6)	C8B—C9B	1.409 (6)
C9A—H9A	0.9500	C9B—H9B	0.9500
C9A—C10A	1.420 (5)	C9B—C10B	1.385 (6)
C10A—H10A	0.9500	C10B—H10B	0.9500
C11A—H11A	0.9500	C11B—H11B	0.9500
C11A—C12A	1.321 (5)	C11B—C12B	1.322 (5)
C12A—H12A	0.9500	C12B—H12C	0.9500
C12A—H12B	0.9500	C12B—H12D	0.9500
C15A—C16A	1.445 (4)	C15B—C16B	1.450 (4)
C15A—C19A	1.438 (4)	C15B—C19B	1.437 (4)
C16A—C17A	1.422 (4)	C16B—C17B	1.429 (4)
C16A—C25A	1.462 (4)	C16B—C25B	1.463 (5)
C17A—H17A	0.9500	C17B—H17B	0.9500
C17A—C18A	1.416 (5)	C17B—C18B	1.404 (5)
C18A—H18A	0.9500	C18B—H18B	0.9500
C18A—C19A	1.415 (4)	C18B—C19B	1.409 (4)
C19A—H19A	0.9500	C19B—H19B	0.9500
C20A—H20A	0.9500	C20B—H20B	0.9500
C20A—C21A	1.418 (6)	C20B—C21B	1.420 (5)
C20A—C24A	1.406 (6)	C20B—C24B	1.405 (5)
C21A—H21A	0.9500	C21B—H21B	0.9500
C21A—C22A	1.397 (6)	C21B—C22B	1.421 (5)
C22A—H22A	0.9500	C22B—H22B	0.9500
C22A—C23A	1.416 (6)	C22B—C23B	1.407 (6)
C23A—H23A	0.9500	C23B—H23B	0.9500
C23A—C24A	1.419 (6)	C23B—C24B	1.426 (5)
C24A—H24A	0.9500	C24B—H24B	0.9500
C25A—H25A	0.9500	C25B—H25B	0.9500
C25A—C26A	1.314 (5)	C25B—C26B	1.305 (5)
C26A—H26A	0.9500	C26B—H26C	0.9500
C26A—H26B	0.9500	C26B—H26D	0.9500

C34A—C35A	1.393 (4)	C34B—C35B	1.393 (4)
C34A—C39A	1.396 (4)	C34B—C39B	1.388 (4)
C35A—H35A	0.9500	C35B—H35B	0.9500
C35A—C36A	1.387 (4)	C35B—C36B	1.392 (4)
C36A—H36A	0.9500	C36B—H36B	0.9500
C36A—C37A	1.386 (5)	C36B—C37B	1.381 (5)
C37A—H37A	0.9500	C37B—H37B	0.9500
C37A—C38A	1.373 (5)	C37B—C38B	1.376 (5)
C38A—H38A	0.9500	C38B—H38B	0.9500
C38A—C39A	1.395 (4)	C38B—C39B	1.391 (4)
C39A—H39A	0.9500	C39B—H39B	0.9500

C1A—Fe1A—C2A	41.88 (11)	C1B—Fe1B—C2B	41.95 (11)
C1A—Fe1A—C3A	69.45 (11)	C1B—Fe1B—C3B	69.53 (12)
C1A—Fe1A—C4A	69.03 (12)	C1B—Fe1B—C4B	69.11 (12)
C1A—Fe1A—C5A	41.41 (11)	C1B—Fe1B—C5B	41.55 (12)
C1A—Fe1A—C6A	108.47 (13)	C1B—Fe1B—C6B	111.05 (14)
C1A—Fe1A—C7A	125.59 (14)	C1B—Fe1B—C7B	126.99 (16)
C1A—Fe1A—C8A	162.38 (16)	C1B—Fe1B—C8B	163.84 (17)
C1A—Fe1A—C9A	156.06 (15)	C1B—Fe1B—C9B	155.05 (15)
C1A—Fe1A—C10A	121.38 (13)	C1B—Fe1B—C10B	122.64 (15)
C2A—Fe1A—C4A	68.68 (12)	C2B—Fe1B—C3B	41.16 (13)
C2A—Fe1A—C9A	160.94 (15)	C2B—Fe1B—C4B	68.82 (14)
C2A—Fe1A—C10A	156.06 (13)	C2B—Fe1B—C6B	123.05 (14)
C3A—Fe1A—C2A	40.91 (11)	C2B—Fe1B—C7B	107.65 (14)
C3A—Fe1A—C4A	40.35 (13)	C2B—Fe1B—C10B	158.35 (15)
C3A—Fe1A—C9A	124.40 (14)	C3B—Fe1B—C4B	40.15 (14)
C3A—Fe1A—C10A	162.62 (13)	C3B—Fe1B—C6B	156.26 (14)
C5A—Fe1A—C2A	69.51 (12)	C3B—Fe1B—C7B	119.73 (15)
C5A—Fe1A—C3A	68.50 (12)	C3B—Fe1B—C10B	159.93 (15)
C5A—Fe1A—C4A	40.46 (12)	C5B—Fe1B—C2B	69.75 (13)
C5A—Fe1A—C9A	120.75 (16)	C5B—Fe1B—C3B	68.46 (13)
C5A—Fe1A—C10A	109.61 (14)	C5B—Fe1B—C4B	40.49 (12)
C6A—Fe1A—C2A	120.05 (13)	C5B—Fe1B—C6B	128.71 (14)
C6A—Fe1A—C3A	154.00 (14)	C5B—Fe1B—C7B	165.29 (16)
C6A—Fe1A—C4A	164.96 (14)	C5B—Fe1B—C9B	118.51 (16)
C6A—Fe1A—C5A	128.04 (13)	C5B—Fe1B—C10B	108.93 (15)
C6A—Fe1A—C8A	68.11 (14)	C6B—Fe1B—C4B	163.54 (15)
C6A—Fe1A—C9A	68.13 (15)	C6B—Fe1B—C10B	40.06 (15)
C6A—Fe1A—C10A	40.52 (14)	C7B—Fe1B—C4B	153.31 (16)
C7A—Fe1A—C2A	105.96 (14)	C7B—Fe1B—C6B	39.77 (16)
C7A—Fe1A—C3A	118.34 (14)	C7B—Fe1B—C10B	67.83 (16)
C7A—Fe1A—C4A	153.03 (14)	C8B—Fe1B—C2B	124.04 (16)
C7A—Fe1A—C5A	164.61 (14)	C8B—Fe1B—C3B	104.77 (16)
C7A—Fe1A—C6A	40.50 (14)	C8B—Fe1B—C4B	116.88 (16)
C7A—Fe1A—C8A	40.65 (16)	C8B—Fe1B—C5B	151.88 (18)
C7A—Fe1A—C9A	68.24 (17)	C8B—Fe1B—C6B	67.79 (17)
C7A—Fe1A—C10A	68.22 (16)	C8B—Fe1B—C7B	41.68 (19)

C8A—Fe1A—C2A	123.54 (15)	C8B—Fe1B—C9B	40.70 (19)
C8A—Fe1A—C3A	105.65 (14)	C8B—Fe1B—C10B	67.65 (18)
C8A—Fe1A—C4A	118.86 (14)	C9B—Fe1B—C2B	160.57 (15)
C8A—Fe1A—C5A	154.08 (15)	C9B—Fe1B—C3B	122.65 (16)
C8A—Fe1A—C9A	40.42 (18)	C9B—Fe1B—C4B	105.26 (16)
C8A—Fe1A—C10A	68.08 (16)	C9B—Fe1B—C6B	67.28 (16)
C9A—Fe1A—C4A	107.76 (15)	C9B—Fe1B—C7B	68.87 (17)
C9A—Fe1A—C10A	40.52 (14)	C9B—Fe1B—C10B	39.68 (17)
C10A—Fe1A—C4A	127.11 (14)	C10B—Fe1B—C4B	125.04 (15)
C15A—Fe2A—C16A	41.61 (11)	C15B—Fe2B—C16B	41.72 (12)
C15A—Fe2A—C17A	69.07 (12)	C15B—Fe2B—C17B	69.40 (12)
C15A—Fe2A—C18A	69.02 (12)	C15B—Fe2B—C18B	69.14 (12)
C15A—Fe2A—C19A	41.33 (11)	C15B—Fe2B—C19B	41.36 (11)
C15A—Fe2A—C20A	110.77 (14)	C15B—Fe2B—C20B	109.69 (12)
C15A—Fe2A—C21A	127.68 (14)	C15B—Fe2B—C21B	122.62 (14)
C15A—Fe2A—C22A	162.74 (14)	C15B—Fe2B—C22B	156.63 (16)
C15A—Fe2A—C23A	156.17 (14)	C15B—Fe2B—C23B	162.42 (17)
C15A—Fe2A—C24A	122.82 (15)	C15B—Fe2B—C24B	126.22 (14)
C16A—Fe2A—C18A	68.80 (12)	C16B—Fe2B—C20B	124.48 (13)
C16A—Fe2A—C19A	69.27 (12)	C16B—Fe2B—C24B	162.13 (13)
C16A—Fe2A—C20A	121.59 (14)	C17B—Fe2B—C16B	41.02 (12)
C16A—Fe2A—C21A	107.14 (14)	C17B—Fe2B—C20B	159.35 (14)
C16A—Fe2A—C24A	157.24 (15)	C17B—Fe2B—C24B	156.64 (14)
C17A—Fe2A—C16A	40.78 (12)	C18B—Fe2B—C16B	68.79 (13)
C17A—Fe2A—C18A	40.49 (13)	C18B—Fe2B—C17B	40.32 (14)
C17A—Fe2A—C19A	68.25 (13)	C18B—Fe2B—C19B	40.50 (12)
C17A—Fe2A—C20A	154.26 (15)	C18B—Fe2B—C20B	160.04 (14)
C17A—Fe2A—C21A	117.96 (15)	C18B—Fe2B—C21B	157.09 (14)
C17A—Fe2A—C23A	122.91 (15)	C18B—Fe2B—C22B	120.62 (14)
C17A—Fe2A—C24A	161.70 (15)	C18B—Fe2B—C23B	106.68 (15)
C18A—Fe2A—C20A	165.12 (15)	C18B—Fe2B—C24B	123.43 (15)
C19A—Fe2A—C18A	40.39 (12)	C19B—Fe2B—C16B	69.34 (13)
C19A—Fe2A—C20A	129.72 (14)	C19B—Fe2B—C17B	68.36 (13)
C19A—Fe2A—C21A	166.74 (14)	C19B—Fe2B—C20B	125.46 (13)
C21A—Fe2A—C18A	151.53 (15)	C19B—Fe2B—C22B	158.33 (15)
C21A—Fe2A—C20A	40.42 (16)	C19B—Fe2B—C24B	110.46 (15)
C22A—Fe2A—C16A	123.28 (15)	C20B—Fe2B—C24B	40.13 (14)
C22A—Fe2A—C17A	104.47 (15)	C21B—Fe2B—C16B	105.89 (16)
C22A—Fe2A—C18A	117.11 (15)	C21B—Fe2B—C17B	121.21 (15)
C22A—Fe2A—C19A	152.72 (15)	C21B—Fe2B—C19B	160.47 (14)
C22A—Fe2A—C20A	67.74 (16)	C21B—Fe2B—C20B	40.71 (15)
C22A—Fe2A—C21A	40.00 (16)	C21B—Fe2B—C22B	40.83 (15)
C22A—Fe2A—C23A	40.69 (16)	C21B—Fe2B—C23B	67.92 (18)
C22A—Fe2A—C24A	67.98 (16)	C21B—Fe2B—C24B	68.01 (17)
C23A—Fe2A—C16A	160.10 (15)	C22B—Fe2B—C16B	118.57 (16)
C23A—Fe2A—C18A	105.78 (15)	C22B—Fe2B—C17B	103.58 (15)
C23A—Fe2A—C19A	119.80 (14)	C22B—Fe2B—C20B	68.73 (14)
C23A—Fe2A—C20A	68.08 (16)	C22B—Fe2B—C24B	68.59 (17)

C23A—Fe2A—C21A	67.97 (16)	C23B—Fe2B—C16B	154.27 (16)
C23A—Fe2A—C24A	40.67 (16)	C23B—Fe2B—C17B	119.17 (14)
C24A—Fe2A—C18A	126.61 (15)	C23B—Fe2B—C19B	124.60 (17)
C24A—Fe2A—C19A	110.37 (15)	C23B—Fe2B—C20B	68.09 (14)
C24A—Fe2A—C20A	40.12 (16)	C23B—Fe2B—C22B	40.39 (18)
C24A—Fe2A—C21A	67.70 (16)	C23B—Fe2B—C24B	40.85 (15)
C1A—P1A—S1A	116.13 (10)	C1B—P1B—S1B	116.14 (10)
C1A—P1A—C34A	103.68 (13)	C1B—P1B—C15B	102.76 (13)
C15A—P1A—S1A	117.58 (10)	C1B—P1B—C34B	103.49 (13)
C15A—P1A—C1A	102.69 (13)	C15B—P1B—S1B	116.81 (10)
C15A—P1A—C34A	103.07 (13)	C15B—P1B—C34B	104.50 (13)
C34A—P1A—S1A	111.94 (9)	C34B—P1B—S1B	111.60 (10)
P1A—C1A—Fe1A	130.23 (15)	P1B—C1B—Fe1B	131.42 (15)
C2A—C1A—Fe1A	70.39 (16)	C2B—C1B—Fe1B	69.70 (16)
C2A—C1A—P1A	129.3 (2)	C2B—C1B—P1B	129.7 (2)
C5A—C1A—Fe1A	70.26 (17)	C5B—C1B—Fe1B	69.83 (17)
C5A—C1A—P1A	122.6 (2)	C5B—C1B—P1B	122.5 (2)
C5A—C1A—C2A	107.8 (2)	C5B—C1B—C2B	107.4 (3)
C1A—C2A—Fe1A	67.73 (16)	C1B—C2B—Fe1B	68.35 (16)
C1A—C2A—C11A	127.6 (3)	C1B—C2B—C11B	128.0 (3)
C3A—C2A—Fe1A	69.43 (17)	C3B—C2B—Fe1B	69.48 (18)
C3A—C2A—C1A	106.6 (3)	C3B—C2B—C1B	106.7 (3)
C3A—C2A—C11A	125.8 (3)	C3B—C2B—C11B	125.3 (3)
C11A—C2A—Fe1A	126.0 (2)	C11B—C2B—Fe1B	124.9 (2)
Fe1A—C3A—H3A	126.0	Fe1B—C3B—H3B	126.1
C2A—C3A—Fe1A	69.65 (16)	C2B—C3B—Fe1B	69.37 (17)
C2A—C3A—H3A	125.5	C2B—C3B—H3B	125.4
C4A—C3A—Fe1A	70.39 (18)	C4B—C3B—Fe1B	70.76 (18)
C4A—C3A—C2A	109.0 (3)	C4B—C3B—C2B	109.3 (3)
C4A—C3A—H3A	125.5	C4B—C3B—H3B	125.4
Fe1A—C4A—H4A	127.6	Fe1B—C4B—H4B	127.9
C3A—C4A—Fe1A	69.25 (17)	C3B—C4B—Fe1B	69.09 (18)
C3A—C4A—H4A	125.8	C3B—C4B—H4B	125.8
C3A—C4A—C5A	108.4 (3)	C3B—C4B—C5B	108.5 (3)
C5A—C4A—Fe1A	68.93 (17)	C5B—C4B—Fe1B	68.79 (17)
C5A—C4A—H4A	125.8	C5B—C4B—H4B	125.8
Fe1A—C5A—H5A	126.7	Fe1B—C5B—H5B	126.4
C1A—C5A—Fe1A	68.32 (17)	C1B—C5B—Fe1B	68.62 (16)
C1A—C5A—H5A	125.9	C1B—C5B—H5B	125.9
C4A—C5A—Fe1A	70.62 (18)	C4B—C5B—Fe1B	70.72 (18)
C4A—C5A—C1A	108.2 (3)	C4B—C5B—C1B	108.3 (3)
C4A—C5A—H5A	125.9	C4B—C5B—H5B	125.9
Fe1A—C6A—H6A	125.8	Fe1B—C6B—H6B	126.1
C7A—C6A—Fe1A	69.62 (19)	C7B—C6B—Fe1B	70.0 (2)
C7A—C6A—H6A	125.8	C7B—C6B—H6B	125.1
C7A—C6A—C10A	108.4 (3)	C7B—C6B—C10B	109.8 (4)
C10A—C6A—Fe1A	70.40 (19)	C10B—C6B—Fe1B	70.4 (2)
C10A—C6A—H6A	125.8	C10B—C6B—H6B	125.1

Fe1A—C7A—H7A	125.8	Fe1B—C7B—H7B	125.9
C6A—C7A—Fe1A	69.9 (2)	C6B—C7B—Fe1B	70.2 (2)
C6A—C7A—H7A	126.1	C6B—C7B—H7B	126.8
C6A—C7A—C8A	107.9 (4)	C6B—C7B—C8B	106.3 (4)
C8A—C7A—Fe1A	69.8 (2)	C8B—C7B—Fe1B	68.7 (2)
C8A—C7A—H7A	126.1	C8B—C7B—H7B	126.8
Fe1A—C8A—H8A	125.9	Fe1B—C8B—H8B	125.6
C7A—C8A—Fe1A	69.53 (19)	C7B—C8B—Fe1B	69.7 (2)
C7A—C8A—H8A	125.8	C7B—C8B—H8B	126.3
C9A—C8A—Fe1A	70.3 (2)	C9B—C8B—Fe1B	70.0 (2)
C9A—C8A—C7A	108.3 (3)	C9B—C8B—C7B	107.4 (4)
C9A—C8A—H8A	125.8	C9B—C8B—H8B	126.3
Fe1A—C9A—H9A	126.3	Fe1B—C9B—H9B	125.6
C8A—C9A—Fe1A	69.3 (2)	C8B—C9B—Fe1B	69.3 (2)
C8A—C9A—H9A	126.1	C8B—C9B—H9B	125.8
C8A—C9A—C10A	107.8 (3)	C10B—C9B—Fe1B	70.9 (2)
C10A—C9A—Fe1A	69.9 (2)	C10B—C9B—C8B	108.4 (4)
C10A—C9A—H9A	126.1	C10B—C9B—H9B	125.8
Fe1A—C10A—H10A	126.6	Fe1B—C10B—H10B	126.6
C6A—C10A—Fe1A	69.08 (19)	C6B—C10B—Fe1B	69.5 (2)
C6A—C10A—C9A	107.5 (3)	C6B—C10B—H10B	126.0
C6A—C10A—H10A	126.2	C9B—C10B—Fe1B	69.5 (2)
C9A—C10A—Fe1A	69.6 (2)	C9B—C10B—C6B	108.1 (4)
C9A—C10A—H10A	126.2	C9B—C10B—H10B	126.0
C2A—C11A—H11A	117.7	C2B—C11B—H11B	117.4
C12A—C11A—C2A	124.6 (3)	C12B—C11B—C2B	125.1 (3)
C12A—C11A—H11A	117.7	C12B—C11B—H11B	117.4
C11A—C12A—H12A	120.0	C11B—C12B—H12C	120.0
C11A—C12A—H12B	120.0	C11B—C12B—H12D	120.0
H12A—C12A—H12B	120.0	H12C—C12B—H12D	120.0
P1A—C15A—Fe2A	133.21 (15)	P1B—C15B—Fe2B	129.25 (15)
C16A—C15A—Fe2A	69.79 (16)	C16B—C15B—Fe2B	69.40 (16)
C16A—C15A—P1A	127.9 (2)	C16B—C15B—P1B	128.8 (2)
C19A—C15A—Fe2A	70.06 (16)	C19B—C15B—Fe2B	69.51 (17)
C19A—C15A—P1A	123.9 (2)	C19B—C15B—P1B	124.2 (2)
C19A—C15A—C16A	107.4 (3)	C19B—C15B—C16B	106.9 (3)
C15A—C16A—Fe2A	68.61 (16)	C15B—C16B—Fe2B	68.88 (16)
C15A—C16A—C25A	126.4 (3)	C15B—C16B—C25B	126.2 (3)
C17A—C16A—Fe2A	69.41 (17)	C17B—C16B—Fe2B	69.44 (17)
C17A—C16A—C15A	107.0 (3)	C17B—C16B—C15B	107.2 (3)
C17A—C16A—C25A	126.7 (3)	C17B—C16B—C25B	126.6 (3)
C25A—C16A—Fe2A	126.7 (2)	C25B—C16B—Fe2B	126.2 (3)
Fe2A—C17A—H17A	126.1	Fe2B—C17B—H17B	126.7
C16A—C17A—Fe2A	69.81 (17)	C16B—C17B—Fe2B	69.53 (17)
C16A—C17A—H17A	125.4	C16B—C17B—H17B	125.7
C18A—C17A—Fe2A	70.33 (19)	C18B—C17B—Fe2B	69.68 (18)
C18A—C17A—C16A	109.3 (3)	C18B—C17B—C16B	108.7 (3)
C18A—C17A—H17A	125.4	C18B—C17B—H17B	125.7

Fe2A—C18A—H18A	126.9	Fe2B—C18B—H18B	126.2
C17A—C18A—Fe2A	69.17 (19)	C17B—C18B—Fe2B	70.00 (18)
C17A—C18A—H18A	126.0	C17B—C18B—H18B	125.5
C19A—C18A—Fe2A	69.56 (18)	C17B—C18B—C19B	109.0 (3)
C19A—C18A—C17A	108.1 (3)	C19B—C18B—Fe2B	69.88 (17)
C19A—C18A—H18A	126.0	C19B—C18B—H18B	125.5
Fe2A—C19A—H19A	127.0	Fe2B—C19B—H19B	127.0
C15A—C19A—Fe2A	68.61 (16)	C15B—C19B—Fe2B	69.13 (17)
C15A—C19A—H19A	125.9	C15B—C19B—H19B	125.9
C18A—C19A—Fe2A	70.05 (18)	C18B—C19B—Fe2B	69.62 (18)
C18A—C19A—C15A	108.2 (3)	C18B—C19B—C15B	108.3 (3)
C18A—C19A—H19A	125.9	C18B—C19B—H19B	125.9
Fe2A—C20A—H20A	126.3	Fe2B—C20B—H20B	126.3
C21A—C20A—Fe2A	69.6 (2)	C21B—C20B—Fe2B	69.29 (19)
C21A—C20A—H20A	126.2	C21B—C20B—H20B	126.0
C24A—C20A—Fe2A	69.5 (2)	C24B—C20B—Fe2B	69.98 (19)
C24A—C20A—H20A	126.2	C24B—C20B—H20B	126.0
C24A—C20A—C21A	107.7 (4)	C24B—C20B—C21B	107.9 (3)
Fe2A—C21A—H21A	126.2	Fe2B—C21B—H21B	126.2
C20A—C21A—Fe2A	70.0 (2)	C20B—C21B—Fe2B	70.0 (2)
C20A—C21A—H21A	125.9	C20B—C21B—H21B	125.8
C22A—C21A—Fe2A	69.4 (2)	C20B—C21B—C22B	108.4 (4)
C22A—C21A—C20A	108.1 (3)	C22B—C21B—Fe2B	69.6 (2)
C22A—C21A—H21A	125.9	C22B—C21B—H21B	125.8
Fe2A—C22A—H22A	125.5	Fe2B—C22B—H22B	125.8
C21A—C22A—Fe2A	70.6 (2)	C21B—C22B—Fe2B	69.55 (19)
C21A—C22A—H22A	125.7	C21B—C22B—H22B	126.4
C21A—C22A—C23A	108.7 (4)	C23B—C22B—Fe2B	69.8 (2)
C23A—C22A—Fe2A	69.9 (2)	C23B—C22B—C21B	107.2 (4)
C23A—C22A—H22A	125.7	C23B—C22B—H22B	126.4
Fe2A—C23A—H23A	125.8	Fe2B—C23B—H23B	126.2
C22A—C23A—Fe2A	69.46 (19)	C22B—C23B—Fe2B	69.8 (2)
C22A—C23A—H23A	126.5	C22B—C23B—H23B	125.6
C22A—C23A—C24A	107.0 (3)	C22B—C23B—C24B	108.7 (3)
C24A—C23A—Fe2A	69.81 (19)	C24B—C23B—Fe2B	69.96 (19)
C24A—C23A—H23A	126.5	C24B—C23B—H23B	125.6
Fe2A—C24A—H24A	125.9	Fe2B—C24B—H24B	126.4
C20A—C24A—Fe2A	70.4 (2)	C20B—C24B—Fe2B	69.89 (19)
C20A—C24A—C23A	108.5 (4)	C20B—C24B—C23B	107.8 (4)
C20A—C24A—H24A	125.8	C20B—C24B—H24B	126.1
C23A—C24A—Fe2A	69.5 (2)	C23B—C24B—Fe2B	69.2 (2)
C23A—C24A—H24A	125.8	C23B—C24B—H24B	126.1
C16A—C25A—H25A	117.4	C16B—C25B—H25B	117.5
C26A—C25A—C16A	125.2 (3)	C26B—C25B—C16B	125.1 (4)
C26A—C25A—H25A	117.4	C26B—C25B—H25B	117.5
C25A—C26A—H26A	120.0	C25B—C26B—H26C	120.0
C25A—C26A—H26B	120.0	C25B—C26B—H26D	120.0
H26A—C26A—H26B	120.0	H26C—C26B—H26D	120.0

C35A—C34A—P1A	119.2 (2)	C35B—C34B—P1B	121.1 (2)
C35A—C34A—C39A	119.7 (3)	C39B—C34B—P1B	119.7 (2)
C39A—C34A—P1A	121.1 (2)	C39B—C34B—C35B	119.2 (3)
C34A—C35A—H35A	120.1	C34B—C35B—H35B	119.9
C36A—C35A—C34A	119.9 (3)	C36B—C35B—C34B	120.3 (3)
C36A—C35A—H35A	120.1	C36B—C35B—H35B	119.9
C35A—C36A—H36A	119.9	C35B—C36B—H36B	120.2
C37A—C36A—C35A	120.3 (3)	C37B—C36B—C35B	119.5 (3)
C37A—C36A—H36A	119.9	C37B—C36B—H36B	120.2
C36A—C37A—H37A	119.9	C36B—C37B—H37B	119.5
C38A—C37A—C36A	120.1 (3)	C38B—C37B—C36B	120.9 (3)
C38A—C37A—H37A	119.9	C38B—C37B—H37B	119.5
C37A—C38A—H38A	119.8	C37B—C38B—H38B	120.2
C37A—C38A—C39A	120.4 (3)	C37B—C38B—C39B	119.6 (3)
C39A—C38A—H38A	119.8	C39B—C38B—H38B	120.2
C34A—C39A—H39A	120.2	C34B—C39B—C38B	120.5 (3)
C38A—C39A—C34A	119.6 (3)	C34B—C39B—H39B	119.7
C38A—C39A—H39A	120.2	C38B—C39B—H39B	119.7

Fe1A—C1A—C2A—C3A	58.8 (2)	Fe1B—C1B—C2B—C3B	59.2 (2)
Fe1A—C1A—C2A—C11A	−119.1 (3)	Fe1B—C1B—C2B—C11B	−118.1 (3)
Fe1A—C1A—C5A—C4A	−59.6 (2)	Fe1B—C1B—C5B—C4B	−59.8 (2)
Fe1A—C2A—C3A—C4A	59.6 (2)	Fe1B—C2B—C3B—C4B	59.7 (2)
Fe1A—C2A—C11A—C12A	99.8 (4)	Fe1B—C2B—C11B—C12B	108.8 (4)
Fe1A—C3A—C4A—C5A	57.9 (2)	Fe1B—C3B—C4B—C5B	57.6 (2)
Fe1A—C4A—C5A—C1A	58.2 (2)	Fe1B—C4B—C5B—C1B	58.5 (2)
Fe1A—C6A—C7A—C8A	−59.7 (2)	Fe1B—C6B—C7B—C8B	−59.5 (3)
Fe1A—C6A—C10A—C9A	59.2 (2)	Fe1B—C6B—C10B—C9B	58.9 (3)
Fe1A—C7A—C8A—C9A	−59.8 (3)	Fe1B—C7B—C8B—C9B	−60.1 (3)
Fe1A—C8A—C9A—C10A	−59.4 (3)	Fe1B—C8B—C9B—C10B	−60.3 (3)
Fe1A—C9A—C10A—C6A	−58.9 (2)	Fe1B—C9B—C10B—C6B	−59.0 (2)
Fe2A—C15A—C16A—C17A	59.0 (2)	Fe2B—C15B—C16B—C17B	59.1 (2)
Fe2A—C15A—C16A—C25A	−120.5 (3)	Fe2B—C15B—C16B—C25B	−120.1 (3)
Fe2A—C15A—C19A—C18A	−59.0 (2)	Fe2B—C15B—C19B—C18B	−58.8 (2)
Fe2A—C16A—C17A—C18A	59.4 (2)	Fe2B—C16B—C17B—C18B	58.9 (2)
Fe2A—C16A—C25A—C26A	111.9 (4)	Fe2B—C16B—C25B—C26B	100.9 (5)
Fe2A—C17A—C18A—C19A	58.9 (2)	Fe2B—C17B—C18B—C19B	59.2 (2)
Fe2A—C18A—C19A—C15A	58.1 (2)	Fe2B—C18B—C19B—C15B	58.5 (2)
Fe2A—C20A—C21A—C22A	−59.1 (2)	Fe2B—C20B—C21B—C22B	−59.2 (2)
Fe2A—C20A—C24A—C23A	59.3 (2)	Fe2B—C20B—C24B—C23B	59.0 (2)
Fe2A—C21A—C22A—C23A	−59.7 (3)	Fe2B—C21B—C22B—C23B	−59.9 (3)
Fe2A—C22A—C23A—C24A	−60.0 (2)	Fe2B—C22B—C23B—C24B	−59.3 (3)
Fe2A—C23A—C24A—C20A	−59.8 (2)	Fe2B—C23B—C24B—C20B	−59.5 (2)
S1A—P1A—C1A—Fe1A	56.0 (2)	S1B—P1B—C1B—Fe1B	58.5 (2)
S1A—P1A—C1A—C2A	−41.1 (3)	S1B—P1B—C1B—C2B	−39.0 (3)
S1A—P1A—C1A—C5A	146.9 (2)	S1B—P1B—C1B—C5B	149.5 (2)
S1A—P1A—C15A—Fe2A	44.7 (2)	S1B—P1B—C15B—Fe2B	45.0 (2)
S1A—P1A—C15A—C16A	−52.8 (3)	S1B—P1B—C15B—C16B	−49.2 (3)

S1A—P1A—C15A—C19A	138.5 (2)	S1B—P1B—C15B—C19B	135.5 (2)
S1A—P1A—C34A—C35A	−32.4 (3)	S1B—P1B—C34B—C35B	150.6 (2)
S1A—P1A—C34A—C39A	149.3 (2)	S1B—P1B—C34B—C39B	−32.2 (3)
P1A—C1A—C2A—Fe1A	126.5 (2)	P1B—C1B—C2B—Fe1B	127.6 (2)
P1A—C1A—C2A—C3A	−174.8 (2)	P1B—C1B—C2B—C3B	−173.3 (2)
P1A—C1A—C2A—C11A	7.4 (5)	P1B—C1B—C2B—C11B	9.5 (5)
P1A—C1A—C5A—Fe1A	−125.8 (2)	P1B—C1B—C5B—Fe1B	−127.0 (2)
P1A—C1A—C5A—C4A	174.6 (2)	P1B—C1B—C5B—C4B	173.2 (2)
P1A—C15A—C16A—Fe2A	129.6 (2)	P1B—C15B—C16B—Fe2B	124.4 (2)
P1A—C15A—C16A—C17A	−171.3 (2)	P1B—C15B—C16B—C17B	−176.5 (2)
P1A—C15A—C16A—C25A	9.1 (5)	P1B—C15B—C16B—C25B	4.3 (5)
P1A—C15A—C19A—Fe2A	−129.3 (2)	P1B—C15B—C19B—Fe2B	−124.2 (2)
P1A—C15A—C19A—C18A	171.7 (2)	P1B—C15B—C19B—C18B	177.0 (2)
P1A—C34A—C35A—C36A	−176.4 (2)	P1B—C34B—C35B—C36B	175.4 (2)
P1A—C34A—C39A—C38A	177.1 (2)	P1B—C34B—C39B—C38B	−175.7 (2)
C1A—P1A—C15A—Fe2A	−84.1 (2)	C1B—P1B—C15B—Fe2B	−83.3 (2)
C1A—P1A—C15A—C16A	178.3 (3)	C1B—P1B—C15B—C16B	−177.6 (3)
C1A—P1A—C15A—C19A	9.7 (3)	C1B—P1B—C15B—C19B	7.1 (3)
C1A—P1A—C34A—C35A	93.5 (2)	C1B—P1B—C34B—C35B	−83.7 (3)
C1A—P1A—C34A—C39A	−84.8 (3)	C1B—P1B—C34B—C39B	93.4 (2)
C1A—C2A—C3A—Fe1A	−57.69 (19)	C1B—C2B—C3B—Fe1B	−58.46 (19)
C1A—C2A—C3A—C4A	1.9 (3)	C1B—C2B—C3B—C4B	1.2 (3)
C1A—C2A—C11A—C12A	−172.1 (4)	C1B—C2B—C11B—C12B	−162.7 (3)
C2A—C1A—C5A—Fe1A	60.7 (2)	C2B—C1B—C5B—Fe1B	59.9 (2)
C2A—C1A—C5A—C4A	1.1 (3)	C2B—C1B—C5B—C4B	0.0 (3)
C2A—C3A—C4A—Fe1A	−59.1 (2)	C2B—C3B—C4B—Fe1B	−58.8 (2)
C2A—C3A—C4A—C5A	−1.2 (4)	C2B—C3B—C4B—C5B	−1.2 (4)
C3A—C2A—C11A—C12A	10.5 (6)	C3B—C2B—C11B—C12B	20.5 (5)
C3A—C4A—C5A—Fe1A	−58.1 (2)	C3B—C4B—C5B—Fe1B	−57.8 (2)
C3A—C4A—C5A—C1A	0.0 (4)	C3B—C4B—C5B—C1B	0.7 (4)
C5A—C1A—C2A—Fe1A	−60.6 (2)	C5B—C1B—C2B—Fe1B	−59.9 (2)
C5A—C1A—C2A—C3A	−1.9 (3)	C5B—C1B—C2B—C3B	−0.8 (3)
C5A—C1A—C2A—C11A	−179.7 (3)	C5B—C1B—C2B—C11B	−178.0 (3)
C6A—C7A—C8A—Fe1A	59.8 (2)	C6B—C7B—C8B—Fe1B	60.5 (2)
C6A—C7A—C8A—C9A	0.0 (4)	C6B—C7B—C8B—C9B	0.3 (4)
C7A—C6A—C10A—Fe1A	−59.4 (2)	C7B—C6B—C10B—Fe1B	−59.1 (3)
C7A—C6A—C10A—C9A	−0.2 (4)	C7B—C6B—C10B—C9B	−0.1 (4)
C7A—C8A—C9A—Fe1A	59.3 (2)	C7B—C8B—C9B—Fe1B	59.9 (3)
C7A—C8A—C9A—C10A	−0.1 (4)	C7B—C8B—C9B—C10B	−0.4 (4)
C8A—C9A—C10A—Fe1A	59.1 (3)	C8B—C9B—C10B—Fe1B	59.3 (3)
C8A—C9A—C10A—C6A	0.2 (4)	C8B—C9B—C10B—C6B	0.4 (4)
C10A—C6A—C7A—Fe1A	59.9 (2)	C10B—C6B—C7B—Fe1B	59.3 (3)
C10A—C6A—C7A—C8A	0.2 (4)	C10B—C6B—C7B—C8B	−0.1 (4)
C11A—C2A—C3A—Fe1A	120.2 (3)	C11B—C2B—C3B—Fe1B	118.9 (3)
C11A—C2A—C3A—C4A	179.8 (3)	C11B—C2B—C3B—C4B	178.6 (3)
C15A—P1A—C1A—Fe1A	−174.24 (19)	C15B—P1B—C1B—Fe1B	−172.69 (19)
C15A—P1A—C1A—C2A	88.6 (3)	C15B—P1B—C1B—C2B	89.8 (3)
C15A—P1A—C1A—C5A	−83.4 (3)	C15B—P1B—C1B—C5B	−81.7 (3)

C15A—P1A—C34A—C35A	−159.7 (2)	C15B—P1B—C34B—C35B	23.5 (3)
C15A—P1A—C34A—C39A	22.0 (3)	C15B—P1B—C34B—C39B	−159.4 (2)
C15A—C16A—C17A—Fe2A	−58.5 (2)	C15B—C16B—C17B—Fe2B	−58.7 (2)
C15A—C16A—C17A—C18A	0.9 (3)	C15B—C16B—C17B—C18B	0.1 (4)
C15A—C16A—C25A—C26A	−159.1 (4)	C15B—C16B—C25B—C26B	−170.2 (4)
C16A—C15A—C19A—Fe2A	60.06 (19)	C16B—C15B—C19B—Fe2B	59.6 (2)
C16A—C15A—C19A—C18A	1.0 (3)	C16B—C15B—C19B—C18B	0.9 (3)
C16A—C17A—C18A—Fe2A	−59.1 (2)	C16B—C17B—C18B—Fe2B	−58.8 (2)
C16A—C17A—C18A—C19A	−0.2 (4)	C16B—C17B—C18B—C19B	0.4 (4)
C17A—C16A—C25A—C26A	21.5 (6)	C17B—C16B—C25B—C26B	10.8 (7)
C17A—C18A—C19A—Fe2A	−58.6 (2)	C17B—C18B—C19B—Fe2B	−59.3 (2)
C17A—C18A—C19A—C15A	−0.5 (4)	C17B—C18B—C19B—C15B	−0.8 (4)
C19A—C15A—C16A—Fe2A	−60.23 (19)	C19B—C15B—C16B—Fe2B	−59.7 (2)
C19A—C15A—C16A—C17A	−1.2 (3)	C19B—C15B—C16B—C17B	−0.6 (3)
C19A—C15A—C16A—C25A	179.3 (3)	C19B—C15B—C16B—C25B	−179.8 (3)
C20A—C21A—C22A—Fe2A	59.5 (2)	C20B—C21B—C22B—Fe2B	59.4 (2)
C20A—C21A—C22A—C23A	−0.2 (4)	C20B—C21B—C22B—C23B	−0.5 (4)
C21A—C20A—C24A—Fe2A	−59.4 (2)	C21B—C20B—C24B—Fe2B	−59.1 (2)
C21A—C20A—C24A—C23A	−0.1 (4)	C21B—C20B—C24B—C23B	−0.1 (4)
C21A—C22A—C23A—Fe2A	60.1 (2)	C21B—C22B—C23B—Fe2B	59.8 (2)
C21A—C22A—C23A—C24A	0.2 (4)	C21B—C22B—C23B—C24B	0.4 (4)
C22A—C23A—C24A—Fe2A	59.8 (2)	C22B—C23B—C24B—Fe2B	59.3 (3)
C22A—C23A—C24A—C20A	−0.1 (4)	C22B—C23B—C24B—C20B	−0.2 (4)
C24A—C20A—C21A—Fe2A	59.3 (2)	C24B—C20B—C21B—Fe2B	59.5 (2)
C24A—C20A—C21A—C22A	0.2 (4)	C24B—C20B—C21B—C22B	0.3 (4)
C25A—C16A—C17A—Fe2A	121.0 (3)	C25B—C16B—C17B—Fe2B	120.4 (4)
C25A—C16A—C17A—C18A	−179.6 (3)	C25B—C16B—C17B—C18B	179.3 (3)
C34A—P1A—C1A—Fe1A	−67.2 (2)	C34B—P1B—C1B—Fe1B	−64.1 (2)
C34A—P1A—C1A—C2A	−164.3 (3)	C34B—P1B—C1B—C2B	−161.7 (3)
C34A—P1A—C1A—C5A	23.7 (3)	C34B—P1B—C1B—C5B	26.9 (3)
C34A—P1A—C15A—Fe2A	168.35 (19)	C34B—P1B—C15B—Fe2B	168.87 (18)
C34A—P1A—C15A—C16A	70.8 (3)	C34B—P1B—C15B—C16B	74.6 (3)
C34A—P1A—C15A—C19A	−97.8 (3)	C34B—P1B—C15B—C19B	−100.7 (3)
C34A—C35A—C36A—C37A	−1.1 (5)	C34B—C35B—C36B—C37B	1.0 (5)
C35A—C34A—C39A—C38A	−1.3 (4)	C35B—C34B—C39B—C38B	1.5 (5)
C35A—C36A—C37A—C38A	−0.6 (5)	C35B—C36B—C37B—C38B	0.0 (5)
C36A—C37A—C38A—C39A	1.3 (5)	C36B—C37B—C38B—C39B	−0.3 (5)
C37A—C38A—C39A—C34A	−0.4 (5)	C37B—C38B—C39B—C34B	−0.5 (5)
C39A—C34A—C35A—C36A	2.0 (4)	C39B—C34B—C35B—C36B	−1.7 (5)

1,1′′-(Phenylphosphanediyl)bis{(2S_p)-2-[(1*R*)-1-\ (acetyloxy)ethyl]ferrocene} (7)

Crystal data

$[Fe_2(C_5H_5)_2(C_{24}H_{25}O_4P)]$
M_r = 650.29
Orthorhombic, $P2_12_12_1$
a = 7.631 (2) Å
b = 10.877 (2) Å
c = 36.025 (8) Å
V = 2990.2 (12) Å^3
Z = 4
F(000) = 1352
D_x = 1.444 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3094 reflections

θ = 2.2–19.9°
μ = 1.06 mm^{-1}
T = 130 K

Block, clear orange
0.15 × 0.08 × 0.06 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: sealed xray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.562, T_{max} = 0.745
46099 measured reflections

5441 independent reflections
4085 reflections with $I > 2\sigma(I)$
R_{int} = 0.150
θ_{max} = 25.4°, θ_{min} = 2.2°
h = −9→9
k = −13→13
l = −38→43

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.122
S = 1.04
5441 reflections
374 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 2.7228P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack x determined using 1235 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (2)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups At 1.5 times of: All C(H,H,H) groups 2.a Ternary CH refined with riding coordinates: C11(H11), C25(H25) 2.b Aromatic/amide H refined with riding coordinates: C3(H3), C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C9(H9), C10(H10), C17(H17), C18(H18), C19(H19), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24), C35(H35), C36(H36), C37(H37), C38(H38), C39(H39) 2.c Idealised Me refined as rotating group: C13(H13A,H13B,H13C), C14(H14A,H14B,H14C), C27(H27A,H27B,H27C), C28(H28A,H28B, H28C)

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

	x	y	z	U_{iso}*/U_{eq}
Fe1	0.79439 (15)	0.89449 (11)	0.38276 (3)	0.0264 (3)
Fe2	1.24405 (15)	0.40848 (10)	0.40108 (3)	0.0235 (3)
P1	0.8827 (3)	0.5855 (2)	0.37276 (5)	0.0218 (5)
O1	0.7061 (8)	0.7131 (5)	0.27691 (15)	0.0339 (15)
O2	0.4850 (9)	0.5800 (7)	0.26629 (19)	0.0519 (19)
O3	0.8911 (7)	0.5751 (5)	0.48204 (14)	0.0275 (14)
O4	0.6319 (8)	0.4892 (6)	0.49674 (18)	0.0430 (18)
C1	0.9068 (11)	0.7452 (7)	0.3578 (2)	0.020 (2)
C2	0.7857 (12)	0.8062 (7)	0.3331 (2)	0.026 (2)
C3	0.8444 (12)	0.9294 (8)	0.3278 (2)	0.033 (2)

H3	0.790570	0.989466	0.312382	0.039*
C4	0.9979 (12)	0.9465 (8)	0.3496 (2)	0.031 (2)
H4	1.061986	1.021088	0.351643	0.037*
C5	1.0401 (12)	0.8347 (8)	0.3678 (2)	0.026 (2)
H5	1.137758	0.820808	0.383551	0.032*
C6	0.7112 (15)	0.8428 (9)	0.4348 (3)	0.044 (3)
H6	0.740860	0.768806	0.447365	0.053*
C7	0.5651 (14)	0.8616 (10)	0.4100 (3)	0.044 (3)
H7	0.480269	0.801654	0.403352	0.053*
C8	0.5702 (12)	0.9839 (8)	0.3975 (3)	0.034 (2)
H8	0.489830	1.020809	0.380758	0.041*
C9	0.7151 (12)	1.0423 (8)	0.4141 (2)	0.033 (2)
H9	0.749057	1.125501	0.410609	0.040*
C10	0.8010 (15)	0.9556 (10)	0.4368 (2)	0.050 (3)
H10	0.903184	0.970965	0.451170	0.060*
C11	0.6349 (12)	0.7474 (8)	0.3133 (2)	0.029 (2)
H11	0.598509	0.671501	0.326949	0.035*
C12	0.6172 (13)	0.6303 (8)	0.2565 (3)	0.036 (2)
C13	0.7073 (15)	0.6108 (9)	0.2201 (2)	0.055 (3)
H13A	0.785645	0.680231	0.215101	0.082*
H13B	0.619605	0.604836	0.200333	0.082*
H13C	0.775670	0.534615	0.221092	0.082*
C14	0.4754 (13)	0.8309 (9)	0.3079 (3)	0.043 (3)
H14A	0.506901	0.899428	0.291501	0.064*
H14B	0.437420	0.863080	0.331953	0.064*
H14C	0.379809	0.783626	0.296612	0.064*
C15	1.0846 (10)	0.5607 (7)	0.3990 (2)	0.0198 (19)
C16	1.0900 (11)	0.5102 (8)	0.4361 (2)	0.021 (2)
C17	1.2691 (13)	0.5118 (8)	0.4482 (2)	0.032 (2)
H17	1.310570	0.484611	0.471699	0.038*
C18	1.3738 (12)	0.5607 (8)	0.4194 (2)	0.029 (2)
H18	1.497201	0.571824	0.420079	0.035*
C19	1.2615 (11)	0.5902 (7)	0.3889 (2)	0.0265 (18)
H19	1.297952	0.623840	0.365846	0.032*
C20	1.1716 (14)	0.2763 (8)	0.3636 (3)	0.038 (3)
H20	1.073876	0.281040	0.347373	0.045*
C21	1.1677 (14)	0.2267 (8)	0.3999 (3)	0.037 (3)
H21	1.069405	0.191373	0.412034	0.044*
C22	1.3408 (14)	0.2401 (9)	0.4146 (3)	0.035 (3)
H22	1.378716	0.215886	0.438661	0.042*
C23	1.4448 (13)	0.2959 (8)	0.3869 (3)	0.036 (2)
H23	1.565586	0.315609	0.389227	0.043*
C24	1.3406 (13)	0.3175 (8)	0.3553 (3)	0.033 (2)
H24	1.378053	0.353351	0.332601	0.039*
C25	0.9380 (12)	0.4680 (7)	0.4591 (2)	0.022 (2)
H25	0.837562	0.444799	0.442727	0.027*
C26	0.7380 (13)	0.5720 (8)	0.4997 (2)	0.031 (2)
C27	0.7112 (14)	0.6845 (8)	0.5235 (2)	0.043 (3)

H27A	0.816621	0.735870	0.522558	0.064*
H27B	0.688940	0.659261	0.549145	0.064*
H27C	0.610816	0.731348	0.514134	0.064*
C28	0.9831 (14)	0.3608 (9)	0.4855 (3)	0.044 (3)
H28A	1.065265	0.389470	0.504559	0.065*
H28B	1.037004	0.293848	0.471332	0.065*
H28C	0.875797	0.330975	0.497440	0.065*
C34	0.9200 (11)	0.5057 (7)	0.3283 (2)	0.0196 (19)
C35	0.7961 (11)	0.4143 (8)	0.3191 (2)	0.033 (2)
H35	0.697616	0.400786	0.334657	0.039*
C36	0.8189 (14)	0.3433 (8)	0.2867 (2)	0.038 (3)
H36	0.734927	0.282046	0.280597	0.046*
C37	0.9591 (13)	0.3611 (9)	0.2643 (3)	0.039 (3)
H37	0.974890	0.311589	0.242803	0.047*
C38	1.0812 (12)	0.4537 (9)	0.2730 (2)	0.036 (2)
H38	1.179345	0.467063	0.257293	0.043*
C39	1.0589 (11)	0.5252 (8)	0.3043 (2)	0.024 (2)
H39	1.140352	0.589012	0.309469	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0298 (7)	0.0221 (6)	0.0273 (7)	0.0056 (6)	0.0064 (5)	0.0017 (6)
Fe2	0.0249 (6)	0.0214 (6)	0.0243 (6)	0.0049 (6)	−0.0004 (5)	−0.0025 (5)
P1	0.0228 (11)	0.0202 (11)	0.0224 (12)	0.0041 (10)	0.0004 (9)	0.0004 (10)
O1	0.043 (4)	0.035 (3)	0.024 (3)	−0.008 (3)	−0.002 (3)	0.000 (3)
O2	0.048 (5)	0.050 (5)	0.058 (5)	−0.009 (4)	−0.003 (4)	0.002 (4)
O3	0.027 (3)	0.031 (4)	0.024 (3)	0.004 (3)	0.009 (3)	−0.008 (3)
O4	0.036 (4)	0.050 (4)	0.043 (4)	−0.013 (4)	0.006 (3)	−0.011 (4)
C1	0.024 (5)	0.014 (4)	0.022 (5)	0.004 (4)	0.005 (4)	0.006 (4)
C2	0.029 (6)	0.020 (4)	0.030 (5)	0.006 (4)	0.001 (4)	0.001 (4)
C3	0.043 (6)	0.033 (6)	0.022 (5)	0.005 (5)	0.010 (4)	0.003 (4)
C4	0.040 (6)	0.022 (5)	0.031 (6)	−0.001 (4)	0.011 (4)	0.001 (4)
C5	0.022 (5)	0.024 (5)	0.032 (6)	−0.003 (4)	0.010 (4)	−0.001 (4)
C6	0.065 (9)	0.033 (6)	0.034 (6)	0.019 (6)	0.025 (6)	0.013 (5)
C7	0.040 (7)	0.043 (6)	0.050 (7)	−0.003 (5)	0.026 (5)	−0.009 (5)
C8	0.029 (5)	0.028 (5)	0.045 (6)	0.017 (4)	0.003 (5)	−0.010 (5)
C9	0.030 (6)	0.028 (5)	0.043 (6)	0.005 (4)	0.005 (5)	−0.004 (4)
C10	0.054 (7)	0.071 (8)	0.024 (5)	0.030 (6)	0.004 (5)	−0.010 (5)
C11	0.030 (6)	0.024 (5)	0.034 (6)	0.005 (4)	−0.004 (4)	0.004 (4)
C12	0.037 (6)	0.034 (6)	0.037 (6)	−0.008 (5)	−0.007 (5)	0.005 (5)
C13	0.085 (8)	0.041 (6)	0.039 (6)	−0.027 (7)	−0.004 (6)	0.002 (5)
C14	0.032 (6)	0.051 (7)	0.045 (7)	0.001 (5)	−0.007 (5)	0.012 (5)
C15	0.020 (5)	0.018 (5)	0.022 (5)	0.004 (3)	0.003 (4)	−0.006 (4)
C16	0.028 (5)	0.019 (5)	0.016 (5)	0.007 (4)	−0.004 (4)	−0.004 (4)
C17	0.044 (6)	0.031 (5)	0.020 (5)	0.010 (5)	−0.009 (5)	0.000 (4)
C18	0.019 (5)	0.026 (5)	0.043 (6)	0.003 (4)	−0.001 (4)	−0.005 (4)
C19	0.033 (5)	0.015 (4)	0.032 (5)	−0.002 (4)	0.006 (4)	−0.003 (4)

C20	0.056 (7)	0.025 (5)	0.032 (6)	0.009 (5)	−0.005 (5)	−0.015 (4)
C21	0.046 (7)	0.022 (5)	0.042 (6)	−0.001 (4)	0.020 (5)	−0.010 (5)
C22	0.053 (8)	0.028 (5)	0.025 (5)	0.011 (5)	0.002 (5)	−0.004 (4)
C23	0.032 (6)	0.036 (6)	0.040 (6)	0.013 (5)	0.002 (5)	−0.001 (5)
C24	0.044 (7)	0.022 (5)	0.033 (5)	0.003 (4)	0.000 (5)	−0.002 (4)
C25	0.033 (5)	0.019 (5)	0.014 (5)	0.003 (4)	−0.001 (4)	−0.002 (4)
C26	0.035 (6)	0.035 (5)	0.023 (5)	0.004 (5)	−0.009 (4)	−0.005 (4)
C27	0.043 (7)	0.049 (6)	0.037 (6)	0.010 (5)	0.004 (5)	−0.009 (5)
C28	0.061 (8)	0.036 (6)	0.034 (6)	0.013 (5)	0.008 (5)	0.014 (5)
C34	0.026 (5)	0.022 (5)	0.012 (4)	0.005 (4)	−0.005 (4)	0.000 (4)
C35	0.029 (5)	0.042 (5)	0.027 (5)	−0.011 (5)	−0.005 (4)	0.002 (5)
C36	0.044 (7)	0.035 (5)	0.037 (6)	−0.009 (5)	−0.006 (5)	−0.006 (5)
C37	0.044 (7)	0.046 (6)	0.028 (6)	0.009 (5)	−0.004 (5)	−0.016 (5)
C38	0.029 (6)	0.052 (7)	0.027 (5)	0.005 (5)	0.003 (4)	0.001 (5)
C39	0.020 (5)	0.034 (5)	0.019 (5)	−0.001 (4)	−0.007 (4)	0.001 (4)

Geometric parameters (Å, º)

Fe1—C1	2.044 (8)	C11—H11	1.0000
Fe1—C2	2.032 (8)	C11—C14	1.531 (12)
Fe1—C3	2.053 (8)	C12—C13	1.496 (13)
Fe1—C4	2.040 (9)	C13—H13A	0.9800
Fe1—C5	2.057 (9)	C13—H13B	0.9800
Fe1—C6	2.059 (9)	C13—H13C	0.9800
Fe1—C7	2.038 (10)	C14—H14A	0.9800
Fe1—C8	2.038 (8)	C14—H14B	0.9800
Fe1—C9	2.056 (8)	C14—H14C	0.9800
Fe1—C10	2.059 (9)	C15—C16	1.446 (11)
Fe2—C15	2.056 (8)	C15—C19	1.434 (11)
Fe2—C16	2.050 (8)	C16—C17	1.435 (12)
Fe2—C17	2.046 (8)	C16—C25	1.497 (12)
Fe2—C18	2.038 (9)	C17—H17	0.9500
Fe2—C19	2.029 (8)	C17—C18	1.415 (12)
Fe2—C20	2.047 (9)	C18—H18	0.9500
Fe2—C21	2.062 (9)	C18—C19	1.428 (11)
Fe2—C22	2.034 (10)	C19—H19	0.9500
Fe2—C23	2.027 (9)	C20—H20	0.9500
Fe2—C24	2.059 (9)	C20—C21	1.412 (12)
P1—C1	1.828 (8)	C20—C24	1.398 (13)
P1—C15	1.828 (8)	C21—H21	0.9500
P1—C34	1.845 (8)	C21—C22	1.432 (13)
O1—C11	1.468 (10)	C22—H22	0.9500
O1—C12	1.345 (10)	C22—C23	1.412 (13)
O2—C12	1.200 (10)	C23—H23	0.9500
O3—C25	1.472 (9)	C23—C24	1.409 (12)
O3—C26	1.331 (10)	C24—H24	0.9500
O4—C26	1.216 (10)	C25—H25	1.0000
C1—C2	1.446 (11)	C25—C28	1.544 (11)

C1—C5	1.452 (12)	C26—C27	1.508 (11)
C2—C3	1.426 (12)	C27—H27A	0.9800
C2—C11	1.497 (12)	C27—H27B	0.9800
C3—H3	0.9500	C27—H27C	0.9800
C3—C4	1.422 (12)	C28—H28A	0.9800
C4—H4	0.9500	C28—H28B	0.9800
C4—C5	1.419 (11)	C28—H28C	0.9800
C5—H5	0.9500	C34—C35	1.411 (11)
C6—H6	0.9500	C34—C39	1.383 (11)
C6—C7	1.443 (14)	C35—H35	0.9500
C6—C10	1.408 (14)	C35—C36	1.409 (12)
C7—H7	0.9500	C36—H36	0.9500
C7—C8	1.406 (13)	C36—C37	1.356 (13)
C8—H8	0.9500	C37—H37	0.9500
C8—C9	1.408 (13)	C37—C38	1.407 (13)
C9—H9	0.9500	C38—H38	0.9500
C9—C10	1.410 (12)	C38—C39	1.380 (12)
C10—H10	0.9500	C39—H39	0.9500

C1—Fe1—C3	69.2 (3)	C7—C8—Fe1	69.8 (5)
C1—Fe1—C5	41.5 (3)	C7—C8—H8	125.9
C1—Fe1—C6	108.2 (3)	C7—C8—C9	108.2 (9)
C1—Fe1—C9	170.4 (4)	C9—C8—Fe1	70.5 (5)
C1—Fe1—C10	131.4 (4)	C9—C8—H8	125.9
C2—Fe1—C1	41.5 (3)	Fe1—C9—H9	126.3
C2—Fe1—C3	40.9 (3)	C8—C9—Fe1	69.2 (5)
C2—Fe1—C4	68.9 (4)	C8—C9—H9	126.0
C2—Fe1—C5	69.4 (4)	C8—C9—C10	108.1 (9)
C2—Fe1—C6	131.6 (4)	C10—C9—Fe1	70.1 (5)
C2—Fe1—C7	108.3 (4)	C10—C9—H9	126.0
C2—Fe1—C8	115.3 (4)	Fe1—C10—H10	126.3
C2—Fe1—C9	147.5 (3)	C6—C10—Fe1	70.0 (5)
C2—Fe1—C10	170.6 (4)	C6—C10—C9	109.1 (9)
C3—Fe1—C5	68.6 (4)	C6—C10—H10	125.5
C3—Fe1—C6	170.8 (4)	C9—C10—Fe1	69.8 (5)
C3—Fe1—C9	116.1 (4)	C9—C10—H10	125.5
C3—Fe1—C10	148.1 (4)	O1—C11—C2	104.4 (7)
C4—Fe1—C1	69.1 (3)	O1—C11—H11	109.4
C4—Fe1—C3	40.7 (3)	O1—C11—C14	109.3 (7)
C4—Fe1—C5	40.5 (3)	C2—C11—H11	109.4
C4—Fe1—C6	147.6 (4)	C2—C11—C14	114.7 (7)
C4—Fe1—C9	109.2 (4)	C14—C11—H11	109.4
C4—Fe1—C10	116.5 (4)	O1—C12—C13	110.0 (8)
C5—Fe1—C6	115.7 (4)	O2—C12—O1	124.7 (9)
C5—Fe1—C10	109.2 (4)	O2—C12—C13	125.4 (9)
C7—Fe1—C1	115.6 (4)	C12—C13—H13A	109.5
C7—Fe1—C3	131.1 (4)	C12—C13—H13B	109.5
C7—Fe1—C4	170.0 (4)	C12—C13—H13C	109.5

C7—Fe1—C5	148.6 (4)	H13A—C13—H13B	109.5
C7—Fe1—C6	41.2 (4)	H13A—C13—H13C	109.5
C7—Fe1—C9	67.7 (4)	H13B—C13—H13C	109.5
C7—Fe1—C10	67.8 (4)	C11—C14—H14A	109.5
C8—Fe1—C1	147.8 (4)	C11—C14—H14B	109.5
C8—Fe1—C3	108.6 (4)	C11—C14—H14C	109.5
C8—Fe1—C4	131.3 (4)	H14A—C14—H14B	109.5
C8—Fe1—C5	169.9 (4)	H14A—C14—H14C	109.5
C8—Fe1—C6	68.5 (4)	H14B—C14—H14C	109.5
C8—Fe1—C7	40.3 (4)	P1—C15—Fe2	129.5 (4)
C8—Fe1—C9	40.2 (4)	C16—C15—Fe2	69.1 (4)
C8—Fe1—C10	67.6 (4)	C16—C15—P1	123.9 (6)
C9—Fe1—C5	131.3 (4)	C19—C15—Fe2	68.4 (4)
C9—Fe1—C6	67.8 (4)	C19—C15—P1	129.0 (6)
C9—Fe1—C10	40.1 (3)	C19—C15—C16	107.0 (7)
C10—Fe1—C6	40.0 (4)	C15—C16—Fe2	69.6 (4)
C15—Fe2—C21	127.2 (4)	C15—C16—C25	127.3 (7)
C15—Fe2—C24	124.7 (3)	C17—C16—Fe2	69.3 (5)
C16—Fe2—C15	41.3 (3)	C17—C16—C15	107.6 (7)
C16—Fe2—C21	111.6 (4)	C17—C16—C25	125.0 (7)
C16—Fe2—C24	163.3 (4)	C25—C16—Fe2	128.3 (6)
C17—Fe2—C15	69.1 (3)	Fe2—C17—H17	126.8
C17—Fe2—C16	41.0 (3)	C16—C17—Fe2	69.7 (5)
C17—Fe2—C20	163.3 (4)	C16—C17—H17	125.7
C17—Fe2—C21	124.8 (4)	C18—C17—Fe2	69.4 (5)
C17—Fe2—C24	153.6 (4)	C18—C17—C16	108.6 (7)
C18—Fe2—C15	69.2 (3)	C18—C17—H17	125.7
C18—Fe2—C16	69.0 (3)	Fe2—C18—H18	126.5
C18—Fe2—C17	40.5 (3)	C17—C18—Fe2	70.0 (5)
C18—Fe2—C20	156.1 (4)	C17—C18—H18	126.0
C18—Fe2—C21	157.4 (4)	C17—C18—C19	108.1 (8)
C18—Fe2—C24	118.4 (4)	C19—C18—Fe2	69.1 (5)
C19—Fe2—C15	41.1 (3)	C19—C18—H18	126.0
C19—Fe2—C16	69.2 (3)	Fe2—C19—H19	125.7
C19—Fe2—C17	68.8 (3)	C15—C19—Fe2	70.5 (4)
C19—Fe2—C18	41.1 (3)	C15—C19—H19	125.7
C19—Fe2—C20	124.0 (3)	C18—C19—Fe2	69.8 (5)
C19—Fe2—C21	161.5 (4)	C18—C19—C15	108.7 (7)
C19—Fe2—C22	154.8 (4)	C18—C19—H19	125.7
C19—Fe2—C24	105.8 (3)	Fe2—C20—H20	125.5
C20—Fe2—C15	112.5 (4)	C21—C20—Fe2	70.5 (5)
C20—Fe2—C16	129.1 (4)	C21—C20—H20	125.0
C20—Fe2—C21	40.2 (4)	C24—C20—Fe2	70.6 (6)
C20—Fe2—C24	39.8 (4)	C24—C20—H20	125.0
C22—Fe2—C15	161.5 (4)	C24—C20—C21	109.9 (9)
C22—Fe2—C16	123.1 (4)	Fe2—C21—H21	127.0
C22—Fe2—C17	105.2 (3)	C20—C21—Fe2	69.3 (5)
C22—Fe2—C18	118.5 (4)	C20—C21—H21	126.7

C22—Fe2—C20	67.9 (4)	C20—C21—C22	106.6 (9)
C22—Fe2—C21	40.9 (4)	C22—C21—Fe2	68.5 (6)
C22—Fe2—C24	68.3 (4)	C22—C21—H21	126.7
C23—Fe2—C15	157.7 (4)	Fe2—C22—H22	125.4
C23—Fe2—C16	156.2 (3)	C21—C22—Fe2	70.6 (6)
C23—Fe2—C17	118.1 (4)	C21—C22—H22	126.3
C23—Fe2—C18	101.8 (4)	C23—C22—Fe2	69.4 (5)
C23—Fe2—C19	119.0 (4)	C23—C22—C21	107.4 (9)
C23—Fe2—C20	67.3 (4)	C23—C22—H22	126.3
C23—Fe2—C21	68.2 (4)	Fe2—C23—H23	125.1
C23—Fe2—C22	40.7 (4)	C22—C23—Fe2	69.9 (5)
C23—Fe2—C24	40.3 (4)	C22—C23—H23	125.5
C24—Fe2—C21	67.9 (4)	C24—C23—Fe2	71.1 (5)
C1—P1—C15	102.0 (4)	C24—C23—C22	109.0 (9)
C1—P1—C34	100.1 (4)	C24—C23—H23	125.5
C15—P1—C34	104.5 (4)	Fe2—C24—H24	126.9
C12—O1—C11	118.1 (7)	C20—C24—Fe2	69.6 (5)
C26—O3—C25	117.5 (7)	C20—C24—C23	107.1 (9)
P1—C1—Fe1	125.7 (4)	C20—C24—H24	126.5
C2—C1—Fe1	68.8 (4)	C23—C24—Fe2	68.6 (5)
C2—C1—P1	123.6 (6)	C23—C24—H24	126.5
C2—C1—C5	107.0 (7)	O3—C25—C16	104.8 (6)
C5—C1—Fe1	69.7 (5)	O3—C25—H25	110.2
C5—C1—P1	129.4 (6)	O3—C25—C28	107.8 (6)
C1—C2—Fe1	69.7 (5)	C16—C25—H25	110.2
C1—C2—C11	126.1 (7)	C16—C25—C28	113.6 (7)
C3—C2—Fe1	70.4 (5)	C28—C25—H25	110.2
C3—C2—C1	108.2 (8)	O3—C26—C27	111.7 (8)
C3—C2—C11	125.4 (8)	O4—C26—O3	124.2 (8)
C11—C2—Fe1	130.3 (6)	O4—C26—C27	124.1 (9)
Fe1—C3—H3	127.6	C26—C27—H27A	109.5
C2—C3—Fe1	68.8 (5)	C26—C27—H27B	109.5
C2—C3—H3	126.0	C26—C27—H27C	109.5
C4—C3—Fe1	69.2 (5)	H27A—C27—H27B	109.5
C4—C3—C2	107.9 (8)	H27A—C27—H27C	109.5
C4—C3—H3	126.0	H27B—C27—H27C	109.5
Fe1—C4—H4	125.7	C25—C28—H28A	109.5
C3—C4—Fe1	70.2 (5)	C25—C28—H28B	109.5
C3—C4—H4	125.4	C25—C28—H28C	109.5
C5—C4—Fe1	70.4 (5)	H28A—C28—H28B	109.5
C5—C4—C3	109.2 (8)	H28A—C28—H28C	109.5
C5—C4—H4	125.4	H28B—C28—H28C	109.5
Fe1—C5—H5	127.5	C35—C34—P1	115.6 (6)
C1—C5—Fe1	68.8 (5)	C39—C34—P1	126.0 (6)
C1—C5—H5	126.2	C39—C34—C35	118.4 (8)
C4—C5—Fe1	69.1 (5)	C34—C35—H35	120.1
C4—C5—C1	107.6 (8)	C36—C35—C34	119.9 (8)
C4—C5—H5	126.2	C36—C35—H35	120.1

Fe1—C6—H6	126.2	C35—C36—H36	119.6
C7—C6—Fe1	68.6 (5)	C37—C36—C35	120.8 (9)
C7—C6—H6	126.7	C37—C36—H36	119.6
C10—C6—Fe1	70.0 (5)	C36—C37—H37	120.3
C10—C6—H6	126.7	C36—C37—C38	119.4 (9)
C10—C6—C7	106.5 (8)	C38—C37—H37	120.3
Fe1—C7—H7	125.7	C37—C38—H38	119.9
C6—C7—Fe1	70.2 (6)	C39—C38—C37	120.3 (9)
C6—C7—H7	125.9	C39—C38—H38	119.9
C8—C7—Fe1	69.8 (6)	C34—C39—H39	119.4
C8—C7—C6	108.1 (10)	C38—C39—C34	121.2 (8)
C8—C7—H7	125.9	C38—C39—H39	119.4
Fe1—C8—H8	125.3		

Fe1—C1—C2—C3	60.0 (6)	C7—C6—C10—C9	−0.1 (10)
Fe1—C1—C2—C11	−125.7 (9)	C7—C8—C9—Fe1	59.9 (6)
Fe1—C1—C5—C4	−58.4 (6)	C7—C8—C9—C10	0.4 (10)
Fe1—C2—C3—C4	58.2 (6)	C8—C9—C10—Fe1	59.0 (6)
Fe1—C2—C11—O1	173.2 (5)	C8—C9—C10—C6	−0.2 (10)
Fe1—C2—C11—C14	53.6 (11)	C10—C6—C7—Fe1	60.1 (6)
Fe1—C3—C4—C5	59.7 (6)	C10—C6—C7—C8	0.3 (10)
Fe1—C4—C5—C1	58.2 (6)	C11—O1—C12—O2	−1.7 (13)
Fe1—C6—C7—C8	−59.7 (6)	C11—O1—C12—C13	178.2 (7)
Fe1—C6—C10—C9	59.1 (6)	C11—C2—C3—Fe1	126.1 (9)
Fe1—C7—C8—C9	−60.4 (6)	C11—C2—C3—C4	−175.7 (8)
Fe1—C8—C9—C10	−59.5 (6)	C12—O1—C11—C2	162.8 (7)
Fe1—C9—C10—C6	−59.2 (6)	C12—O1—C11—C14	−74.0 (9)
Fe2—C15—C16—C17	59.1 (6)	C15—P1—C1—Fe1	−98.9 (5)
Fe2—C15—C16—C25	−123.2 (8)	C15—P1—C1—C2	174.5 (7)
Fe2—C15—C19—C18	−59.5 (5)	C15—P1—C1—C5	−6.7 (8)
Fe2—C16—C17—C18	58.6 (6)	C15—P1—C34—C35	122.9 (6)
Fe2—C16—C25—O3	173.3 (5)	C15—P1—C34—C39	−55.1 (8)
Fe2—C16—C25—C28	55.9 (10)	C15—C16—C17—Fe2	−59.3 (5)
Fe2—C17—C18—C19	58.8 (6)	C15—C16—C17—C18	−0.6 (9)
Fe2—C18—C19—C15	60.0 (5)	C15—C16—C25—O3	−94.2 (9)
Fe2—C20—C21—C22	−58.6 (6)	C15—C16—C25—C28	148.4 (8)
Fe2—C20—C24—C23	58.6 (6)	C16—C15—C19—Fe2	58.6 (5)
Fe2—C21—C22—C23	−59.8 (6)	C16—C15—C19—C18	−1.0 (9)
Fe2—C22—C23—C24	−60.6 (6)	C16—C17—C18—Fe2	−58.8 (6)
Fe2—C23—C24—C20	−59.2 (6)	C16—C17—C18—C19	0.0 (9)
P1—C1—C2—Fe1	119.6 (6)	C17—C16—C25—O3	83.1 (9)
P1—C1—C2—C3	179.6 (6)	C17—C16—C25—C28	−34.3 (12)
P1—C1—C2—C11	−6.1 (12)	C17—C18—C19—Fe2	−59.4 (6)
P1—C1—C5—Fe1	−120.1 (7)	C17—C18—C19—C15	0.6 (9)
P1—C1—C5—C4	−178.5 (6)	C19—C15—C16—Fe2	−58.1 (5)
P1—C15—C16—Fe2	124.3 (6)	C19—C15—C16—C17	1.0 (9)
P1—C15—C16—C17	−176.5 (6)	C19—C15—C16—C25	178.7 (8)
P1—C15—C16—C25	1.2 (12)	C20—C21—C22—Fe2	59.2 (6)

P1—C15—C19—Fe2	−124.1 (7)	C20—C21—C22—C23	−0.7 (10)
P1—C15—C19—C18	176.4 (6)	C21—C20—C24—Fe2	−59.7 (6)
P1—C34—C35—C36	−176.3 (7)	C21—C20—C24—C23	−1.1 (10)
P1—C34—C39—C38	175.0 (6)	C21—C22—C23—Fe2	60.6 (6)
C1—P1—C15—Fe2	−140.8 (5)	C21—C22—C23—C24	0.0 (11)
C1—P1—C15—C16	129.3 (7)	C22—C23—C24—Fe2	59.9 (6)
C1—P1—C15—C19	−47.6 (8)	C22—C23—C24—C20	0.6 (10)
C1—P1—C34—C35	−131.8 (6)	C24—C20—C21—Fe2	59.7 (6)
C1—P1—C34—C39	50.2 (8)	C24—C20—C21—C22	1.1 (10)
C1—C2—C3—Fe1	−59.6 (6)	C25—O3—C26—O4	−3.3 (12)
C1—C2—C3—C4	−1.4 (9)	C25—O3—C26—C27	177.2 (7)
C1—C2—C11—O1	−93.7 (10)	C25—C16—C17—Fe2	123.0 (8)
C1—C2—C11—C14	146.7 (8)	C25—C16—C17—C18	−178.4 (7)
C2—C1—C5—Fe1	58.9 (6)	C26—O3—C25—C16	166.5 (6)
C2—C1—C5—C4	0.5 (9)	C26—O3—C25—C28	−72.2 (9)
C2—C3—C4—Fe1	−58.0 (6)	C34—P1—C1—Fe1	153.8 (5)
C2—C3—C4—C5	1.7 (10)	C34—P1—C1—C2	67.1 (7)
C3—C2—C11—O1	79.6 (9)	C34—P1—C1—C5	−114.0 (8)
C3—C2—C11—C14	−40.0 (12)	C34—P1—C15—Fe2	−36.8 (6)
C3—C4—C5—Fe1	−59.6 (6)	C34—P1—C15—C16	−126.8 (7)
C3—C4—C5—C1	−1.4 (10)	C34—P1—C15—C19	56.3 (8)
C5—C1—C2—Fe1	−59.5 (6)	C34—C35—C36—C37	0.3 (14)
C5—C1—C2—C3	0.5 (9)	C35—C34—C39—C38	−2.9 (12)
C5—C1—C2—C11	174.8 (8)	C35—C36—C37—C38	−1.4 (14)
C6—C7—C8—Fe1	59.9 (6)	C36—C37—C38—C39	0.4 (14)
C6—C7—C8—C9	−0.5 (10)	C37—C38—C39—C34	1.8 (13)
C7—C6—C10—Fe1	−59.2 (6)	C39—C34—C35—C36	1.9 (12)

{(2*S*$_p$)-2-[(1*R*)-1-(Acetyloxy)ethyl]ferrocen-1-yl}[(2*S*$_p$)-2-ethenylferrocen-1-yl]phenyl-(*S*)-phosphane sulfide (8a)

Crystal data

$[Fe_2(C_5H_5)_2(C_{22}H_{21}O_2PS)]$
M_r = 622.30
Orthorhombic, $P2_12_12_1$
a = 7.4923 (3) Å
b = 12.0133 (4) Å
c = 31.758 (1) Å
V = 2858.45 (17) Å^3
Z = 4
$F(000)$ = 1288
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9862 reflections
θ = 2.6–29.6°
μ = 1.17 mm^{-1}
T = 100 K
Plate, clear orange
0.21 × 0.14 × 0.05 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: sealed xray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.607, T_{max} = 0.746
52739 measured reflections
8330 independent reflections
7214 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 30.0°, θ_{min} = 2.6°
h = −10→10
k = −16→15
l = −44→40

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.062$
$S = 1.04$
8330 reflections
345 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 0.8513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Absolute structure: Flack *x* determined using 2809 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.007 (5)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups At 1.5 times of: All C(H,H,H) groups 2.a Ternary CH refined with riding coordinates: C25(H25) 2.b Aromatic/amide H refined with riding coordinates: C3(H3), C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C9(H9), C10(H10), C11(H11), C17(H17), C18(H18), C19(H19), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24), C35(H35), C36(H36), C37(H37), C38(H38), C39(H39) 2.c X=CH2 refined with riding coordinates: C12(H12A,H12B) 2.d Idealised Me refined as rotating group: C27(H27A,H27B,H27C), C28(H28A,H28B,H28C)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.84121 (5)	−0.18090 (3)	0.40555 (2)	0.01684 (9)
Fe2	0.60566 (5)	0.30603 (3)	0.41975 (2)	0.01652 (9)
S1	0.45722 (9)	0.02593 (6)	0.34750 (2)	0.01925 (14)
P1	0.70409 (9)	0.06730 (5)	0.35977 (2)	0.01195 (13)
O1	0.6817 (2)	0.30513 (15)	0.28448 (5)	0.0175 (4)
O2	0.4435 (3)	0.26315 (16)	0.24431 (6)	0.0236 (4)
C1	0.8179 (4)	−0.01370 (19)	0.39926 (7)	0.0148 (5)
C2	0.7513 (4)	−0.0495 (2)	0.43976 (8)	0.0183 (6)
C3	0.8949 (4)	−0.1031 (2)	0.46113 (8)	0.0230 (6)
H3	0.888873	−0.135570	0.488372	0.028*
C4	1.0480 (4)	−0.0999 (2)	0.43502 (9)	0.0254 (6)
H4	1.161922	−0.129537	0.441885	0.030*
C5	1.0028 (4)	−0.0452 (2)	0.39690 (8)	0.0190 (6)
H5	1.080914	−0.031729	0.373894	0.023*
C6	0.7115 (5)	−0.2603 (2)	0.35696 (9)	0.0329 (8)
H6	0.659643	−0.226079	0.332938	0.039*
C7	0.6251 (4)	−0.2816 (2)	0.39548 (9)	0.0275 (7)
H7	0.504649	−0.264033	0.402018	0.033*
C8	0.7482 (4)	−0.3334 (2)	0.42265 (9)	0.0265 (6)
H8	0.724760	−0.357321	0.450621	0.032*
C9	0.9111 (5)	−0.3437 (2)	0.40135 (10)	0.0301 (7)

H9	1.017630	−0.375068	0.412418	0.036*
C10	0.8890 (5)	−0.2990 (2)	0.36035 (9)	0.0346 (7)
H10	0.977676	−0.295624	0.339000	0.042*
C11	0.5680 (4)	−0.0391 (2)	0.45499 (8)	0.0246 (6)
H11	0.476791	−0.027092	0.434716	0.030*
C12	0.5201 (5)	−0.0454 (3)	0.49504 (9)	0.0380 (8)
H12A	0.607820	−0.057404	0.516165	0.046*
H12B	0.398118	−0.037912	0.502653	0.046*
C15	0.7387 (3)	0.2077 (2)	0.37792 (7)	0.0133 (5)
C16	0.6821 (3)	0.3103 (2)	0.35835 (7)	0.0154 (5)
C17	0.7645 (4)	0.3989 (2)	0.38082 (8)	0.0183 (5)
H17	0.752333	0.475814	0.374486	0.022*
C18	0.8673 (4)	0.3543 (2)	0.41406 (8)	0.0191 (5)
H18	0.934574	0.395864	0.433926	0.023*
C19	0.8526 (4)	0.2363 (2)	0.41266 (7)	0.0168 (5)
H19	0.908377	0.185425	0.431394	0.020*
C20	0.3838 (4)	0.2247 (2)	0.44182 (9)	0.0270 (6)
H20	0.345910	0.151978	0.434147	0.032*
C21	0.3342 (4)	0.3246 (2)	0.42145 (9)	0.0294 (6)
H21	0.257300	0.330909	0.397791	0.035*
C22	0.4204 (4)	0.4145 (3)	0.44278 (10)	0.0312 (7)
H22	0.411066	0.491136	0.435758	0.037*
C23	0.5225 (5)	0.3691 (3)	0.47631 (9)	0.0306 (7)
H23	0.593323	0.409909	0.495730	0.037*
C24	0.4997 (4)	0.2512 (3)	0.47563 (9)	0.0291 (7)
H24	0.552832	0.199583	0.494519	0.035*
C25	0.5635 (3)	0.3234 (2)	0.32061 (7)	0.0166 (5)
H25	0.468303	0.265037	0.321063	0.020*
C26	0.6027 (4)	0.2739 (2)	0.24842 (8)	0.0193 (6)
C27	0.7367 (4)	0.2552 (2)	0.21417 (8)	0.0261 (6)
H27A	0.785854	0.326950	0.205125	0.039*
H27B	0.678720	0.218646	0.190224	0.039*
H27C	0.833351	0.207881	0.224748	0.039*
C28	0.4786 (4)	0.4381 (2)	0.31699 (9)	0.0250 (6)
H28A	0.571985	0.495146	0.317601	0.037*
H28B	0.396514	0.449686	0.340620	0.037*
H28C	0.412520	0.443228	0.290430	0.037*
C34	0.8497 (3)	0.05608 (19)	0.31425 (7)	0.0142 (5)
C35	0.9988 (4)	0.1234 (2)	0.30989 (8)	0.0186 (5)
H35	1.024300	0.178211	0.330583	0.022*
C36	1.1110 (4)	0.1110 (2)	0.27541 (9)	0.0247 (6)
H36	1.211512	0.158452	0.272101	0.030*
C37	1.0754 (4)	0.0290 (3)	0.24583 (8)	0.0268 (7)
H37	1.152680	0.019673	0.222391	0.032*
C38	0.9290 (4)	−0.0387 (2)	0.25025 (8)	0.0265 (7)
H38	0.906227	−0.095129	0.229993	0.032*
C39	0.8142 (4)	−0.0252 (2)	0.28415 (8)	0.0195 (5)
H39	0.711711	−0.071215	0.286801	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0231 (2)	0.01293 (16)	0.01450 (16)	−0.00341 (15)	−0.00318 (14)	0.00026 (14)
Fe2	0.01752 (19)	0.01750 (17)	0.01454 (16)	−0.00029 (15)	0.00374 (14)	−0.00430 (14)
S1	0.0127 (3)	0.0242 (3)	0.0209 (3)	−0.0063 (3)	−0.0003 (3)	−0.0018 (3)
P1	0.0113 (3)	0.0130 (3)	0.0116 (3)	−0.0025 (2)	0.0007 (2)	−0.0012 (2)
O1	0.0184 (9)	0.0206 (8)	0.0136 (8)	−0.0016 (8)	0.0010 (7)	0.0006 (7)
O2	0.0214 (11)	0.0287 (10)	0.0207 (9)	−0.0047 (9)	−0.0054 (8)	0.0040 (8)
C1	0.0188 (13)	0.0124 (10)	0.0133 (11)	−0.0021 (10)	−0.0010 (10)	−0.0003 (9)
C2	0.0269 (15)	0.0146 (12)	0.0134 (11)	−0.0072 (11)	−0.0002 (10)	−0.0033 (10)
C3	0.0358 (17)	0.0188 (12)	0.0144 (11)	−0.0083 (12)	−0.0098 (12)	0.0003 (10)
C4	0.0277 (16)	0.0198 (13)	0.0287 (14)	−0.0040 (12)	−0.0142 (13)	0.0005 (11)
C5	0.0198 (14)	0.0150 (12)	0.0221 (13)	−0.0034 (10)	−0.0025 (11)	−0.0004 (10)
C6	0.057 (2)	0.0205 (13)	0.0216 (14)	−0.0149 (14)	−0.0163 (15)	0.0001 (11)
C7	0.0308 (18)	0.0168 (12)	0.0350 (16)	−0.0085 (12)	−0.0030 (14)	−0.0040 (11)
C8	0.0429 (19)	0.0139 (12)	0.0226 (13)	−0.0077 (12)	−0.0001 (13)	0.0016 (11)
C9	0.0397 (19)	0.0150 (12)	0.0357 (15)	0.0006 (12)	−0.0045 (15)	−0.0046 (11)
C10	0.049 (2)	0.0257 (14)	0.0292 (15)	−0.0113 (15)	0.0122 (15)	−0.0129 (13)
C11	0.0329 (18)	0.0222 (14)	0.0186 (12)	−0.0047 (12)	0.0068 (12)	−0.0007 (10)
C12	0.044 (2)	0.0470 (19)	0.0227 (14)	−0.0067 (17)	0.0117 (14)	0.0002 (14)
C15	0.0116 (12)	0.0145 (11)	0.0138 (11)	−0.0021 (9)	0.0023 (9)	−0.0031 (9)
C16	0.0139 (12)	0.0160 (11)	0.0164 (11)	−0.0021 (11)	0.0042 (9)	−0.0008 (10)
C17	0.0181 (14)	0.0157 (12)	0.0210 (12)	−0.0017 (10)	0.0046 (11)	−0.0031 (10)
C18	0.0167 (14)	0.0205 (12)	0.0200 (12)	−0.0029 (10)	−0.0013 (11)	−0.0072 (10)
C19	0.0178 (14)	0.0185 (11)	0.0142 (11)	−0.0008 (10)	0.0000 (10)	−0.0023 (9)
C20	0.0249 (16)	0.0296 (14)	0.0265 (14)	−0.0057 (13)	0.0144 (13)	−0.0052 (11)
C21	0.0189 (14)	0.0390 (16)	0.0304 (14)	0.0033 (13)	0.0090 (12)	−0.0015 (14)
C22	0.0305 (18)	0.0254 (14)	0.0379 (16)	0.0057 (13)	0.0168 (14)	−0.0085 (13)
C23	0.0371 (19)	0.0316 (15)	0.0230 (14)	0.0005 (14)	0.0134 (13)	−0.0124 (12)
C24	0.035 (2)	0.0334 (16)	0.0192 (13)	−0.0010 (14)	0.0133 (13)	−0.0008 (12)
C25	0.0151 (13)	0.0180 (12)	0.0168 (11)	0.0013 (10)	0.0028 (9)	0.0001 (10)
C26	0.0243 (16)	0.0142 (11)	0.0195 (12)	0.0009 (11)	−0.0018 (11)	0.0043 (9)
C27	0.0283 (17)	0.0325 (16)	0.0176 (13)	0.0052 (13)	−0.0007 (12)	−0.0006 (12)
C28	0.0253 (16)	0.0253 (14)	0.0242 (13)	0.0065 (12)	0.0005 (12)	0.0018 (11)
C34	0.0145 (13)	0.0162 (11)	0.0119 (10)	0.0038 (10)	0.0001 (9)	0.0015 (9)
C35	0.0161 (14)	0.0204 (13)	0.0194 (12)	−0.0002 (10)	0.0010 (10)	−0.0015 (10)
C36	0.0164 (14)	0.0315 (15)	0.0261 (14)	0.0021 (12)	0.0066 (12)	0.0080 (11)
C37	0.0252 (17)	0.0359 (16)	0.0195 (13)	0.0146 (14)	0.0089 (11)	0.0051 (12)
C38	0.0336 (18)	0.0271 (15)	0.0187 (12)	0.0080 (13)	0.0020 (12)	−0.0056 (11)
C39	0.0230 (15)	0.0182 (12)	0.0171 (11)	0.0001 (11)	−0.0005 (11)	−0.0002 (10)

Geometric parameters (Å, º)

Fe1—C1	2.026 (2)	C10—H10	0.9500
Fe1—C2	2.032 (3)	C11—H11	0.9500
Fe1—C3	2.038 (2)	C11—C12	1.324 (4)
Fe1—C4	2.055 (3)	C12—H12A	0.9500

Fe1—C5	2.049 (3)	C12—H12B	0.9500
Fe1—C6	2.058 (3)	C15—C16	1.444 (3)
Fe1—C7	2.046 (3)	C15—C19	1.437 (3)
Fe1—C8	2.034 (3)	C16—C17	1.423 (4)
Fe1—C9	2.029 (3)	C16—C25	1.500 (3)
Fe1—C10	2.050 (3)	C17—H17	0.9500
Fe2—C15	2.038 (2)	C17—C18	1.412 (4)
Fe2—C16	2.033 (2)	C18—H18	0.9500
Fe2—C17	2.047 (3)	C18—C19	1.422 (3)
Fe2—C18	2.052 (3)	C19—H19	0.9500
Fe2—C19	2.043 (3)	C20—H20	0.9500
Fe2—C20	2.052 (3)	C20—C21	1.414 (4)
Fe2—C21	2.047 (3)	C20—C24	1.417 (4)
Fe2—C22	2.039 (3)	C21—H21	0.9500
Fe2—C23	2.047 (3)	C21—C22	1.429 (4)
Fe2—C24	2.053 (3)	C22—H22	0.9500
S1—P1	1.9544 (9)	C22—C23	1.420 (5)
P1—C1	1.802 (2)	C23—H23	0.9500
P1—C15	1.801 (2)	C23—C24	1.427 (4)
P1—C34	1.816 (2)	C24—H24	0.9500
O1—C25	1.466 (3)	C25—H25	1.0000
O1—C26	1.343 (3)	C25—C28	1.522 (4)
O2—C26	1.207 (3)	C26—C27	1.497 (4)
C1—C2	1.445 (3)	C27—H27A	0.9800
C1—C5	1.438 (4)	C27—H27B	0.9800
C2—C3	1.426 (4)	C27—H27C	0.9800
C2—C11	1.461 (4)	C28—H28A	0.9800
C3—H3	0.9500	C28—H28B	0.9800
C3—C4	1.416 (4)	C28—H28C	0.9800
C4—H4	0.9500	C34—C35	1.386 (4)
C4—C5	1.419 (4)	C34—C39	1.392 (3)
C5—H5	0.9500	C35—H35	0.9500
C6—H6	0.9500	C35—C36	1.388 (4)
C6—C7	1.407 (4)	C36—H36	0.9500
C6—C10	1.413 (5)	C36—C37	1.387 (4)
C7—H7	0.9500	C37—H37	0.9500
C7—C8	1.408 (4)	C37—C38	1.372 (4)
C8—H8	0.9500	C38—H38	0.9500
C8—C9	1.401 (4)	C38—C39	1.388 (4)
C9—H9	0.9500	C39—H39	0.9500
C9—C10	1.418 (4)		

C1—Fe1—C2	41.73 (10)	C10—C6—Fe1	69.56 (17)
C1—Fe1—C3	69.38 (10)	C10—C6—H6	126.1
C1—Fe1—C4	68.95 (11)	Fe1—C7—H7	125.9
C1—Fe1—C5	41.33 (11)	C6—C7—Fe1	70.41 (17)
C1—Fe1—C6	110.18 (11)	C6—C7—H7	125.9
C1—Fe1—C7	120.16 (11)	C6—C7—C8	108.2 (3)

C1—Fe1—C8	152.84 (12)	C8—C7—Fe1	69.36 (17)
C1—Fe1—C9	166.25 (12)	C8—C7—H7	125.9
C1—Fe1—C10	129.21 (11)	Fe1—C8—H8	125.8
C2—Fe1—C3	41.03 (11)	C7—C8—Fe1	70.28 (15)
C2—Fe1—C4	68.80 (12)	C7—C8—H8	125.9
C2—Fe1—C5	69.47 (11)	C9—C8—Fe1	69.63 (15)
C2—Fe1—C6	127.22 (13)	C9—C8—C7	108.3 (3)
C2—Fe1—C7	106.31 (12)	C9—C8—H8	125.9
C2—Fe1—C8	116.34 (11)	Fe1—C9—H9	125.1
C2—Fe1—C10	166.03 (12)	C8—C9—Fe1	70.03 (16)
C3—Fe1—C4	40.48 (12)	C8—C9—H9	126.0
C3—Fe1—C5	68.56 (11)	C8—C9—C10	108.0 (3)
C3—Fe1—C6	162.84 (14)	C10—C9—Fe1	70.44 (16)
C3—Fe1—C7	124.25 (12)	C10—C9—H9	126.0
C3—Fe1—C10	152.83 (13)	Fe1—C10—H10	126.3
C4—Fe1—C6	156.49 (13)	C6—C10—Fe1	70.21 (17)
C5—Fe1—C4	40.45 (10)	C6—C10—C9	107.7 (3)
C5—Fe1—C6	123.19 (11)	C6—C10—H10	126.1
C5—Fe1—C10	110.70 (12)	C9—C10—Fe1	68.87 (15)
C7—Fe1—C4	161.36 (11)	C9—C10—H10	126.1
C7—Fe1—C5	156.48 (11)	C2—C11—H11	117.7
C7—Fe1—C6	40.10 (12)	C12—C11—C2	124.6 (3)
C7—Fe1—C10	67.65 (13)	C12—C11—H11	117.7
C8—Fe1—C3	104.45 (11)	C11—C12—H12A	120.0
C8—Fe1—C4	124.27 (11)	C11—C12—H12B	120.0
C8—Fe1—C5	162.71 (12)	H12A—C12—H12B	120.0
C8—Fe1—C6	67.71 (12)	P1—C15—Fe2	132.94 (14)
C8—Fe1—C7	40.36 (12)	C16—C15—Fe2	69.03 (13)
C8—Fe1—C10	67.88 (12)	C16—C15—P1	128.28 (18)
C9—Fe1—C2	150.44 (11)	C19—C15—Fe2	69.58 (14)
C9—Fe1—C3	116.62 (12)	C19—C15—P1	123.75 (19)
C9—Fe1—C4	106.95 (13)	C19—C15—C16	107.5 (2)
C9—Fe1—C5	127.26 (13)	C15—C16—Fe2	69.43 (13)
C9—Fe1—C6	68.02 (13)	C15—C16—C25	127.4 (2)
C9—Fe1—C7	67.92 (13)	C17—C16—Fe2	70.12 (14)
C9—Fe1—C8	40.34 (13)	C17—C16—C15	107.2 (2)
C9—Fe1—C10	40.69 (12)	C17—C16—C25	125.4 (2)
C10—Fe1—C4	120.98 (14)	C25—C16—Fe2	127.01 (17)
C10—Fe1—C6	40.23 (14)	Fe2—C17—H17	127.0
C15—Fe2—C17	68.78 (10)	C16—C17—Fe2	69.06 (14)
C15—Fe2—C18	68.85 (10)	C16—C17—H17	125.5
C15—Fe2—C19	41.22 (9)	C18—C17—Fe2	70.03 (16)
C15—Fe2—C20	110.03 (10)	C18—C17—C16	109.1 (2)
C15—Fe2—C21	124.49 (11)	C18—C17—H17	125.5
C15—Fe2—C22	159.53 (12)	Fe2—C18—H18	126.7
C15—Fe2—C23	159.31 (12)	C17—C18—Fe2	69.66 (16)
C15—Fe2—C24	124.51 (11)	C17—C18—H18	125.9
C16—Fe2—C15	41.54 (10)	C17—C18—C19	108.2 (2)

C16—Fe2—C17	40.82 (10)	C19—C18—Fe2	69.37 (16)
C16—Fe2—C18	68.85 (10)	C19—C18—H18	125.9
C16—Fe2—C19	69.47 (10)	Fe2—C19—H19	126.4
C16—Fe2—C20	124.60 (11)	C15—C19—Fe2	69.19 (15)
C16—Fe2—C21	107.61 (11)	C15—C19—H19	126.0
C16—Fe2—C22	121.31 (12)	C18—C19—Fe2	70.00 (16)
C16—Fe2—C23	156.69 (11)	C18—C19—C15	108.0 (2)
C16—Fe2—C24	161.13 (11)	C18—C19—H19	126.0
C17—Fe2—C18	40.31 (10)	Fe2—C20—H20	126.3
C17—Fe2—C20	159.57 (12)	C21—C20—Fe2	69.63 (16)
C17—Fe2—C24	157.21 (12)	C21—C20—H20	125.8
C18—Fe2—C20	159.80 (12)	C21—C20—C24	108.5 (3)
C18—Fe2—C24	122.43 (12)	C24—C20—Fe2	69.85 (17)
C19—Fe2—C17	68.30 (10)	C24—C20—H20	125.8
C19—Fe2—C18	40.63 (10)	Fe2—C21—H21	126.2
C19—Fe2—C20	125.16 (11)	C20—C21—Fe2	70.01 (17)
C19—Fe2—C21	161.33 (11)	C20—C21—H21	126.1
C19—Fe2—C23	121.61 (12)	C20—C21—C22	107.8 (3)
C19—Fe2—C24	108.30 (12)	C22—C21—Fe2	69.26 (17)
C20—Fe2—C24	40.40 (12)	C22—C21—H21	126.1
C21—Fe2—C17	122.29 (12)	Fe2—C22—H22	125.8
C21—Fe2—C18	157.03 (11)	C21—C22—Fe2	69.81 (16)
C21—Fe2—C20	40.36 (12)	C21—C22—H22	126.0
C21—Fe2—C23	68.53 (13)	C23—C22—Fe2	69.94 (17)
C21—Fe2—C24	68.16 (13)	C23—C22—C21	108.0 (3)
C22—Fe2—C17	105.31 (12)	C23—C22—H22	126.0
C22—Fe2—C18	120.09 (12)	Fe2—C23—H23	126.2
C22—Fe2—C19	156.58 (12)	C22—C23—Fe2	69.38 (16)
C22—Fe2—C20	68.32 (12)	C22—C23—H23	126.1
C22—Fe2—C21	40.93 (12)	C22—C23—C24	107.8 (3)
C22—Fe2—C23	40.68 (13)	C24—C23—Fe2	69.87 (16)
C22—Fe2—C24	68.40 (13)	C24—C23—H23	126.1
C23—Fe2—C17	120.36 (12)	Fe2—C24—H24	126.4
C23—Fe2—C18	105.29 (12)	C20—C24—Fe2	69.76 (16)
C23—Fe2—C20	68.27 (12)	C20—C24—C23	107.9 (3)
C23—Fe2—C24	40.73 (12)	C20—C24—H24	126.0
C1—P1—S1	116.69 (9)	C23—C24—Fe2	69.40 (17)
C1—P1—C34	103.27 (11)	C23—C24—H24	126.0
C15—P1—S1	115.98 (9)	O1—C25—C16	104.57 (19)
C15—P1—C1	102.41 (11)	O1—C25—H25	109.7
C15—P1—C34	103.76 (11)	O1—C25—C28	109.2 (2)
C34—P1—S1	113.02 (9)	C16—C25—H25	109.7
C26—O1—C25	116.3 (2)	C16—C25—C28	113.8 (2)
P1—C1—Fe1	130.16 (13)	C28—C25—H25	109.7
C2—C1—Fe1	69.34 (13)	O1—C26—C27	111.4 (2)
C2—C1—P1	128.1 (2)	O2—C26—O1	123.9 (3)
C5—C1—Fe1	70.20 (14)	O2—C26—C27	124.6 (3)
C5—C1—P1	124.18 (19)	C26—C27—H27A	109.5

C5—C1—C2	107.5 (2)	C26—C27—H27B	109.5
C1—C2—Fe1	68.93 (14)	C26—C27—H27C	109.5
C1—C2—C11	126.4 (2)	H27A—C27—H27B	109.5
C3—C2—Fe1	69.71 (15)	H27A—C27—H27C	109.5
C3—C2—C1	107.3 (2)	H27B—C27—H27C	109.5
C3—C2—C11	126.2 (2)	C25—C28—H28A	109.5
C11—C2—Fe1	123.68 (18)	C25—C28—H28B	109.5
Fe1—C3—H3	126.2	C25—C28—H28C	109.5
C2—C3—Fe1	69.26 (14)	H28A—C28—H28B	109.5
C2—C3—H3	125.7	H28A—C28—H28C	109.5
C4—C3—Fe1	70.42 (15)	H28B—C28—H28C	109.5
C4—C3—C2	108.7 (2)	C35—C34—P1	121.37 (19)
C4—C3—H3	125.7	C35—C34—C39	119.6 (2)
Fe1—C4—H4	127.2	C39—C34—P1	118.9 (2)
C3—C4—Fe1	69.10 (16)	C34—C35—H35	119.8
C3—C4—H4	125.7	C34—C35—C36	120.3 (2)
C3—C4—C5	108.6 (3)	C36—C35—H35	119.8
C5—C4—Fe1	69.56 (15)	C35—C36—H36	120.2
C5—C4—H4	125.7	C37—C36—C35	119.5 (3)
Fe1—C5—H5	127.1	C37—C36—H36	120.2
C1—C5—Fe1	68.47 (14)	C36—C37—H37	119.8
C1—C5—H5	126.0	C38—C37—C36	120.4 (3)
C4—C5—Fe1	69.99 (15)	C38—C37—H37	119.8
C4—C5—C1	107.9 (2)	C37—C38—H38	119.8
C4—C5—H5	126.0	C37—C38—C39	120.3 (3)
Fe1—C6—H6	126.5	C39—C38—H38	119.8
C7—C6—Fe1	69.49 (16)	C34—C39—H39	120.1
C7—C6—H6	126.1	C38—C39—C34	119.8 (3)
C7—C6—C10	107.9 (3)	C38—C39—H39	120.1

Fe1—C1—C2—C3	59.38 (17)	C5—C1—C2—C11	−177.1 (2)
Fe1—C1—C2—C11	−117.0 (3)	C6—C7—C8—Fe1	59.95 (19)
Fe1—C1—C5—C4	−59.07 (18)	C6—C7—C8—C9	0.5 (3)
Fe1—C2—C3—C4	59.58 (18)	C7—C6—C10—Fe1	−59.12 (18)
Fe1—C2—C11—C12	110.9 (3)	C7—C6—C10—C9	−0.3 (3)
Fe1—C3—C4—C5	58.48 (18)	C7—C8—C9—Fe1	59.88 (18)
Fe1—C4—C5—C1	58.13 (17)	C7—C8—C9—C10	−0.6 (3)
Fe1—C6—C7—C8	−59.30 (19)	C8—C9—C10—Fe1	60.26 (19)
Fe1—C6—C10—C9	58.86 (19)	C8—C9—C10—C6	0.6 (3)
Fe1—C7—C8—C9	−59.48 (19)	C10—C6—C7—Fe1	59.17 (19)
Fe1—C8—C9—C10	−60.52 (19)	C10—C6—C7—C8	−0.1 (3)
Fe1—C9—C10—C6	−59.70 (19)	C11—C2—C3—Fe1	117.5 (3)
Fe2—C15—C16—C17	60.23 (16)	C11—C2—C3—C4	177.1 (2)
Fe2—C15—C16—C25	−121.5 (2)	C15—P1—C1—Fe1	177.61 (17)
Fe2—C15—C19—C18	−59.48 (19)	C15—P1—C1—C2	83.3 (2)
Fe2—C16—C17—C18	58.72 (19)	C15—P1—C1—C5	−90.3 (2)
Fe2—C16—C25—O1	−172.23 (16)	C15—P1—C34—C35	24.6 (2)
Fe2—C16—C25—C28	68.7 (3)	C15—P1—C34—C39	−158.1 (2)

Fe2—C17—C18—C19	58.81 (19)	C15—C16—C17—Fe2	−59.79 (16)
Fe2—C18—C19—C15	58.97 (18)	C15—C16—C17—C18	−1.1 (3)
Fe2—C20—C21—C22	−59.15 (19)	C15—C16—C25—O1	−81.0 (3)
Fe2—C20—C24—C23	59.1 (2)	C15—C16—C25—C28	160.0 (2)
Fe2—C21—C22—C23	−59.8 (2)	C16—C15—C19—Fe2	58.83 (16)
Fe2—C22—C23—C24	−59.5 (2)	C16—C15—C19—C18	−0.6 (3)
Fe2—C23—C24—C20	−59.3 (2)	C16—C17—C18—Fe2	−58.13 (18)
S1—P1—C1—Fe1	49.8 (2)	C16—C17—C18—C19	0.7 (3)
S1—P1—C1—C2	−44.5 (2)	C17—C16—C25—O1	97.0 (3)
S1—P1—C1—C5	141.96 (19)	C17—C16—C25—C28	−22.0 (3)
S1—P1—C15—Fe2	42.7 (2)	C17—C18—C19—Fe2	−58.99 (19)
S1—P1—C15—C16	−53.7 (2)	C17—C18—C19—C15	0.0 (3)
S1—P1—C15—C19	135.49 (19)	C19—C15—C16—Fe2	−59.18 (17)
S1—P1—C34—C35	151.04 (18)	C19—C15—C16—C17	1.0 (3)
S1—P1—C34—C39	−31.7 (2)	C19—C15—C16—C25	179.3 (2)
P1—C1—C2—Fe1	125.5 (2)	C20—C21—C22—Fe2	59.62 (19)
P1—C1—C2—C3	−175.15 (18)	C20—C21—C22—C23	−0.1 (3)
P1—C1—C2—C11	8.5 (4)	C21—C20—C24—Fe2	−59.1 (2)
P1—C1—C5—Fe1	−125.74 (19)	C21—C20—C24—C23	0.0 (3)
P1—C1—C5—C4	175.19 (18)	C21—C22—C23—Fe2	59.68 (19)
P1—C15—C16—Fe2	128.8 (2)	C21—C22—C23—C24	0.1 (3)
P1—C15—C16—C17	−171.0 (2)	C22—C23—C24—Fe2	59.2 (2)
P1—C15—C16—C25	7.3 (4)	C22—C23—C24—C20	−0.1 (4)
P1—C15—C19—Fe2	−128.71 (19)	C24—C20—C21—Fe2	59.2 (2)
P1—C15—C19—C18	171.81 (19)	C24—C20—C21—C22	0.1 (3)
P1—C34—C35—C36	178.1 (2)	C25—O1—C26—O2	1.8 (3)
P1—C34—C39—C38	−176.8 (2)	C25—O1—C26—C27	−178.7 (2)
C1—P1—C15—Fe2	−85.5 (2)	C25—C16—C17—Fe2	121.9 (2)
C1—P1—C15—C16	178.1 (2)	C25—C16—C17—C18	−179.4 (2)
C1—P1—C15—C19	7.2 (2)	C26—O1—C25—C16	157.5 (2)
C1—P1—C34—C35	−82.0 (2)	C26—O1—C25—C28	−80.4 (3)
C1—P1—C34—C39	95.3 (2)	C34—P1—C1—Fe1	−74.80 (19)
C1—C2—C3—Fe1	−58.89 (16)	C34—P1—C1—C2	−169.1 (2)
C1—C2—C3—C4	0.7 (3)	C34—P1—C1—C5	17.3 (2)
C1—C2—C11—C12	−161.7 (3)	C34—P1—C15—Fe2	167.25 (17)
C2—C1—C5—Fe1	59.56 (16)	C34—P1—C15—C16	70.9 (2)
C2—C1—C5—C4	0.5 (3)	C34—P1—C15—C19	−100.0 (2)
C2—C3—C4—Fe1	−58.87 (18)	C34—C35—C36—C37	−1.5 (4)
C2—C3—C4—C5	−0.4 (3)	C35—C34—C39—C38	0.5 (4)
C3—C2—C11—C12	22.6 (4)	C35—C36—C37—C38	0.8 (4)
C3—C4—C5—Fe1	−58.20 (18)	C36—C37—C38—C39	0.6 (4)
C3—C4—C5—C1	−0.1 (3)	C37—C38—C39—C34	−1.3 (4)
C5—C1—C2—Fe1	−60.11 (16)	C39—C34—C35—C36	0.9 (4)
C5—C1—C2—C3	−0.7 (3)		

[(2S_p)-2-Ethenylferrocen-1-yl]{(2S_p)-2-[(1*R*)-1-hydroxyethyl]ferrocen-1-yl}phenyl-(*S*)-phosphane sulfide (8b)

Crystal data

$[Fe_2(C_5H_5)_2(C_{20}H_{19}OPS)]$
M_r = 580.26
Orthorhombic, $P2_12_12_1$
a = 7.5285 (3) Å
b = 17.6463 (7) Å
c = 39.3333 (15) Å
V = 5225.4 (4) Å^3
Z = 8
F(000) = 2400
D_x = 1.475 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9990 reflections
θ = 2.4–29.3°
μ = 1.27 mm^{-1}
T = 130 K
Block, clear orange
0.25 × 0.2 × 0.17 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: sealed xray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.650, T_{max} = 0.746
38763 measured reflections
14944 independent reflections
11780 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 30.0°, θ_{min} = 1.0°
h = −9→10
k = −24→24
l = −49→55

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.137
S = 1.04
14944 reflections
635 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 6.896P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.80 e Å^{-3}
Absolute structure: Flack x determined using 4140 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.010 (7)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups At 1.5 times of: All C(H,H,H) groups, All O(H) groups 2. Restrained distances H1B-C34B 2.5 with sigma of 0.05 3.a Ternary CH refined with riding coordinates: C25A(H25A), C25B(H25B) 3.b Aromatic/amide H refined with riding coordinates: C3A(H3A), C4A(H4A), C5A(H5A), C6A(H6A), C7A(H7A), C8A(H8A), C9A(H9A), C10A(H10A), C11A(H11A), C17A(H17A), C18A(H18A), C19A(H19A), C20A(H20A), C21A(H21A), C22A(H22A), C23A(H23A), C24A(H24A), C35A(H35A), C36A(H36A), C37A(H37A), C38A(H38A), C39A(H39A), C3B(H3B), C4B(H4B), C5B(H5B), C6B(H6B), C7B(H7B), C8B(H8B), C9B(H9B), C10B(H10B), C11B(H11B), C17B(H17B), C18B(H18B), C19B(H19B), C20B(H20B), C21B(H21B), C22B(H22B), C23B(H23B), C24B(H24B), C35B(H35B), C36B(H36B), C37B(H37B), C38B(H38B), C39B(H39B) 3.c X=CH2 refined with riding coordinates: C12A(H12A,H12B), C12B(H12C,H12D) 3.d Idealised Me refined as rotating group: C26A(H26A,H26B,H26C), C26B(H26D,H26E,H26F) 3.e Idealised tetrahedral OH refined as rotating group: O1A(H1A), O1B(H1B)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1A	0.72689 (11)	0.58337 (4)	0.56427 (2)	0.02723 (17)
Fe2A	0.90817 (12)	0.50676 (5)	0.41673 (2)	0.03364 (19)
S1A	0.4437 (2)	0.55690 (8)	0.47076 (4)	0.0329 (3)
P1A	0.63867 (18)	0.49477 (7)	0.48811 (3)	0.0215 (2)
O1A	0.4921 (7)	0.3319 (3)	0.42896 (12)	0.0496 (12)
H1A	0.481829	0.339883	0.449923	0.074*
C1A	0.7859 (7)	0.5377 (3)	0.51848 (12)	0.0249 (10)
C2A	0.8462 (8)	0.6159 (3)	0.52000 (13)	0.0319 (12)
C3A	0.9682 (9)	0.6202 (4)	0.54785 (15)	0.0399 (14)
H3A	1.027855	0.664803	0.555144	0.048*
C4A	0.9862 (8)	0.5476 (4)	0.56284 (15)	0.0368 (13)
H4A	1.060591	0.535142	0.581538	0.044*
C5A	0.8742 (7)	0.4968 (3)	0.54515 (13)	0.0294 (11)
H5A	0.859724	0.444446	0.550079	0.035*
C6A	0.4564 (8)	0.5854 (3)	0.56956 (14)	0.0354 (12)
H6A	0.371524	0.568517	0.553370	0.042*
C7A	0.5267 (9)	0.6602 (3)	0.57211 (15)	0.0388 (14)
H7A	0.497184	0.701982	0.557971	0.047*
C8A	0.6488 (9)	0.6610 (3)	0.59955 (15)	0.0388 (14)
H8A	0.715712	0.703531	0.606930	0.047*
C9A	0.6541 (8)	0.5874 (4)	0.61417 (14)	0.0362 (12)
H9A	0.724229	0.572079	0.633029	0.043*
C10A	0.5349 (8)	0.5409 (3)	0.59534 (14)	0.0355 (13)
H10A	0.512097	0.488778	0.599418	0.043*
C11A	0.7839 (10)	0.6800 (3)	0.49998 (16)	0.0434 (15)
H11A	0.702283	0.669007	0.482224	0.052*
C12A	0.8284 (12)	0.7509 (4)	0.5039 (2)	0.063 (2)
H12A	0.909615	0.764937	0.521286	0.076*
H12B	0.779709	0.788540	0.489354	0.076*
C15A	0.7888 (7)	0.4568 (3)	0.45709 (12)	0.0228 (9)
C16A	0.7459 (7)	0.4173 (3)	0.42600 (12)	0.0267 (10)
C17A	0.9091 (8)	0.3920 (3)	0.41194 (14)	0.0342 (12)
H17A	0.920726	0.364127	0.391387	0.041*
C18A	1.0508 (8)	0.4141 (3)	0.43292 (16)	0.0376 (13)
H18A	1.172981	0.403694	0.429057	0.045*
C19A	0.9793 (7)	0.4550 (3)	0.46105 (14)	0.0307 (11)
H19A	1.045205	0.477083	0.479122	0.037*
C20A	0.8220 (12)	0.6174 (4)	0.41152 (19)	0.056 (2)
H20A	0.736712	0.642900	0.425144	0.067*
C21A	0.7885 (12)	0.5742 (4)	0.38160 (17)	0.059 (2)
H21A	0.674693	0.565730	0.371867	0.070*
C22A	0.9473 (14)	0.5464 (5)	0.36890 (19)	0.068 (3)
H22A	0.961400	0.516048	0.349142	0.082*
C23A	1.0842 (12)	0.5715 (5)	0.3907 (2)	0.067 (2)
H23A	1.207123	0.560776	0.387988	0.080*

C24A	1.0091 (13)	0.6148 (4)	0.4169 (2)	0.064 (2)
H24A	1.071804	0.638125	0.435086	0.077*
C25A	0.5625 (9)	0.3995 (3)	0.41240 (15)	0.0395 (14)
H25A	0.482977	0.442919	0.418328	0.047*
C26A	0.5476 (13)	0.3864 (5)	0.37579 (18)	0.068 (2)
H26A	0.600296	0.429109	0.363484	0.102*
H26B	0.422028	0.381616	0.369580	0.102*
H26C	0.610430	0.339620	0.369791	0.102*
C34A	0.5525 (8)	0.4108 (3)	0.50942 (12)	0.0263 (10)
C35A	0.6566 (9)	0.3457 (3)	0.51330 (14)	0.0356 (13)
H35A	0.774718	0.344963	0.504835	0.043*
C36A	0.5878 (11)	0.2816 (3)	0.52957 (15)	0.0460 (17)
H36A	0.659011	0.237537	0.532309	0.055*
C37A	0.4154 (11)	0.2828 (4)	0.54164 (15)	0.0497 (18)
H37A	0.367680	0.239471	0.552681	0.060*
C38A	0.3126 (10)	0.3468 (4)	0.53767 (16)	0.0473 (17)
H38A	0.194223	0.347044	0.546014	0.057*
C39A	0.3786 (8)	0.4105 (3)	0.52181 (14)	0.0345 (12)
H39A	0.306022	0.454216	0.519319	0.041*
Fe1B	0.26525 (12)	0.28793 (6)	0.17616 (3)	0.0465 (3)
Fe2B	0.08660 (14)	0.18732 (5)	0.32286 (2)	0.0406 (2)
S1B	0.5324 (2)	0.27642 (8)	0.27046 (4)	0.0373 (3)
P1B	0.36294 (19)	0.20308 (7)	0.25184 (4)	0.0276 (3)
O1B	0.5684 (10)	0.0491 (7)	0.3061 (2)	0.146 (5)
H1B	0.541816	0.050393	0.285400	0.219*
C1B	0.2073 (7)	0.2372 (3)	0.22072 (14)	0.0306 (11)
C2B	0.1185 (8)	0.3093 (3)	0.21902 (16)	0.0376 (13)
C3B	0.0059 (8)	0.3084 (4)	0.18994 (17)	0.0412 (15)
H3B	−0.068780	0.348483	0.182527	0.049*
C4B	0.0253 (9)	0.2368 (4)	0.17407 (17)	0.0463 (16)
H4B	−0.034289	0.221283	0.153948	0.056*
C5B	0.1462 (8)	0.1919 (4)	0.19258 (15)	0.0380 (13)
H5B	0.180846	0.141432	0.187474	0.046*
C6B	0.5317 (9)	0.3057 (6)	0.1728 (3)	0.077 (3)
H6B	0.616455	0.294239	0.189959	0.092*
C7B	0.4419 (11)	0.3746 (6)	0.1698 (2)	0.079 (3)
H7B	0.453339	0.417800	0.184019	0.095*
C8B	0.3284 (10)	0.3667 (6)	0.1405 (2)	0.077 (3)
H8B	0.250993	0.404793	0.132038	0.092*
C9B	0.3492 (12)	0.2946 (7)	0.1265 (2)	0.076 (3)
H9B	0.288574	0.275542	0.107075	0.092*
C10B	0.4776 (12)	0.2543 (7)	0.1463 (3)	0.083 (3)
H10B	0.518752	0.204057	0.142677	0.100*
C11B	0.1372 (10)	0.3735 (3)	0.24254 (19)	0.0456 (16)
H11B	0.243928	0.378078	0.255245	0.055*
C12B	0.0112 (13)	0.4253 (4)	0.2468 (3)	0.071 (2)
H12C	−0.096649	0.421812	0.234374	0.086*
H12D	0.028965	0.465902	0.262315	0.086*

C15B	0.2279 (8)	0.1535 (3)	0.28203 (14)	0.0305 (11)
C16B	0.2868 (10)	0.1137 (3)	0.31220 (16)	0.0437 (15)
C17B	0.1361 (10)	0.0741 (4)	0.32479 (17)	0.0471 (16)
H17B	0.135397	0.043146	0.344550	0.056*
C18B	−0.0110 (9)	0.0873 (4)	0.30393 (15)	0.0404 (14)
H18B	−0.127006	0.067313	0.307058	0.049*
C19B	0.0442 (8)	0.1361 (3)	0.27724 (14)	0.0337 (12)
H19B	−0.028663	0.154085	0.259240	0.040*
C20B	0.1274 (11)	0.2999 (4)	0.3314 (2)	0.0533 (18)
H20B	0.207787	0.331261	0.319193	0.064*
C21B	0.1659 (18)	0.2564 (5)	0.3615 (2)	0.087 (4)
H21B	0.276115	0.253832	0.373252	0.104*
C22B	0.009 (3)	0.2188 (6)	0.3701 (2)	0.124 (7)
H22B	−0.005504	0.185628	0.388905	0.149*
C23B	−0.1198 (18)	0.2371 (6)	0.3472 (3)	0.103 (5)
H23B	−0.238357	0.218687	0.347330	0.123*
C24B	−0.0492 (12)	0.2871 (5)	0.3236 (2)	0.062 (2)
H24B	−0.112028	0.309028	0.305134	0.074*
C25B	0.4773 (14)	0.1103 (5)	0.3239 (3)	0.085 (3)
H25B	0.537917	0.159761	0.319410	0.103*
C26B	0.4888 (14)	0.0901 (5)	0.3619 (2)	0.080 (3)
H26D	0.422548	0.127650	0.375211	0.119*
H26E	0.613428	0.090148	0.369085	0.119*
H26F	0.437638	0.039739	0.365642	0.119*
C34B	0.4751 (8)	0.1251 (3)	0.22994 (14)	0.0297 (11)
C35B	0.3919 (9)	0.0551 (3)	0.22620 (16)	0.0396 (13)
H35B	0.276944	0.047290	0.235515	0.048*
C36B	0.4760 (10)	−0.0031 (4)	0.20895 (18)	0.0487 (16)
H36B	0.420204	−0.051125	0.206828	0.058*
C37B	0.6413 (10)	0.0091 (4)	0.19488 (18)	0.0491 (16)
H37B	0.697762	−0.030307	0.182485	0.059*
C38B	0.7259 (10)	0.0783 (4)	0.19864 (17)	0.0474 (15)
H38B	0.840391	0.086177	0.189128	0.057*
C39B	0.6420 (8)	0.1360 (3)	0.21639 (14)	0.0344 (12)
H39B	0.699993	0.183439	0.219237	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1A	0.0270 (4)	0.0313 (3)	0.0234 (3)	−0.0057 (3)	0.0012 (3)	−0.0056 (3)
Fe2A	0.0356 (4)	0.0386 (4)	0.0267 (4)	−0.0072 (4)	0.0068 (4)	0.0052 (3)
S1A	0.0298 (7)	0.0314 (6)	0.0374 (7)	0.0090 (6)	−0.0027 (6)	0.0018 (5)
P1A	0.0220 (6)	0.0218 (5)	0.0208 (5)	−0.0001 (5)	−0.0001 (5)	0.0003 (4)
O1A	0.047 (3)	0.053 (3)	0.048 (3)	−0.015 (2)	−0.005 (2)	0.000 (2)
C1A	0.024 (2)	0.030 (2)	0.021 (2)	−0.003 (2)	0.003 (2)	0.0002 (17)
C2A	0.035 (3)	0.035 (2)	0.025 (2)	−0.013 (2)	0.005 (2)	−0.006 (2)
C3A	0.037 (3)	0.050 (3)	0.033 (3)	−0.018 (3)	0.004 (3)	−0.010 (3)
C4A	0.026 (3)	0.056 (3)	0.028 (3)	−0.005 (3)	−0.001 (2)	−0.004 (3)

C5A	0.026 (3)	0.038 (3)	0.024 (2)	0.003 (2)	−0.003 (2)	0.001 (2)
C6A	0.027 (3)	0.047 (3)	0.032 (3)	0.000 (3)	0.007 (2)	−0.013 (2)
C7A	0.041 (3)	0.045 (3)	0.031 (3)	0.007 (3)	0.007 (3)	−0.004 (2)
C8A	0.046 (4)	0.039 (3)	0.032 (3)	−0.007 (3)	0.005 (3)	−0.013 (2)
C9A	0.038 (3)	0.048 (3)	0.022 (2)	−0.001 (3)	−0.001 (2)	−0.002 (2)
C10A	0.035 (3)	0.043 (3)	0.029 (3)	−0.002 (3)	0.008 (2)	−0.002 (2)
C11A	0.058 (4)	0.035 (3)	0.037 (3)	−0.011 (3)	0.006 (3)	0.002 (2)
C12A	0.070 (6)	0.042 (3)	0.077 (5)	−0.022 (4)	−0.010 (5)	0.006 (3)
C15A	0.023 (2)	0.025 (2)	0.020 (2)	0.002 (2)	0.004 (2)	0.0043 (17)
C16A	0.027 (3)	0.030 (2)	0.023 (2)	−0.001 (2)	0.000 (2)	0.0026 (18)
C17A	0.037 (3)	0.037 (3)	0.028 (3)	0.001 (3)	0.007 (3)	−0.003 (2)
C18A	0.027 (3)	0.044 (3)	0.042 (3)	0.004 (3)	0.009 (3)	−0.003 (3)
C19A	0.024 (3)	0.038 (3)	0.031 (3)	−0.001 (2)	−0.003 (2)	−0.001 (2)
C20A	0.077 (6)	0.040 (3)	0.050 (4)	−0.005 (4)	0.010 (4)	0.019 (3)
C21A	0.071 (5)	0.067 (4)	0.037 (3)	−0.012 (4)	−0.001 (4)	0.027 (3)
C22A	0.106 (8)	0.063 (4)	0.036 (4)	−0.018 (5)	0.019 (5)	0.015 (3)
C23A	0.061 (5)	0.065 (5)	0.074 (5)	−0.021 (4)	0.026 (5)	0.026 (4)
C24A	0.078 (6)	0.048 (4)	0.066 (5)	−0.027 (4)	0.005 (5)	0.016 (4)
C25A	0.037 (3)	0.044 (3)	0.037 (3)	−0.001 (3)	−0.010 (3)	−0.003 (2)
C26A	0.072 (6)	0.087 (6)	0.044 (4)	−0.020 (5)	−0.020 (4)	0.000 (4)
C34A	0.035 (3)	0.026 (2)	0.018 (2)	−0.006 (2)	0.000 (2)	−0.0009 (17)
C35A	0.046 (3)	0.029 (2)	0.032 (3)	−0.001 (2)	0.001 (3)	0.001 (2)
C36A	0.074 (5)	0.028 (2)	0.036 (3)	−0.006 (3)	−0.004 (4)	0.002 (2)
C37A	0.075 (5)	0.043 (3)	0.031 (3)	−0.032 (4)	0.000 (3)	0.007 (2)
C38A	0.048 (4)	0.060 (4)	0.034 (3)	−0.024 (3)	0.002 (3)	0.000 (3)
C39A	0.031 (3)	0.039 (3)	0.034 (3)	−0.008 (3)	−0.001 (2)	−0.004 (2)
Fe1B	0.0244 (4)	0.0691 (6)	0.0460 (5)	−0.0012 (4)	0.0028 (4)	0.0336 (5)
Fe2B	0.0566 (6)	0.0410 (4)	0.0242 (4)	−0.0133 (4)	0.0019 (4)	−0.0041 (3)
S1B	0.0309 (7)	0.0297 (6)	0.0515 (9)	−0.0042 (6)	−0.0037 (7)	0.0023 (6)
P1B	0.0249 (7)	0.0259 (5)	0.0320 (7)	−0.0017 (5)	0.0000 (6)	0.0063 (5)
O1B	0.063 (5)	0.275 (12)	0.100 (6)	0.064 (7)	0.015 (4)	0.114 (7)
C1B	0.024 (3)	0.035 (3)	0.033 (3)	0.001 (2)	0.006 (2)	0.010 (2)
C2B	0.027 (3)	0.037 (3)	0.049 (3)	−0.001 (2)	−0.003 (3)	0.017 (2)
C3B	0.024 (3)	0.052 (3)	0.048 (3)	0.000 (3)	0.000 (3)	0.025 (3)
C4B	0.030 (3)	0.072 (4)	0.037 (3)	−0.002 (3)	−0.002 (3)	0.018 (3)
C5B	0.034 (3)	0.046 (3)	0.034 (3)	−0.004 (3)	0.003 (3)	0.007 (2)
C6B	0.023 (3)	0.119 (7)	0.088 (6)	−0.004 (4)	0.009 (4)	0.073 (6)
C7B	0.046 (5)	0.100 (6)	0.090 (7)	−0.021 (5)	0.002 (5)	0.061 (5)
C8B	0.031 (4)	0.128 (8)	0.070 (6)	−0.004 (5)	0.002 (4)	0.074 (6)
C9B	0.056 (5)	0.120 (8)	0.053 (5)	−0.001 (6)	0.010 (4)	0.044 (5)
C10B	0.042 (5)	0.133 (9)	0.075 (6)	0.015 (6)	0.019 (5)	0.052 (6)
C11B	0.041 (4)	0.027 (2)	0.068 (4)	0.003 (3)	−0.013 (3)	0.006 (3)
C12B	0.066 (6)	0.047 (4)	0.101 (7)	0.017 (4)	−0.025 (5)	−0.005 (4)
C15B	0.031 (3)	0.028 (2)	0.032 (3)	−0.005 (2)	−0.001 (2)	0.0065 (19)
C16B	0.048 (4)	0.039 (3)	0.044 (3)	−0.009 (3)	−0.008 (3)	0.019 (3)
C17B	0.054 (4)	0.049 (3)	0.038 (3)	−0.015 (3)	0.004 (3)	0.012 (3)
C18B	0.041 (3)	0.044 (3)	0.036 (3)	−0.015 (3)	0.008 (3)	−0.003 (3)
C19B	0.033 (3)	0.040 (3)	0.028 (3)	−0.005 (3)	0.004 (2)	−0.005 (2)

C20B	0.056 (4)	0.040 (3)	0.064 (5)	−0.011 (3)	−0.001 (4)	−0.011 (3)
C21B	0.137 (10)	0.057 (5)	0.066 (6)	0.007 (6)	−0.056 (6)	−0.030 (4)
C22B	0.26 (2)	0.063 (5)	0.044 (5)	−0.046 (9)	0.052 (8)	−0.030 (4)
C23B	0.112 (9)	0.096 (7)	0.101 (8)	−0.040 (7)	0.067 (8)	−0.070 (7)
C24B	0.063 (5)	0.066 (4)	0.055 (4)	0.000 (4)	−0.001 (4)	−0.027 (4)
C25B	0.075 (6)	0.076 (5)	0.105 (8)	−0.020 (5)	−0.041 (6)	0.061 (6)
C26B	0.090 (7)	0.061 (5)	0.088 (6)	−0.018 (5)	−0.053 (6)	0.033 (4)
C34B	0.031 (3)	0.030 (2)	0.028 (3)	0.002 (2)	−0.002 (2)	0.007 (2)
C35B	0.041 (3)	0.032 (2)	0.046 (3)	−0.003 (3)	0.001 (3)	0.004 (2)
C36B	0.057 (4)	0.033 (3)	0.056 (4)	0.003 (3)	0.002 (3)	0.000 (3)
C37B	0.057 (4)	0.042 (3)	0.048 (4)	0.011 (3)	0.007 (3)	−0.004 (3)
C38B	0.047 (4)	0.051 (3)	0.045 (3)	0.001 (3)	0.015 (3)	0.001 (3)
C39B	0.036 (3)	0.036 (3)	0.031 (3)	−0.002 (3)	0.001 (3)	0.005 (2)

Geometric parameters (Å, º)

Fe1A—C1A	2.023 (5)	Fe1B—C1B	2.016 (5)
Fe1A—C2A	2.041 (5)	Fe1B—C2B	2.050 (7)
Fe1A—C3A	2.035 (6)	Fe1B—C3B	2.058 (6)
Fe1A—C4A	2.053 (6)	Fe1B—C4B	2.021 (7)
Fe1A—C5A	2.032 (5)	Fe1B—C5B	2.022 (6)
Fe1A—C6A	2.048 (6)	Fe1B—C6B	2.035 (7)
Fe1A—C7A	2.050 (6)	Fe1B—C7B	2.043 (8)
Fe1A—C8A	2.036 (6)	Fe1B—C8B	2.031 (7)
Fe1A—C9A	2.039 (5)	Fe1B—C9B	2.058 (8)
Fe1A—C10A	2.035 (6)	Fe1B—C10B	2.071 (9)
Fe2A—C15A	2.026 (5)	Fe2B—C15B	2.017 (6)
Fe2A—C16A	2.029 (5)	Fe2B—C16B	2.034 (7)
Fe2A—C17A	2.034 (5)	Fe2B—C17B	2.034 (7)
Fe2A—C18A	2.057 (6)	Fe2B—C18B	2.051 (6)
Fe2A—C19A	2.039 (6)	Fe2B—C19B	2.035 (6)
Fe2A—C20A	2.067 (7)	Fe2B—C20B	2.038 (6)
Fe2A—C21A	2.034 (7)	Fe2B—C21B	2.039 (7)
Fe2A—C22A	2.029 (7)	Fe2B—C22B	2.024 (8)
Fe2A—C23A	2.028 (7)	Fe2B—C23B	2.025 (10)
Fe2A—C24A	2.052 (7)	Fe2B—C24B	2.036 (8)
S1A—P1A	1.9552 (18)	S1B—P1B	1.959 (2)
P1A—C1A	1.797 (5)	P1B—C1B	1.798 (6)
P1A—C15A	1.793 (5)	P1B—C15B	1.791 (5)
P1A—C34A	1.822 (5)	P1B—C34B	1.830 (6)
O1A—H1A	0.8400	O1B—H1B	0.8400
O1A—C25A	1.460 (7)	O1B—C25B	1.458 (14)
C1A—C2A	1.454 (7)	C1B—C2B	1.439 (8)
C1A—C5A	1.436 (7)	C1B—C5B	1.440 (8)
C2A—C3A	1.432 (8)	C2B—C3B	1.424 (9)
C2A—C11A	1.456 (8)	C2B—C11B	1.469 (9)
C3A—H3A	0.9500	C3B—H3B	0.9500
C3A—C4A	1.418 (9)	C3B—C4B	1.417 (10)

C4A—H4A	0.9500	C4B—H4B	0.9500
C4A—C5A	1.413 (8)	C4B—C5B	1.408 (9)
C5A—H5A	0.9500	C5B—H5B	0.9500
C6A—H6A	0.9500	C6B—H6B	0.9500
C6A—C7A	1.425 (8)	C6B—C7B	1.398 (13)
C6A—C10A	1.412 (8)	C6B—C10B	1.441 (15)
C7A—H7A	0.9500	C7B—H7B	0.9500
C7A—C8A	1.417 (9)	C7B—C8B	1.440 (13)
C8A—H8A	0.9500	C8B—H8B	0.9500
C8A—C9A	1.420 (8)	C8B—C9B	1.396 (14)
C9A—H9A	0.9500	C9B—H9B	0.9500
C9A—C10A	1.424 (8)	C9B—C10B	1.431 (12)
C10A—H10A	0.9500	C10B—H10B	0.9500
C11A—H11A	0.9500	C11B—H11B	0.9500
C11A—C12A	1.305 (9)	C11B—C12B	1.329 (10)
C12A—H12A	0.9500	C12B—H12C	0.9500
C12A—H12B	0.9500	C12B—H12D	0.9500
C15A—C16A	1.444 (7)	C15B—C16B	1.449 (8)
C15A—C19A	1.443 (7)	C15B—C19B	1.430 (8)
C16A—C17A	1.420 (8)	C16B—C17B	1.421 (9)
C16A—C25A	1.513 (8)	C16B—C25B	1.507 (11)
C17A—H17A	0.9500	C17B—H17B	0.9500
C17A—C18A	1.404 (9)	C17B—C18B	1.398 (10)
C18A—H18A	0.9500	C18B—H18B	0.9500
C18A—C19A	1.427 (8)	C18B—C19B	1.420 (8)
C19A—H19A	0.9500	C19B—H19B	0.9500
C20A—H20A	0.9500	C20B—H20B	0.9500
C20A—C21A	1.425 (11)	C20B—C21B	1.443 (12)
C20A—C24A	1.425 (12)	C20B—C24B	1.383 (11)
C21A—H21A	0.9500	C21B—H21B	0.9500
C21A—C22A	1.385 (12)	C21B—C22B	1.395 (18)
C22A—H22A	0.9500	C22B—H22B	0.9500
C22A—C23A	1.411 (13)	C22B—C23B	1.364 (19)
C23A—H23A	0.9500	C23B—H23B	0.9500
C23A—C24A	1.404 (12)	C23B—C24B	1.385 (14)
C24A—H24A	0.9500	C24B—H24B	0.9500
C25A—H25A	1.0000	C25B—H25B	1.0000
C25A—C26A	1.463 (9)	C25B—C26B	1.540 (12)
C26A—H26A	0.9800	C26B—H26D	0.9800
C26A—H26B	0.9800	C26B—H26E	0.9800
C26A—H26C	0.9800	C26B—H26F	0.9800
C34A—C35A	1.399 (8)	C34B—C35B	1.392 (8)
C34A—C39A	1.397 (8)	C34B—C39B	1.379 (8)
C35A—H35A	0.9500	C35B—H35B	0.9500
C35A—C36A	1.399 (8)	C35B—C36B	1.384 (9)
C36A—H36A	0.9500	C36B—H36B	0.9500
C36A—C37A	1.382 (11)	C36B—C37B	1.379 (10)
C37A—H37A	0.9500	C37B—H37B	0.9500

C37A—C38A	1.378 (10)	C37B—C38B	1.385 (9)
C38A—H38A	0.9500	C38B—H38B	0.9500
C38A—C39A	1.379 (8)	C38B—C39B	1.387 (9)
C39A—H39A	0.9500	C39B—H39B	0.9500

C1A—Fe1A—C2A	41.91 (19)	C1B—Fe1B—C2B	41.4 (2)
C1A—Fe1A—C3A	69.4 (2)	C1B—Fe1B—C3B	69.1 (2)
C1A—Fe1A—C4A	69.1 (2)	C1B—Fe1B—C4B	69.1 (2)
C1A—Fe1A—C5A	41.5 (2)	C1B—Fe1B—C5B	41.8 (2)
C1A—Fe1A—C6A	108.4 (2)	C1B—Fe1B—C6B	109.7 (3)
C1A—Fe1A—C7A	124.0 (2)	C1B—Fe1B—C7B	125.5 (3)
C1A—Fe1A—C8A	159.8 (2)	C1B—Fe1B—C8B	162.8 (4)
C1A—Fe1A—C9A	158.5 (2)	C1B—Fe1B—C9B	156.6 (4)
C1A—Fe1A—C10A	123.0 (2)	C1B—Fe1B—C10B	122.2 (3)
C2A—Fe1A—C4A	69.2 (3)	C2B—Fe1B—C3B	40.5 (2)
C2A—Fe1A—C6A	121.3 (2)	C2B—Fe1B—C9B	159.4 (3)
C2A—Fe1A—C7A	105.4 (2)	C2B—Fe1B—C10B	159.2 (3)
C3A—Fe1A—C2A	41.1 (2)	C3B—Fe1B—C10B	158.7 (4)
C3A—Fe1A—C4A	40.6 (3)	C4B—Fe1B—C2B	68.5 (3)
C3A—Fe1A—C6A	156.2 (3)	C4B—Fe1B—C3B	40.6 (3)
C3A—Fe1A—C7A	119.5 (3)	C4B—Fe1B—C5B	40.8 (3)
C3A—Fe1A—C8A	105.0 (3)	C4B—Fe1B—C6B	161.3 (4)
C3A—Fe1A—C9A	122.3 (2)	C4B—Fe1B—C7B	155.7 (3)
C3A—Fe1A—C10A	160.4 (3)	C4B—Fe1B—C8B	119.1 (3)
C5A—Fe1A—C2A	69.9 (2)	C4B—Fe1B—C9B	105.2 (4)
C5A—Fe1A—C3A	68.6 (2)	C4B—Fe1B—C10B	122.6 (4)
C5A—Fe1A—C4A	40.5 (2)	C5B—Fe1B—C2B	69.7 (2)
C5A—Fe1A—C6A	126.4 (2)	C5B—Fe1B—C3B	69.0 (3)
C5A—Fe1A—C7A	162.5 (2)	C5B—Fe1B—C6B	125.9 (3)
C5A—Fe1A—C8A	156.3 (2)	C5B—Fe1B—C7B	162.8 (3)
C5A—Fe1A—C9A	122.0 (2)	C5B—Fe1B—C8B	153.8 (4)
C5A—Fe1A—C10A	109.5 (2)	C5B—Fe1B—C9B	119.2 (4)
C6A—Fe1A—C4A	162.6 (3)	C5B—Fe1B—C10B	106.5 (4)
C6A—Fe1A—C7A	40.7 (2)	C6B—Fe1B—C2B	123.8 (4)
C7A—Fe1A—C4A	155.0 (3)	C6B—Fe1B—C3B	157.7 (4)
C8A—Fe1A—C2A	121.3 (2)	C6B—Fe1B—C7B	40.1 (4)
C8A—Fe1A—C4A	120.0 (3)	C6B—Fe1B—C9B	68.1 (4)
C8A—Fe1A—C6A	68.4 (3)	C6B—Fe1B—C10B	41.1 (4)
C8A—Fe1A—C7A	40.6 (3)	C7B—Fe1B—C2B	108.3 (4)
C8A—Fe1A—C9A	40.8 (2)	C7B—Fe1B—C3B	121.3 (4)
C9A—Fe1A—C2A	158.3 (2)	C7B—Fe1B—C9B	68.9 (4)
C9A—Fe1A—C4A	107.0 (2)	C7B—Fe1B—C10B	69.0 (5)
C9A—Fe1A—C6A	68.5 (2)	C8B—Fe1B—C2B	124.6 (4)
C9A—Fe1A—C7A	68.6 (2)	C8B—Fe1B—C3B	106.5 (3)
C10A—Fe1A—C2A	158.1 (2)	C8B—Fe1B—C6B	67.6 (3)
C10A—Fe1A—C4A	125.3 (2)	C8B—Fe1B—C7B	41.4 (4)
C10A—Fe1A—C6A	40.5 (2)	C8B—Fe1B—C9B	39.9 (4)
C10A—Fe1A—C7A	68.4 (3)	C8B—Fe1B—C10B	67.9 (4)

C10A—Fe1A—C8A	68.5 (2)	C9B—Fe1B—C3B	122.1 (3)
C10A—Fe1A—C9A	40.9 (2)	C9B—Fe1B—C10B	40.5 (4)
C15A—Fe2A—C16A	41.73 (19)	C15B—Fe2B—C16B	41.9 (2)
C15A—Fe2A—C17A	69.0 (2)	C15B—Fe2B—C17B	69.1 (2)
C15A—Fe2A—C18A	69.1 (2)	C15B—Fe2B—C18B	69.2 (2)
C15A—Fe2A—C19A	41.6 (2)	C15B—Fe2B—C19B	41.3 (2)
C15A—Fe2A—C20A	110.4 (3)	C15B—Fe2B—C20B	109.9 (3)
C15A—Fe2A—C21A	126.2 (3)	C15B—Fe2B—C21B	128.1 (4)
C15A—Fe2A—C22A	160.2 (3)	C15B—Fe2B—C22B	164.5 (6)
C15A—Fe2A—C23A	158.6 (3)	C15B—Fe2B—C23B	155.4 (5)
C15A—Fe2A—C24A	124.4 (3)	C15B—Fe2B—C24B	122.2 (3)
C16A—Fe2A—C17A	40.9 (2)	C16B—Fe2B—C18B	69.0 (3)
C16A—Fe2A—C18A	68.9 (2)	C16B—Fe2B—C19B	69.5 (3)
C16A—Fe2A—C19A	69.9 (2)	C16B—Fe2B—C20B	123.0 (3)
C16A—Fe2A—C20A	124.3 (3)	C16B—Fe2B—C21B	108.6 (4)
C16A—Fe2A—C21A	108.1 (3)	C16B—Fe2B—C24B	158.1 (3)
C16A—Fe2A—C22A	121.5 (3)	C17B—Fe2B—C16B	40.9 (3)
C16A—Fe2A—C24A	160.9 (3)	C17B—Fe2B—C18B	40.0 (3)
C17A—Fe2A—C18A	40.1 (2)	C17B—Fe2B—C19B	68.0 (3)
C17A—Fe2A—C19A	68.4 (2)	C17B—Fe2B—C20B	157.5 (3)
C17A—Fe2A—C20A	158.8 (3)	C17B—Fe2B—C21B	120.4 (3)
C17A—Fe2A—C24A	157.5 (3)	C17B—Fe2B—C24B	160.2 (3)
C18A—Fe2A—C20A	160.9 (3)	C19B—Fe2B—C18B	40.7 (2)
C19A—Fe2A—C18A	40.8 (2)	C19B—Fe2B—C20B	127.0 (3)
C19A—Fe2A—C20A	126.2 (3)	C19B—Fe2B—C21B	165.9 (4)
C19A—Fe2A—C24A	108.4 (3)	C19B—Fe2B—C24B	108.6 (3)
C21A—Fe2A—C17A	121.4 (3)	C20B—Fe2B—C18B	162.2 (3)
C21A—Fe2A—C18A	155.0 (3)	C20B—Fe2B—C21B	41.5 (3)
C21A—Fe2A—C19A	163.5 (3)	C21B—Fe2B—C18B	152.9 (4)
C21A—Fe2A—C20A	40.6 (3)	C22B—Fe2B—C16B	125.3 (5)
C21A—Fe2A—C24A	67.9 (3)	C22B—Fe2B—C17B	106.7 (4)
C22A—Fe2A—C17A	104.9 (3)	C22B—Fe2B—C18B	117.8 (4)
C22A—Fe2A—C18A	119.0 (3)	C22B—Fe2B—C19B	152.4 (5)
C22A—Fe2A—C19A	155.4 (4)	C22B—Fe2B—C20B	68.0 (4)
C22A—Fe2A—C20A	68.1 (3)	C22B—Fe2B—C21B	40.2 (5)
C22A—Fe2A—C21A	39.9 (4)	C22B—Fe2B—C23B	39.4 (6)
C22A—Fe2A—C24A	68.2 (3)	C22B—Fe2B—C24B	66.7 (5)
C23A—Fe2A—C16A	157.3 (3)	C23B—Fe2B—C16B	160.6 (5)
C23A—Fe2A—C17A	120.8 (3)	C23B—Fe2B—C17B	123.3 (4)
C23A—Fe2A—C18A	105.2 (3)	C23B—Fe2B—C18B	105.6 (3)
C23A—Fe2A—C19A	120.8 (3)	C23B—Fe2B—C19B	119.3 (4)
C23A—Fe2A—C20A	67.9 (3)	C23B—Fe2B—C20B	67.4 (4)
C23A—Fe2A—C21A	67.5 (4)	C23B—Fe2B—C21B	67.2 (5)
C23A—Fe2A—C22A	40.7 (4)	C23B—Fe2B—C24B	39.9 (4)
C23A—Fe2A—C24A	40.3 (3)	C24B—Fe2B—C18B	124.7 (3)
C24A—Fe2A—C18A	122.9 (3)	C24B—Fe2B—C20B	39.7 (3)
C24A—Fe2A—C20A	40.5 (3)	C24B—Fe2B—C21B	67.6 (4)
C1A—P1A—S1A	117.33 (18)	C1B—P1B—S1B	117.24 (19)

C1A—P1A—C34A	104.9 (2)	C1B—P1B—C34B	103.4 (3)
C15A—P1A—S1A	116.44 (17)	C15B—P1B—S1B	116.4 (2)
C15A—P1A—C1A	102.8 (2)	C15B—P1B—C1B	104.2 (3)
C15A—P1A—C34A	103.5 (2)	C15B—P1B—C34B	101.9 (2)
C34A—P1A—S1A	110.5 (2)	C34B—P1B—S1B	111.9 (2)
C25A—O1A—H1A	109.5	C25B—O1B—H1B	109.5
P1A—C1A—Fe1A	128.6 (3)	P1B—C1B—Fe1B	126.8 (3)
C2A—C1A—Fe1A	69.7 (3)	C2B—C1B—Fe1B	70.6 (3)
C2A—C1A—P1A	128.3 (4)	C2B—C1B—P1B	129.1 (5)
C5A—C1A—Fe1A	69.6 (3)	C2B—C1B—C5B	107.8 (5)
C5A—C1A—P1A	124.0 (4)	C5B—C1B—Fe1B	69.3 (3)
C5A—C1A—C2A	107.6 (5)	C5B—C1B—P1B	123.1 (4)
C1A—C2A—Fe1A	68.4 (3)	C1B—C2B—Fe1B	68.0 (3)
C1A—C2A—C11A	127.9 (5)	C1B—C2B—C11B	127.5 (5)
C3A—C2A—Fe1A	69.2 (3)	C3B—C2B—Fe1B	70.0 (4)
C3A—C2A—C1A	106.4 (5)	C3B—C2B—C1B	107.7 (6)
C3A—C2A—C11A	125.4 (5)	C3B—C2B—C11B	124.9 (6)
C11A—C2A—Fe1A	122.5 (5)	C11B—C2B—Fe1B	127.4 (5)
Fe1A—C3A—H3A	126.2	Fe1B—C3B—H3B	127.7
C2A—C3A—Fe1A	69.7 (3)	C2B—C3B—Fe1B	69.4 (4)
C2A—C3A—H3A	125.3	C2B—C3B—H3B	126.2
C4A—C3A—Fe1A	70.4 (3)	C4B—C3B—Fe1B	68.3 (4)
C4A—C3A—C2A	109.3 (5)	C4B—C3B—C2B	107.6 (5)
C4A—C3A—H3A	125.3	C4B—C3B—H3B	126.2
Fe1A—C4A—H4A	127.6	Fe1B—C4B—H4B	125.8
C3A—C4A—Fe1A	69.0 (4)	C3B—C4B—Fe1B	71.1 (4)
C3A—C4A—H4A	125.9	C3B—C4B—H4B	125.1
C5A—C4A—Fe1A	69.0 (3)	C5B—C4B—Fe1B	69.7 (4)
C5A—C4A—C3A	108.2 (5)	C5B—C4B—C3B	109.9 (6)
C5A—C4A—H4A	125.9	C5B—C4B—H4B	125.1
Fe1A—C5A—H5A	126.4	Fe1B—C5B—H5B	126.6
C1A—C5A—Fe1A	68.9 (3)	C1B—C5B—Fe1B	68.9 (3)
C1A—C5A—H5A	125.8	C1B—C5B—H5B	126.5
C4A—C5A—Fe1A	70.5 (3)	C4B—C5B—Fe1B	69.6 (4)
C4A—C5A—C1A	108.5 (5)	C4B—C5B—C1B	107.0 (6)
C4A—C5A—H5A	125.8	C4B—C5B—H5B	126.5
Fe1A—C6A—H6A	126.5	Fe1B—C6B—H6B	125.7
C7A—C6A—Fe1A	69.8 (3)	C7B—C6B—Fe1B	70.3 (4)
C7A—C6A—H6A	126.0	C7B—C6B—H6B	124.8
C10A—C6A—Fe1A	69.3 (3)	C7B—C6B—C10B	110.4 (8)
C10A—C6A—H6A	126.0	C10B—C6B—Fe1B	70.8 (5)
C10A—C6A—C7A	108.0 (5)	C10B—C6B—H6B	124.8
Fe1A—C7A—H7A	126.7	Fe1B—C7B—H7B	125.9
C6A—C7A—Fe1A	69.5 (3)	C6B—C7B—Fe1B	69.6 (5)
C6A—C7A—H7A	126.2	C6B—C7B—H7B	127.1
C8A—C7A—Fe1A	69.2 (4)	C6B—C7B—C8B	105.7 (10)
C8A—C7A—C6A	107.7 (5)	C8B—C7B—Fe1B	68.9 (5)
C8A—C7A—H7A	126.2	C8B—C7B—H7B	127.1

Fe1A—C8A—H8A	125.9	Fe1B—C8B—H8B	125.6
C7A—C8A—Fe1A	70.2 (3)	C7B—C8B—Fe1B	69.7 (4)
C7A—C8A—H8A	125.7	C7B—C8B—H8B	125.1
C7A—C8A—C9A	108.5 (5)	C9B—C8B—Fe1B	71.1 (5)
C9A—C8A—Fe1A	69.7 (3)	C9B—C8B—C7B	109.8 (8)
C9A—C8A—H8A	125.7	C9B—C8B—H8B	125.1
Fe1A—C9A—H9A	126.3	Fe1B—C9B—H9B	126.5
C8A—C9A—Fe1A	69.5 (3)	C8B—C9B—Fe1B	69.0 (5)
C8A—C9A—H9A	126.3	C8B—C9B—H9B	125.9
C8A—C9A—C10A	107.3 (5)	C8B—C9B—C10B	108.2 (10)
C10A—C9A—Fe1A	69.4 (3)	C10B—C9B—Fe1B	70.2 (5)
C10A—C9A—H9A	126.3	C10B—C9B—H9B	125.9
Fe1A—C10A—H10A	125.9	Fe1B—C10B—H10B	127.1
C6A—C10A—Fe1A	70.2 (3)	C6B—C10B—Fe1B	68.1 (5)
C6A—C10A—C9A	108.5 (5)	C6B—C10B—H10B	127.1
C6A—C10A—H10A	125.8	C9B—C10B—Fe1B	69.2 (5)
C9A—C10A—Fe1A	69.7 (3)	C9B—C10B—C6B	105.9 (10)
C9A—C10A—H10A	125.8	C9B—C10B—H10B	127.1
C2A—C11A—H11A	116.6	C2B—C11B—H11B	118.6
C12A—C11A—C2A	126.8 (7)	C12B—C11B—C2B	122.9 (7)
C12A—C11A—H11A	116.6	C12B—C11B—H11B	118.6
C11A—C12A—H12A	120.0	C11B—C12B—H12C	120.0
C11A—C12A—H12B	120.0	C11B—C12B—H12D	120.0
H12A—C12A—H12B	120.0	H12C—C12B—H12D	120.0
P1A—C15A—Fe2A	130.6 (3)	P1B—C15B—Fe2B	133.1 (3)
C16A—C15A—Fe2A	69.2 (3)	C16B—C15B—Fe2B	69.7 (4)
C16A—C15A—P1A	128.0 (4)	C16B—C15B—P1B	127.3 (5)
C19A—C15A—Fe2A	69.7 (3)	C19B—C15B—Fe2B	70.0 (3)
C19A—C15A—P1A	124.2 (4)	C19B—C15B—P1B	124.5 (4)
C19A—C15A—C16A	107.7 (5)	C19B—C15B—C16B	107.4 (5)
C15A—C16A—Fe2A	69.0 (3)	C15B—C16B—Fe2B	68.4 (4)
C15A—C16A—C25A	127.1 (5)	C15B—C16B—C25B	124.0 (6)
C17A—C16A—Fe2A	69.8 (3)	C17B—C16B—Fe2B	69.5 (4)
C17A—C16A—C15A	106.8 (5)	C17B—C16B—C15B	106.2 (6)
C17A—C16A—C25A	125.9 (5)	C17B—C16B—C25B	129.4 (6)
C25A—C16A—Fe2A	130.4 (4)	C25B—C16B—Fe2B	131.8 (7)
Fe2A—C17A—H17A	126.4	Fe2B—C17B—H17B	126.5
C16A—C17A—Fe2A	69.3 (3)	C16B—C17B—Fe2B	69.6 (4)
C16A—C17A—H17A	125.0	C16B—C17B—H17B	124.9
C18A—C17A—Fe2A	70.8 (3)	C18B—C17B—Fe2B	70.7 (4)
C18A—C17A—C16A	109.9 (5)	C18B—C17B—C16B	110.2 (5)
C18A—C17A—H17A	125.0	C18B—C17B—H17B	124.9
Fe2A—C18A—H18A	127.6	Fe2B—C18B—H18B	127.0
C17A—C18A—Fe2A	69.1 (3)	C17B—C18B—Fe2B	69.3 (4)
C17A—C18A—H18A	126.0	C17B—C18B—H18B	126.2
C17A—C18A—C19A	108.1 (5)	C17B—C18B—C19B	107.7 (6)
C19A—C18A—Fe2A	69.0 (3)	C19B—C18B—Fe2B	69.0 (3)
C19A—C18A—H18A	126.0	C19B—C18B—H18B	126.2

Fe2A—C19A—H19A	126.4	Fe2B—C19B—H19B	126.8
C15A—C19A—Fe2A	68.7 (3)	C15B—C19B—Fe2B	68.7 (3)
C15A—C19A—H19A	126.2	C15B—C19B—H19B	125.8
C18A—C19A—Fe2A	70.3 (3)	C18B—C19B—Fe2B	70.3 (3)
C18A—C19A—C15A	107.6 (5)	C18B—C19B—C15B	108.4 (5)
C18A—C19A—H19A	126.2	C18B—C19B—H19B	125.8
Fe2A—C20A—H20A	127.1	Fe2B—C20B—H20B	125.5
C21A—C20A—Fe2A	68.4 (4)	C21B—C20B—Fe2B	69.3 (4)
C21A—C20A—H20A	126.8	C21B—C20B—H20B	126.6
C21A—C20A—C24A	106.3 (8)	C24B—C20B—Fe2B	70.1 (4)
C24A—C20A—Fe2A	69.2 (5)	C24B—C20B—H20B	126.6
C24A—C20A—H20A	126.8	C24B—C20B—C21B	106.7 (8)
Fe2A—C21A—H21A	125.5	Fe2B—C21B—H21B	126.1
C20A—C21A—Fe2A	70.9 (4)	C20B—C21B—Fe2B	69.2 (4)
C20A—C21A—H21A	125.2	C20B—C21B—H21B	126.8
C22A—C21A—Fe2A	69.9 (5)	C22B—C21B—Fe2B	69.4 (5)
C22A—C21A—C20A	109.5 (8)	C22B—C21B—C20B	106.3 (10)
C22A—C21A—H21A	125.2	C22B—C21B—H21B	126.8
Fe2A—C22A—H22A	125.5	Fe2B—C22B—H22B	125.4
C21A—C22A—Fe2A	70.3 (4)	C21B—C22B—Fe2B	70.5 (6)
C21A—C22A—H22A	126.2	C21B—C22B—H22B	125.4
C21A—C22A—C23A	107.5 (7)	C23B—C22B—Fe2B	70.4 (5)
C23A—C22A—Fe2A	69.6 (4)	C23B—C22B—C21B	109.3 (9)
C23A—C22A—H22A	126.2	C23B—C22B—H22B	125.4
Fe2A—C23A—H23A	125.5	Fe2B—C23B—H23B	125.1
C22A—C23A—Fe2A	69.7 (4)	C22B—C23B—Fe2B	70.3 (7)
C22A—C23A—H23A	125.6	C22B—C23B—H23B	125.7
C24A—C23A—Fe2A	70.8 (4)	C22B—C23B—C24B	108.7 (11)
C24A—C23A—C22A	108.8 (8)	C24B—C23B—Fe2B	70.5 (5)
C24A—C23A—H23A	125.6	C24B—C23B—H23B	125.7
Fe2A—C24A—H24A	126.2	Fe2B—C24B—H24B	126.2
C20A—C24A—Fe2A	70.4 (4)	C20B—C24B—Fe2B	70.2 (5)
C20A—C24A—H24A	126.1	C20B—C24B—C23B	109.0 (10)
C23A—C24A—Fe2A	69.0 (4)	C20B—C24B—H24B	125.5
C23A—C24A—C20A	107.8 (8)	C23B—C24B—Fe2B	69.6 (6)
C23A—C24A—H24A	126.1	C23B—C24B—H24B	125.5
O1A—C25A—C16A	110.1 (5)	O1B—C25B—C16B	109.3 (8)
O1A—C25A—H25A	107.7	O1B—C25B—H25B	110.3
O1A—C25A—C26A	106.4 (6)	O1B—C25B—C26B	105.5 (7)
C16A—C25A—H25A	107.7	C16B—C25B—H25B	110.3
C26A—C25A—C16A	116.8 (6)	C16B—C25B—C26B	111.0 (9)
C26A—C25A—H25A	107.7	C26B—C25B—H25B	110.3
C25A—C26A—H26A	109.5	C25B—C26B—H26D	109.5
C25A—C26A—H26B	109.5	C25B—C26B—H26E	109.5
C25A—C26A—H26C	109.5	C25B—C26B—H26F	109.5
H26A—C26A—H26B	109.5	H26D—C26B—H26E	109.5
H26A—C26A—H26C	109.5	H26D—C26B—H26F	109.5
H26B—C26A—H26C	109.5	H26E—C26B—H26F	109.5

C35A—C34A—P1A	121.3 (4)	C35B—C34B—P1B	120.6 (5)
C39A—C34A—P1A	119.8 (4)	C39B—C34B—P1B	119.8 (4)
C39A—C34A—C35A	119.0 (5)	C39B—C34B—C35B	119.6 (6)
C34A—C35A—H35A	119.8	C34B—C35B—H35B	119.9
C36A—C35A—C34A	120.5 (6)	C36B—C35B—C34B	120.3 (6)
C36A—C35A—H35A	119.8	C36B—C35B—H35B	119.9
C35A—C36A—H36A	120.3	C35B—C36B—H36B	120.2
C37A—C36A—C35A	119.5 (6)	C37B—C36B—C35B	119.6 (6)
C37A—C36A—H36A	120.3	C37B—C36B—H36B	120.2
C36A—C37A—H37A	120.0	C36B—C37B—H37B	119.7
C38A—C37A—C36A	120.1 (6)	C36B—C37B—C38B	120.6 (6)
C38A—C37A—H37A	120.0	C38B—C37B—H37B	119.7
C37A—C38A—H38A	119.4	C37B—C38B—H38B	120.3
C37A—C38A—C39A	121.2 (6)	C37B—C38B—C39B	119.5 (6)
C39A—C38A—H38A	119.4	C39B—C38B—H38B	120.3
C34A—C39A—H39A	120.1	C34B—C39B—C38B	120.4 (6)
C38A—C39A—C34A	119.9 (6)	C34B—C39B—H39B	119.8
C38A—C39A—H39A	120.1	C38B—C39B—H39B	119.8

Fe1A—C1A—C2A—C3A	59.0 (4)	Fe1B—C1B—C2B—C3B	59.0 (4)
Fe1A—C1A—C2A—C11A	−115.1 (6)	Fe1B—C1B—C2B—C11B	−121.1 (7)
Fe1A—C1A—C5A—C4A	−59.6 (4)	Fe1B—C1B—C5B—C4B	−59.4 (4)
Fe1A—C2A—C3A—C4A	59.4 (4)	Fe1B—C2B—C3B—C4B	57.7 (4)
Fe1A—C2A—C11A—C12A	86.6 (9)	Fe1B—C2B—C11B—C12B	115.3 (8)
Fe1A—C3A—C4A—C5A	58.0 (4)	Fe1B—C3B—C4B—C5B	59.1 (4)
Fe1A—C4A—C5A—C1A	58.6 (4)	Fe1B—C4B—C5B—C1B	58.9 (4)
Fe1A—C6A—C7A—C8A	−58.9 (4)	Fe1B—C6B—C7B—C8B	−59.7 (5)
Fe1A—C6A—C10A—C9A	59.4 (4)	Fe1B—C6B—C10B—C9B	59.2 (6)
Fe1A—C7A—C8A—C9A	−59.4 (4)	Fe1B—C7B—C8B—C9B	−60.0 (6)
Fe1A—C8A—C9A—C10A	−59.3 (4)	Fe1B—C8B—C9B—C10B	−59.5 (6)
Fe1A—C9A—C10A—C6A	−59.7 (4)	Fe1B—C9B—C10B—C6B	−58.5 (5)
Fe2A—C15A—C16A—C17A	59.8 (4)	Fe2B—C15B—C16B—C17B	59.5 (5)
Fe2A—C15A—C16A—C25A	−125.4 (5)	Fe2B—C15B—C16B—C25B	−126.8 (9)
Fe2A—C15A—C19A—C18A	−59.8 (4)	Fe2B—C15B—C19B—C18B	−59.2 (4)
Fe2A—C16A—C17A—C18A	59.3 (4)	Fe2B—C16B—C17B—C18B	59.1 (5)
Fe2A—C16A—C25A—O1A	−174.7 (4)	Fe2B—C16B—C25B—O1B	−175.1 (5)
Fe2A—C16A—C25A—C26A	63.9 (8)	Fe2B—C16B—C25B—C26B	68.9 (9)
Fe2A—C17A—C18A—C19A	58.1 (4)	Fe2B—C17B—C18B—C19B	58.6 (4)
Fe2A—C18A—C19A—C15A	58.8 (4)	Fe2B—C18B—C19B—C15B	58.2 (4)
Fe2A—C20A—C21A—C22A	−59.4 (5)	Fe2B—C20B—C21B—C22B	−59.8 (6)
Fe2A—C20A—C24A—C23A	59.0 (5)	Fe2B—C20B—C24B—C23B	59.0 (6)
Fe2A—C21A—C22A—C23A	−59.9 (5)	Fe2B—C21B—C22B—C23B	−59.9 (6)
Fe2A—C22A—C23A—C24A	−60.2 (5)	Fe2B—C22B—C23B—C24B	−60.3 (6)
Fe2A—C23A—C24A—C20A	−59.9 (5)	Fe2B—C23B—C24B—C20B	−59.4 (6)
S1A—P1A—C1A—Fe1A	58.3 (4)	S1B—P1B—C1B—Fe1B	57.4 (4)
S1A—P1A—C1A—C2A	−35.4 (6)	S1B—P1B—C1B—C2B	−36.8 (6)
S1A—P1A—C1A—C5A	148.4 (4)	S1B—P1B—C1B—C5B	145.2 (4)
S1A—P1A—C15A—Fe2A	45.8 (4)	S1B—P1B—C15B—Fe2B	46.2 (5)

S1A—P1A—C15A—C16A	−48.6 (5)	S1B—P1B—C15B—C16B	−50.4 (6)
S1A—P1A—C15A—C19A	137.5 (4)	S1B—P1B—C15B—C19B	140.5 (4)
S1A—P1A—C34A—C35A	157.1 (4)	S1B—P1B—C34B—C35B	155.8 (4)
S1A—P1A—C34A—C39A	−22.1 (4)	S1B—P1B—C34B—C39B	−25.5 (5)
P1A—C1A—C2A—Fe1A	123.8 (5)	P1B—C1B—C2B—Fe1B	122.2 (5)
P1A—C1A—C2A—C3A	−177.2 (4)	P1B—C1B—C2B—C3B	−178.9 (4)
P1A—C1A—C2A—C11A	8.7 (9)	P1B—C1B—C2B—C11B	1.1 (10)
P1A—C1A—C5A—Fe1A	−123.5 (4)	P1B—C1B—C5B—Fe1B	−121.3 (4)
P1A—C1A—C5A—C4A	176.8 (4)	P1B—C1B—C5B—C4B	179.4 (4)
P1A—C15A—C16A—Fe2A	125.9 (4)	P1B—C15B—C16B—Fe2B	129.3 (5)
P1A—C15A—C16A—C17A	−174.2 (4)	P1B—C15B—C16B—C17B	−171.2 (5)
P1A—C15A—C16A—C25A	0.5 (8)	P1B—C15B—C16B—C25B	2.5 (11)
P1A—C15A—C19A—Fe2A	−126.0 (4)	P1B—C15B—C19B—Fe2B	−129.2 (4)
P1A—C15A—C19A—C18A	174.3 (4)	P1B—C15B—C19B—C18B	171.6 (4)
P1A—C34A—C35A—C36A	−179.7 (4)	P1B—C34B—C35B—C36B	178.6 (5)
P1A—C34A—C39A—C38A	179.4 (4)	P1B—C34B—C39B—C38B	−177.6 (5)
C1A—P1A—C15A—Fe2A	−83.8 (4)	C1B—P1B—C15B—Fe2B	−84.5 (5)
C1A—P1A—C15A—C16A	−178.2 (4)	C1B—P1B—C15B—C16B	178.9 (5)
C1A—P1A—C15A—C19A	7.9 (5)	C1B—P1B—C15B—C19B	9.8 (5)
C1A—P1A—C34A—C35A	−75.6 (5)	C1B—P1B—C34B—C35B	−77.1 (5)
C1A—P1A—C34A—C39A	105.2 (4)	C1B—P1B—C34B—C39B	101.5 (5)
C1A—C2A—C3A—Fe1A	−58.4 (4)	C1B—C2B—C3B—Fe1B	−57.7 (4)
C1A—C2A—C3A—C4A	0.9 (7)	C1B—C2B—C3B—C4B	0.0 (7)
C1A—C2A—C11A—C12A	173.3 (8)	C1B—C2B—C11B—C12B	−155.1 (7)
C2A—C1A—C5A—Fe1A	59.6 (4)	C2B—C1B—C5B—Fe1B	60.3 (4)
C2A—C1A—C5A—C4A	0.0 (6)	C2B—C1B—C5B—C4B	1.0 (7)
C2A—C3A—C4A—Fe1A	−58.9 (4)	C2B—C3B—C4B—Fe1B	−58.4 (4)
C2A—C3A—C4A—C5A	−1.0 (7)	C2B—C3B—C4B—C5B	0.6 (7)
C3A—C2A—C11A—C12A	0.3 (12)	C3B—C2B—C11B—C12B	24.8 (11)
C3A—C4A—C5A—Fe1A	−58.0 (4)	C3B—C4B—C5B—Fe1B	−59.9 (5)
C3A—C4A—C5A—C1A	0.6 (6)	C3B—C4B—C5B—C1B	−1.0 (7)
C5A—C1A—C2A—Fe1A	−59.5 (4)	C5B—C1B—C2B—Fe1B	−59.6 (4)
C5A—C1A—C2A—C3A	−0.6 (6)	C5B—C1B—C2B—C3B	−0.6 (7)
C5A—C1A—C2A—C11A	−174.6 (6)	C5B—C1B—C2B—C11B	179.3 (6)
C6A—C7A—C8A—Fe1A	59.1 (4)	C6B—C7B—C8B—Fe1B	60.2 (5)
C6A—C7A—C8A—C9A	−0.3 (7)	C6B—C7B—C8B—C9B	0.2 (8)
C7A—C6A—C10A—Fe1A	−59.2 (4)	C7B—C6B—C10B—Fe1B	−59.3 (5)
C7A—C6A—C10A—C9A	0.2 (7)	C7B—C6B—C10B—C9B	−0.1 (9)
C7A—C8A—C9A—Fe1A	59.7 (4)	C7B—C8B—C9B—Fe1B	59.2 (5)
C7A—C8A—C9A—C10A	0.4 (7)	C7B—C8B—C9B—C10B	−0.3 (9)
C8A—C9A—C10A—Fe1A	59.4 (4)	C8B—C9B—C10B—Fe1B	58.7 (6)
C8A—C9A—C10A—C6A	−0.3 (7)	C8B—C9B—C10B—C6B	0.2 (9)
C10A—C6A—C7A—Fe1A	58.9 (4)	C10B—C6B—C7B—Fe1B	59.6 (6)
C10A—C6A—C7A—C8A	0.1 (7)	C10B—C6B—C7B—C8B	−0.1 (8)
C11A—C2A—C3A—Fe1A	115.8 (6)	C11B—C2B—C3B—Fe1B	122.4 (6)
C11A—C2A—C3A—C4A	175.2 (6)	C11B—C2B—C3B—C4B	−179.9 (6)
C15A—P1A—C1A—Fe1A	−172.6 (3)	C15B—P1B—C1B—Fe1B	−172.4 (3)
C15A—P1A—C1A—C2A	93.7 (5)	C15B—P1B—C1B—C2B	93.4 (5)

C15A—P1A—C1A—C5A	−82.5 (5)	C15B—P1B—C1B—C5B	−84.6 (5)
C15A—P1A—C34A—C35A	31.8 (5)	C15B—P1B—C34B—C35B	30.8 (5)
C15A—P1A—C34A—C39A	−147.4 (4)	C15B—P1B—C34B—C39B	−150.5 (4)
C15A—C16A—C17A—Fe2A	−59.4 (3)	C15B—C16B—C17B—Fe2B	−58.8 (4)
C15A—C16A—C17A—C18A	−0.1 (6)	C15B—C16B—C17B—C18B	0.3 (8)
C15A—C16A—C25A—O1A	−81.6 (7)	C15B—C16B—C25B—O1B	−84.6 (8)
C15A—C16A—C25A—C26A	157.0 (6)	C15B—C16B—C25B—C26B	159.4 (7)
C16A—C15A—C19A—Fe2A	59.1 (3)	C16B—C15B—C19B—Fe2B	59.9 (4)
C16A—C15A—C19A—C18A	−0.7 (6)	C16B—C15B—C19B—C18B	0.7 (7)
C16A—C17A—C18A—Fe2A	−58.4 (4)	C16B—C17B—C18B—Fe2B	−58.4 (5)
C16A—C17A—C18A—C19A	−0.3 (7)	C16B—C17B—C18B—C19B	0.1 (8)
C17A—C16A—C25A—O1A	92.2 (6)	C17B—C16B—C25B—O1B	87.6 (11)
C17A—C16A—C25A—C26A	−29.2 (9)	C17B—C16B—C25B—C26B	−28.4 (14)
C17A—C18A—C19A—Fe2A	−58.1 (4)	C17B—C18B—C19B—Fe2B	−58.7 (5)
C17A—C18A—C19A—C15A	0.6 (7)	C17B—C18B—C19B—C15B	−0.5 (7)
C19A—C15A—C16A—Fe2A	−59.4 (4)	C19B—C15B—C16B—Fe2B	−60.1 (4)
C19A—C15A—C16A—C17A	0.5 (6)	C19B—C15B—C16B—C17B	−0.6 (7)
C19A—C15A—C16A—C25A	175.2 (5)	C19B—C15B—C16B—C25B	173.1 (8)
C20A—C21A—C22A—Fe2A	60.1 (5)	C20B—C21B—C22B—Fe2B	59.7 (6)
C20A—C21A—C22A—C23A	0.2 (8)	C20B—C21B—C22B—C23B	−0.2 (10)
C21A—C20A—C24A—Fe2A	−58.6 (5)	C21B—C20B—C24B—Fe2B	−59.9 (5)
C21A—C20A—C24A—C23A	0.4 (8)	C21B—C20B—C24B—C23B	−0.9 (8)
C21A—C22A—C23A—Fe2A	60.3 (5)	C21B—C22B—C23B—Fe2B	59.9 (7)
C21A—C22A—C23A—C24A	0.1 (8)	C21B—C22B—C23B—C24B	−0.4 (11)
C22A—C23A—C24A—Fe2A	59.5 (5)	C22B—C23B—C24B—Fe2B	60.2 (7)
C22A—C23A—C24A—C20A	−0.3 (8)	C22B—C23B—C24B—C20B	0.8 (10)
C24A—C20A—C21A—Fe2A	59.0 (5)	C24B—C20B—C21B—Fe2B	60.4 (5)
C24A—C20A—C21A—C22A	−0.4 (8)	C24B—C20B—C21B—C22B	0.7 (9)
C25A—C16A—C17A—Fe2A	125.8 (5)	C25B—C16B—C17B—Fe2B	127.9 (10)
C25A—C16A—C17A—C18A	−174.9 (5)	C25B—C16B—C17B—C18B	−173.0 (9)
C34A—P1A—C1A—Fe1A	−64.6 (4)	C34B—P1B—C1B—Fe1B	−66.2 (4)
C34A—P1A—C1A—C2A	−158.4 (5)	C34B—P1B—C1B—C2B	−160.4 (5)
C34A—P1A—C1A—C5A	25.4 (5)	C34B—P1B—C1B—C5B	21.6 (5)
C34A—P1A—C15A—Fe2A	167.2 (3)	C34B—P1B—C15B—Fe2B	168.2 (4)
C34A—P1A—C15A—C16A	72.8 (5)	C34B—P1B—C15B—C16B	71.6 (6)
C34A—P1A—C15A—C19A	−101.1 (5)	C34B—P1B—C15B—C19B	−97.5 (5)
C34A—C35A—C36A—C37A	0.4 (9)	C34B—C35B—C36B—C37B	−1.3 (10)
C35A—C34A—C39A—C38A	0.2 (8)	C35B—C34B—C39B—C38B	1.1 (9)
C35A—C36A—C37A—C38A	−0.1 (9)	C35B—C36B—C37B—C38B	1.8 (11)
C36A—C37A—C38A—C39A	−0.1 (10)	C36B—C37B—C38B—C39B	−0.8 (11)
C37A—C38A—C39A—C34A	0.1 (9)	C37B—C38B—C39B—C34B	−0.6 (10)
C39A—C34A—C35A—C36A	−0.5 (8)	C39B—C34B—C35B—C36B	−0.1 (9)

{(2S_p)-2-[(1*R*)-1-(Acetyloxy)ethyl]ferrocen-1-yl}{(2S_p)-2-[(1*R*)-1-hydroxyethyl]ferrocen-1-yl}phenyl-(*R*)-phosphane sulfide (8c)

Crystal data

$[Fe_2(C_5H_5)_2(C_{22}H_{23}O_3PS)]$
M_r = 640.31
Orthorhombic, $P2_12_12_1$
a = 7.8204 (11) Å
b = 17.835 (3) Å
c = 20.394 (2) Å
V = 2844.5 (7) Å^3
Z = 4
$F(000)$ = 1328
D_x = 1.495 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1636 reflections
θ = 2.3–17.7°
μ = 1.18 mm^{-1}
T = 130 K
Plate, clear orange
0.1 × 0.06 × 0.01 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: sealed xray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.568, T_{max} = 0.745
35430 measured reflections
5258 independent reflections
3417 reflections with $I > 2\sigma(I)$
R_{int} = 0.167
θ_{max} = 25.5°, θ_{min} = 2.3°
h = −9→9
k = −21→21
l = −20→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.093
S = 1.02
5258 reflections
356 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0262P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack x determined using 1051 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.00 (2)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups At 1.5 times of: All C(H,H,H) groups, All O(H) groups 2.a Ternary CH refined with riding coordinates: C11(H11), C25(H25) 2.b Aromatic/amide H refined with riding coordinates: C3(H3A), C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C9(H9), C10(H10), C17(H17), C18(H18), C19(H19), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24), C39(H39), C38(H38), C37(H37), C36(H36), C35(H35) 2.c Idealised Me refined as rotating group: C13(H13A,H13B,H13C), C14(H14A,H14B,H14C), C26(H26A,H26B,H26C) 2.d Idealised tetrahedral OH refined as rotating group: O3(H3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.49633 (16)	0.66812 (6)	0.63443 (5)	0.0260 (3)
Fe2	0.09126 (14)	0.49141 (7)	0.85171 (5)	0.0295 (3)
S1	−0.0032 (3)	0.68244 (11)	0.73939 (9)	0.0282 (5)
P1	0.2250 (3)	0.65243 (12)	0.76895 (9)	0.0201 (5)
O1	0.1576 (7)	0.4879 (3)	0.5949 (2)	0.0354 (15)
O2	−0.1257 (9)	0.4851 (4)	0.5812 (4)	0.076 (2)
O3	0.1577 (10)	0.7052 (4)	0.9575 (3)	0.064 (2)
H3	0.239200	0.718829	0.933439	0.096*
C1	0.3634 (9)	0.6151 (4)	0.7074 (3)	0.0175 (18)
C2	0.3235 (10)	0.5812 (4)	0.6444 (4)	0.0223 (19)
C3	0.4802 (11)	0.5554 (4)	0.6176 (3)	0.029 (2)
H3A	0.492286	0.531214	0.576413	0.034*
C4	0.6161 (11)	0.5711 (4)	0.6614 (4)	0.029 (2)
H4	0.733257	0.559028	0.655074	0.035*
C5	0.5444 (9)	0.6084 (4)	0.7166 (3)	0.024 (2)
H5	0.606541	0.626007	0.753536	0.029*
C6	0.4284 (16)	0.7782 (6)	0.6237 (7)	0.075 (4)
H6	0.332502	0.801953	0.643394	0.090*
C7	0.4345 (19)	0.7422 (8)	0.5627 (7)	0.085 (5)
H7	0.341397	0.737606	0.533030	0.102*
C8	0.597 (2)	0.7144 (6)	0.5525 (5)	0.065 (3)
H8	0.634698	0.687015	0.515338	0.077*
C9	0.6920 (13)	0.7334 (5)	0.6053 (5)	0.046 (3)
H9	0.809738	0.721973	0.610997	0.056*
C10	0.5926 (16)	0.7719 (5)	0.6495 (5)	0.050 (3)
H10	0.629610	0.790900	0.690615	0.060*
C11	0.1529 (11)	0.5671 (5)	0.6137 (4)	0.029 (2)
H11	0.061959	0.574419	0.647608	0.035*
C12	0.0085 (15)	0.4537 (5)	0.5805 (4)	0.047 (3)
C13	0.0325 (14)	0.3729 (5)	0.5656 (5)	0.072 (4)
H13A	0.132793	0.366649	0.537278	0.108*
H13B	−0.069137	0.353707	0.543079	0.108*
H13C	0.049797	0.345138	0.606494	0.108*
C14	0.1115 (12)	0.6151 (5)	0.5548 (4)	0.046 (3)
H14A	0.201853	0.609504	0.521892	0.068*
H14B	0.103807	0.667728	0.568276	0.068*
H14C	0.001983	0.599150	0.536085	0.068*
C15	0.2338 (10)	0.5832 (4)	0.8332 (3)	0.021 (2)
C16	0.1549 (11)	0.5889 (5)	0.8967 (4)	0.029 (2)
C17	0.2137 (11)	0.5271 (5)	0.9342 (4)	0.033 (2)
H17	0.183025	0.516780	0.978410	0.040*
C18	0.3254 (10)	0.4832 (5)	0.8954 (3)	0.027 (2)
H18	0.380377	0.438271	0.908827	0.033*
C19	0.3413 (9)	0.5175 (4)	0.8332 (4)	0.0236 (19)
H19	0.410138	0.500408	0.797835	0.028*

C20	−0.1633 (11)	0.4916 (6)	0.8299 (6)	0.060 (3)
H20	−0.237723	0.533607	0.832684	0.072*
C21	−0.0686 (13)	0.4712 (6)	0.7752 (5)	0.054 (3)
H21	−0.066901	0.496847	0.734343	0.064*
C22	0.0249 (14)	0.4057 (5)	0.7906 (5)	0.061 (3)
H22	0.099446	0.379034	0.762211	0.073*
C23	−0.0135 (13)	0.3878 (5)	0.8557 (6)	0.059 (3)
H23	0.032814	0.346702	0.879414	0.071*
C24	−0.1310 (12)	0.4400 (6)	0.8807 (5)	0.056 (3)
H24	−0.179235	0.440467	0.923453	0.068*
C25	0.0485 (11)	0.6538 (5)	0.9215 (4)	0.044 (3)
H25	−0.002628	0.680689	0.883175	0.053*
C26	−0.0922 (13)	0.6312 (6)	0.9678 (4)	0.060 (3)
H26A	−0.043240	0.603747	1.004978	0.090*
H26B	−0.174199	0.599062	0.944821	0.090*
H26C	−0.150811	0.676181	0.983920	0.090*
C34	0.3455 (10)	0.7300 (4)	0.8041 (3)	0.024 (2)
C39	0.3041 (11)	0.8034 (5)	0.7878 (4)	0.033 (2)
H39	0.209659	0.812782	0.759629	0.039*
C38	0.3979 (12)	0.8626 (5)	0.8117 (4)	0.039 (2)
H38	0.368464	0.912456	0.799876	0.047*
C37	0.5340 (12)	0.8496 (5)	0.8527 (4)	0.045 (3)
H37	0.600124	0.890575	0.868362	0.054*
C36	0.5758 (12)	0.7764 (5)	0.8717 (4)	0.046 (3)
H36	0.668270	0.767494	0.900850	0.056*
C35	0.4802 (11)	0.7171 (4)	0.8472 (3)	0.031 (2)
H35	0.507092	0.667211	0.859997	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0204 (6)	0.0320 (7)	0.0257 (6)	0.0000 (7)	0.0010 (6)	0.0092 (5)
Fe2	0.0249 (6)	0.0264 (7)	0.0372 (7)	−0.0019 (6)	−0.0037 (6)	0.0093 (6)
S1	0.0204 (10)	0.0325 (12)	0.0318 (11)	0.0038 (12)	−0.0019 (12)	0.0021 (9)
P1	0.0197 (12)	0.0214 (13)	0.0192 (11)	0.0011 (10)	−0.0014 (9)	0.0017 (10)
O1	0.022 (3)	0.041 (4)	0.044 (3)	−0.008 (3)	−0.007 (3)	−0.009 (3)
O2	0.031 (4)	0.074 (6)	0.123 (6)	−0.012 (4)	0.006 (4)	−0.060 (5)
O3	0.099 (7)	0.046 (5)	0.047 (4)	0.004 (4)	0.022 (4)	−0.014 (4)
C1	0.014 (4)	0.020 (5)	0.018 (4)	−0.002 (4)	−0.007 (3)	0.006 (3)
C2	0.024 (5)	0.031 (5)	0.011 (4)	0.001 (4)	0.000 (4)	0.002 (4)
C3	0.017 (5)	0.044 (5)	0.025 (4)	0.000 (5)	0.010 (4)	−0.001 (4)
C4	0.024 (5)	0.026 (5)	0.038 (5)	0.007 (4)	0.002 (4)	0.008 (4)
C5	0.025 (6)	0.027 (5)	0.019 (4)	−0.001 (4)	0.000 (4)	0.004 (4)
C6	0.050 (8)	0.056 (8)	0.119 (11)	0.026 (6)	0.041 (8)	0.062 (8)
C7	0.075 (10)	0.095 (11)	0.085 (10)	−0.049 (9)	−0.045 (9)	0.077 (9)
C8	0.093 (10)	0.060 (8)	0.041 (7)	−0.030 (8)	0.017 (8)	0.014 (5)
C9	0.034 (6)	0.042 (7)	0.063 (7)	−0.004 (5)	0.008 (6)	0.016 (5)
C10	0.078 (8)	0.026 (6)	0.046 (6)	−0.008 (6)	0.011 (7)	0.011 (5)

C11	0.029 (5)	0.033 (6)	0.024 (5)	0.000 (4)	0.000 (4)	−0.011 (4)
C12	0.026 (6)	0.066 (7)	0.050 (6)	0.008 (7)	−0.001 (6)	−0.022 (5)
C13	0.069 (9)	0.047 (7)	0.100 (8)	−0.016 (6)	−0.017 (7)	−0.013 (6)
C14	0.049 (7)	0.048 (6)	0.039 (5)	0.000 (6)	−0.027 (5)	−0.002 (5)
C15	0.021 (5)	0.026 (5)	0.018 (4)	−0.003 (4)	−0.004 (4)	0.005 (4)
C16	0.035 (6)	0.030 (6)	0.023 (5)	0.003 (4)	−0.002 (4)	0.001 (4)
C17	0.045 (6)	0.043 (6)	0.012 (4)	0.006 (5)	0.001 (4)	0.009 (4)
C18	0.027 (5)	0.029 (5)	0.026 (5)	0.003 (4)	−0.005 (4)	0.008 (4)
C19	0.019 (4)	0.024 (5)	0.027 (4)	0.002 (4)	−0.002 (3)	0.002 (4)
C20	0.030 (6)	0.045 (7)	0.104 (9)	−0.002 (6)	−0.016 (6)	0.030 (7)
C21	0.047 (7)	0.060 (8)	0.054 (6)	−0.027 (6)	−0.028 (6)	0.013 (6)
C22	0.052 (8)	0.040 (7)	0.090 (8)	−0.010 (6)	−0.031 (7)	−0.010 (6)
C23	0.038 (6)	0.039 (6)	0.101 (9)	−0.016 (6)	−0.039 (8)	0.022 (6)
C24	0.035 (6)	0.048 (7)	0.086 (8)	−0.011 (6)	0.004 (6)	0.034 (6)
C25	0.055 (8)	0.050 (6)	0.028 (5)	0.015 (5)	0.011 (5)	0.004 (5)
C26	0.059 (7)	0.066 (8)	0.056 (7)	0.014 (6)	0.008 (6)	−0.002 (5)
C34	0.026 (5)	0.025 (5)	0.022 (4)	0.001 (4)	−0.006 (4)	−0.005 (4)
C39	0.030 (5)	0.028 (6)	0.040 (5)	−0.002 (4)	−0.002 (4)	0.002 (4)
C38	0.041 (6)	0.021 (5)	0.055 (6)	0.001 (5)	−0.009 (5)	0.002 (4)
C37	0.052 (7)	0.030 (5)	0.053 (6)	−0.005 (5)	−0.005 (5)	−0.015 (5)
C36	0.056 (6)	0.039 (6)	0.045 (5)	−0.003 (5)	−0.017 (5)	−0.004 (5)
C35	0.038 (5)	0.020 (4)	0.036 (5)	−0.007 (4)	−0.007 (5)	−0.002 (4)

Geometric parameters (Å, º)

Fe1—C1	2.048 (7)	C9—C10	1.373 (12)
Fe1—C2	2.067 (7)	C10—H10	0.9500
Fe1—C3	2.043 (8)	C11—H11	1.0000
Fe1—C4	2.043 (8)	C11—C14	1.509 (10)
Fe1—C5	2.021 (7)	C12—C13	1.485 (12)
Fe1—C6	2.046 (10)	C13—H13A	0.9800
Fe1—C7	2.029 (10)	C13—H13B	0.9800
Fe1—C8	2.022 (9)	C13—H13C	0.9800
Fe1—C9	2.013 (9)	C14—H14A	0.9800
Fe1—C10	2.021 (9)	C14—H14B	0.9800
Fe2—C15	2.016 (8)	C14—H14C	0.9800
Fe2—C16	2.028 (8)	C15—C16	1.438 (10)
Fe2—C17	2.038 (8)	C15—C19	1.442 (10)
Fe2—C18	2.041 (8)	C16—C17	1.419 (10)
Fe2—C19	2.045 (7)	C16—C25	1.512 (11)
Fe2—C20	2.039 (9)	C17—H17	0.9500
Fe2—C21	2.032 (8)	C17—C18	1.415 (10)
Fe2—C22	2.039 (9)	C18—H18	0.9500
Fe2—C23	2.022 (9)	C18—C19	1.414 (9)
Fe2—C24	2.052 (9)	C19—H19	0.9500
S1—P1	1.958 (3)	C20—H20	0.9500
P1—C1	1.786 (8)	C20—C21	1.389 (13)
P1—C15	1.802 (7)	C20—C24	1.408 (12)

P1—C34	1.820 (8)	C21—H21	0.9500
O1—C11	1.465 (9)	C21—C22	1.413 (12)
O1—C12	1.348 (11)	C22—H22	0.9500
O2—C12	1.190 (11)	C22—C23	1.399 (13)
O3—H3	0.8400	C23—H23	0.9500
O3—C25	1.453 (10)	C23—C24	1.404 (13)
C1—C2	1.456 (10)	C24—H24	0.9500
C1—C5	1.433 (10)	C25—H25	1.0000
C2—C3	1.417 (10)	C25—C26	1.506 (11)
C2—C11	1.495 (10)	C26—H26A	0.9800
C3—H3A	0.9500	C26—H26B	0.9800
C3—C4	1.416 (10)	C26—H26C	0.9800
C4—H4	0.9500	C34—C39	1.389 (10)
C4—C5	1.422 (10)	C34—C35	1.391 (10)
C5—H5	0.9500	C39—H39	0.9500
C6—H6	0.9500	C39—C38	1.376 (11)
C6—C7	1.402 (15)	C38—H38	0.9500
C6—C10	1.392 (14)	C38—C37	1.374 (11)
C7—H7	0.9500	C37—H37	0.9500
C7—C8	1.378 (16)	C37—C36	1.400 (11)
C8—H8	0.9500	C36—H36	0.9500
C8—C9	1.353 (13)	C36—C35	1.389 (10)
C9—H9	0.9500	C35—H35	0.9500

C1—Fe1—C2	41.4 (3)	C6—C7—Fe1	70.5 (6)
C3—Fe1—C1	68.6 (3)	C6—C7—H7	125.4
C3—Fe1—C2	40.3 (3)	C8—C7—Fe1	69.8 (7)
C3—Fe1—C4	40.5 (3)	C8—C7—C6	109.2 (11)
C3—Fe1—C6	155.6 (5)	C8—C7—H7	125.4
C4—Fe1—C1	69.2 (3)	Fe1—C8—H8	124.8
C4—Fe1—C2	68.8 (3)	C7—C8—Fe1	70.4 (6)
C4—Fe1—C6	163.9 (5)	C7—C8—H8	126.3
C5—Fe1—C1	41.2 (3)	C9—C8—Fe1	70.1 (6)
C5—Fe1—C2	69.2 (3)	C9—C8—C7	107.3 (11)
C5—Fe1—C3	68.4 (3)	C9—C8—H8	126.3
C5—Fe1—C4	41.0 (3)	Fe1—C9—H9	125.2
C5—Fe1—C6	130.0 (5)	C8—C9—Fe1	70.8 (6)
C5—Fe1—C7	170.1 (6)	C8—C9—H9	125.2
C5—Fe1—C8	145.9 (5)	C8—C9—C10	109.6 (10)
C5—Fe1—C10	106.7 (4)	C10—C9—Fe1	70.4 (6)
C6—Fe1—C1	112.9 (4)	C10—C9—H9	125.2
C6—Fe1—C2	124.1 (4)	Fe1—C10—H10	125.1
C7—Fe1—C1	134.7 (5)	C6—C10—Fe1	70.9 (6)
C7—Fe1—C2	113.8 (4)	C6—C10—H10	125.8
C7—Fe1—C3	120.3 (5)	C9—C10—Fe1	69.8 (5)
C7—Fe1—C4	148.7 (6)	C9—C10—C6	108.4 (10)
C7—Fe1—C6	40.2 (4)	C9—C10—H10	125.8
C8—Fe1—C1	170.6 (5)	O1—C11—C2	104.4 (6)

C8—Fe1—C2	129.9 (4)	O1—C11—H11	108.9
C8—Fe1—C3	106.7 (4)	O1—C11—C14	110.1 (6)
C8—Fe1—C4	113.0 (5)	C2—C11—H11	108.9
C8—Fe1—C6	67.7 (5)	C2—C11—C14	115.4 (7)
C8—Fe1—C7	39.8 (4)	C14—C11—H11	108.9
C9—Fe1—C1	150.2 (4)	O1—C12—C13	112.0 (9)
C9—Fe1—C2	163.8 (4)	O2—C12—O1	123.2 (8)
C9—Fe1—C3	124.5 (4)	O2—C12—C13	124.8 (10)
C9—Fe1—C4	102.8 (4)	C12—C13—H13A	109.5
C9—Fe1—C5	114.1 (4)	C12—C13—H13B	109.5
C9—Fe1—C6	67.1 (4)	C12—C13—H13C	109.5
C9—Fe1—C7	65.9 (4)	H13A—C13—H13B	109.5
C9—Fe1—C8	39.2 (4)	H13A—C13—H13C	109.5
C9—Fe1—C10	39.8 (4)	H13B—C13—H13C	109.5
C10—Fe1—C1	120.1 (4)	C11—C14—H14A	109.5
C10—Fe1—C2	156.3 (4)	C11—C14—H14B	109.5
C10—Fe1—C3	161.7 (4)	C11—C14—H14C	109.5
C10—Fe1—C4	124.3 (4)	H14A—C14—H14B	109.5
C10—Fe1—C6	40.0 (4)	H14A—C14—H14C	109.5
C10—Fe1—C7	66.6 (4)	H14B—C14—H14C	109.5
C10—Fe1—C8	66.9 (4)	P1—C15—Fe2	132.2 (4)
C15—Fe2—C16	41.6 (3)	C16—C15—Fe2	69.6 (4)
C15—Fe2—C17	69.0 (3)	C16—C15—P1	126.2 (6)
C15—Fe2—C18	69.1 (3)	C16—C15—C19	107.9 (6)
C15—Fe2—C19	41.6 (3)	C19—C15—Fe2	70.3 (4)
C15—Fe2—C20	119.8 (4)	C19—C15—P1	125.3 (6)
C15—Fe2—C21	109.9 (3)	C15—C16—Fe2	68.8 (4)
C15—Fe2—C22	129.4 (4)	C15—C16—C25	126.2 (7)
C15—Fe2—C23	166.7 (4)	C17—C16—Fe2	70.0 (5)
C15—Fe2—C24	152.2 (4)	C17—C16—C15	107.0 (7)
C16—Fe2—C17	40.8 (3)	C17—C16—C25	126.3 (7)
C16—Fe2—C18	69.1 (3)	C25—C16—Fe2	132.2 (6)
C16—Fe2—C19	69.7 (3)	Fe2—C17—H17	127.2
C16—Fe2—C20	109.7 (4)	C16—C17—Fe2	69.2 (4)
C16—Fe2—C21	130.6 (4)	C16—C17—H17	125.5
C16—Fe2—C22	169.0 (4)	C18—C17—Fe2	69.8 (4)
C16—Fe2—C24	117.4 (4)	C18—C17—C16	109.1 (7)
C17—Fe2—C18	40.6 (3)	C18—C17—H17	125.5
C17—Fe2—C19	68.4 (3)	Fe2—C18—H18	126.3
C17—Fe2—C20	129.6 (4)	C17—C18—Fe2	69.6 (5)
C17—Fe2—C22	149.1 (4)	C17—C18—H18	125.7
C17—Fe2—C24	107.4 (4)	C19—C18—Fe2	69.9 (4)
C18—Fe2—C19	40.5 (3)	C19—C18—C17	108.5 (7)
C18—Fe2—C24	127.0 (3)	C19—C18—H18	125.7
C19—Fe2—C24	164.7 (4)	Fe2—C19—H19	127.5
C20—Fe2—C18	166.1 (4)	C15—C19—Fe2	68.1 (4)
C20—Fe2—C19	153.2 (3)	C15—C19—H19	126.3
C20—Fe2—C24	40.3 (3)	C18—C19—Fe2	69.6 (4)

C21—Fe2—C17	168.2 (4)	C18—C19—C15	107.4 (7)
C21—Fe2—C18	151.0 (4)	C18—C19—H19	126.3
C21—Fe2—C19	119.1 (4)	Fe2—C20—H20	125.9
C21—Fe2—C20	39.9 (4)	C21—C20—Fe2	69.8 (5)
C21—Fe2—C22	40.6 (4)	C21—C20—H20	125.5
C21—Fe2—C24	67.7 (4)	C21—C20—C24	108.9 (9)
C22—Fe2—C18	116.2 (4)	C24—C20—Fe2	70.3 (5)
C22—Fe2—C19	107.5 (4)	C24—C20—H20	125.5
C22—Fe2—C20	67.7 (5)	Fe2—C21—H21	125.4
C22—Fe2—C24	68.0 (4)	C20—C21—Fe2	70.3 (5)
C23—Fe2—C16	149.8 (4)	C20—C21—H21	125.9
C23—Fe2—C17	116.2 (4)	C20—C21—C22	108.3 (9)
C23—Fe2—C18	106.3 (4)	C22—C21—Fe2	69.9 (5)
C23—Fe2—C19	127.1 (4)	C22—C21—H21	125.9
C23—Fe2—C20	67.4 (4)	Fe2—C22—H22	126.3
C23—Fe2—C21	67.7 (4)	C21—C22—Fe2	69.4 (5)
C23—Fe2—C22	40.3 (4)	C21—C22—H22	126.6
C23—Fe2—C24	40.3 (4)	C23—C22—Fe2	69.2 (5)
C1—P1—S1	116.0 (2)	C23—C22—C21	106.8 (10)
C1—P1—C15	103.4 (3)	C23—C22—H22	126.6
C1—P1—C34	104.3 (4)	Fe2—C23—H23	124.9
C15—P1—S1	116.5 (3)	C22—C23—Fe2	70.5 (5)
C15—P1—C34	102.4 (3)	C22—C23—H23	125.3
C34—P1—S1	112.7 (3)	C22—C23—C24	109.5 (9)
C12—O1—C11	118.1 (7)	C24—C23—Fe2	71.0 (5)
C25—O3—H3	109.5	C24—C23—H23	125.3
P1—C1—Fe1	130.2 (4)	Fe2—C24—H24	126.7
C2—C1—Fe1	70.0 (4)	C20—C24—Fe2	69.4 (5)
C2—C1—P1	130.2 (6)	C20—C24—H24	126.8
C5—C1—Fe1	68.4 (4)	C23—C24—Fe2	68.7 (5)
C5—C1—P1	122.6 (6)	C23—C24—C20	106.5 (10)
C5—C1—C2	107.0 (7)	C23—C24—H24	126.8
C1—C2—Fe1	68.6 (4)	O3—C25—C16	109.2 (7)
C1—C2—C11	129.1 (7)	O3—C25—H25	109.1
C3—C2—Fe1	68.9 (4)	O3—C25—C26	106.3 (7)
C3—C2—C1	106.8 (6)	C16—C25—H25	109.1
C3—C2—C11	123.9 (7)	C26—C25—C16	114.1 (8)
C11—C2—Fe1	131.9 (5)	C26—C25—H25	109.1
Fe1—C3—H3A	126.1	C25—C26—H26A	109.5
C2—C3—Fe1	70.8 (4)	C25—C26—H26B	109.5
C2—C3—H3A	125.0	C25—C26—H26C	109.5
C4—C3—Fe1	69.7 (4)	H26A—C26—H26B	109.5
C4—C3—C2	110.1 (7)	H26A—C26—H26C	109.5
C4—C3—H3A	125.0	H26B—C26—H26C	109.5
Fe1—C4—H4	126.7	C39—C34—P1	120.0 (6)
C3—C4—Fe1	69.7 (4)	C39—C34—C35	119.0 (7)
C3—C4—H4	126.4	C35—C34—P1	121.0 (6)
C3—C4—C5	107.2 (7)	C34—C39—H39	119.5

C5—C4—Fe1	68.7 (4)	C38—C39—C34	120.9 (8)
C5—C4—H4	126.4	C38—C39—H39	119.5
Fe1—C5—H5	125.3	C39—C38—H38	120.0
C1—C5—Fe1	70.4 (4)	C37—C38—C39	120.0 (8)
C1—C5—H5	125.5	C37—C38—H38	120.0
C4—C5—Fe1	70.3 (4)	C38—C37—H37	119.8
C4—C5—C1	109.0 (7)	C38—C37—C36	120.4 (8)
C4—C5—H5	125.5	C36—C37—H37	119.8
Fe1—C6—H6	126.0	C37—C36—H36	120.5
C7—C6—Fe1	69.3 (7)	C35—C36—C37	119.1 (8)
C7—C6—H6	127.3	C35—C36—H36	120.5
C10—C6—Fe1	69.0 (6)	C34—C35—H35	119.7
C10—C6—H6	127.3	C36—C35—C34	120.6 (8)
C10—C6—C7	105.5 (11)	C36—C35—H35	119.7
Fe1—C7—H7	125.9		

Fe1—C1—C2—C3	58.5 (5)	C5—C1—C2—Fe1	−58.6 (5)
Fe1—C1—C2—C11	−127.3 (8)	C5—C1—C2—C3	−0.1 (8)
Fe1—C1—C5—C4	−60.0 (5)	C5—C1—C2—C11	174.1 (7)
Fe1—C2—C3—C4	58.8 (5)	C6—C7—C8—Fe1	59.7 (7)
Fe1—C2—C11—O1	135.7 (6)	C6—C7—C8—C9	−1.0 (13)
Fe1—C2—C11—C14	14.7 (11)	C7—C6—C10—Fe1	−60.0 (7)
Fe1—C3—C4—C5	58.7 (5)	C7—C6—C10—C9	−0.1 (11)
Fe1—C4—C5—C1	60.0 (5)	C7—C8—C9—Fe1	60.9 (8)
Fe1—C6—C7—C8	−59.3 (8)	C7—C8—C9—C10	0.9 (12)
Fe1—C6—C10—C9	60.0 (6)	C8—C9—C10—Fe1	60.2 (7)
Fe1—C7—C8—C9	−60.6 (7)	C8—C9—C10—C6	−0.5 (11)
Fe1—C8—C9—C10	−60.0 (7)	C10—C6—C7—Fe1	59.9 (7)
Fe1—C9—C10—C6	−60.7 (7)	C10—C6—C7—C8	0.6 (12)
Fe2—C15—C16—C17	59.8 (6)	C11—O1—C12—O2	1.4 (13)
Fe2—C15—C16—C25	−127.5 (8)	C11—O1—C12—C13	−177.3 (7)
Fe2—C15—C19—C18	−58.7 (5)	C11—C2—C3—Fe1	127.1 (7)
Fe2—C16—C17—C18	58.5 (6)	C11—C2—C3—C4	−174.1 (7)
Fe2—C16—C25—O3	172.7 (6)	C12—O1—C11—C2	164.2 (7)
Fe2—C16—C25—C26	53.9 (10)	C12—O1—C11—C14	−71.3 (9)
Fe2—C17—C18—C19	59.3 (5)	C15—P1—C1—Fe1	−155.6 (5)
Fe2—C18—C19—C15	57.8 (5)	C15—P1—C1—C2	106.9 (7)
Fe2—C20—C21—C22	59.9 (6)	C15—P1—C1—C5	−67.5 (7)
Fe2—C20—C24—C23	−59.0 (6)	C15—P1—C34—C39	−148.6 (6)
Fe2—C21—C22—C23	59.4 (7)	C15—P1—C34—C35	31.8 (7)
Fe2—C22—C23—C24	60.5 (7)	C15—C16—C17—Fe2	−59.0 (5)
Fe2—C23—C24—C20	59.4 (6)	C15—C16—C17—C18	−0.5 (9)
S1—P1—C1—Fe1	75.6 (5)	C15—C16—C25—O3	−94.0 (9)
S1—P1—C1—C2	−21.8 (8)	C15—C16—C25—C26	147.3 (8)
S1—P1—C1—C5	163.8 (5)	C16—C15—C19—Fe2	59.7 (5)
S1—P1—C15—Fe2	37.9 (6)	C16—C15—C19—C18	1.0 (8)
S1—P1—C15—C16	−56.7 (7)	C16—C17—C18—Fe2	−58.1 (6)
S1—P1—C15—C19	132.7 (6)	C16—C17—C18—C19	1.1 (9)

S1—P1—C34—C39	−22.8 (7)	C17—C16—C25—O3	77.3 (10)
S1—P1—C34—C35	157.7 (5)	C17—C16—C25—C26	−41.5 (12)
P1—C1—C2—Fe1	126.3 (6)	C17—C18—C19—Fe2	−59.1 (6)
P1—C1—C2—C3	−175.2 (6)	C17—C18—C19—C15	−1.3 (8)
P1—C1—C2—C11	−1.0 (12)	C19—C15—C16—Fe2	−60.1 (5)
P1—C1—C5—Fe1	−124.8 (6)	C19—C15—C16—C17	−0.3 (9)
P1—C1—C5—C4	175.2 (5)	C19—C15—C16—C25	172.4 (8)
P1—C15—C16—Fe2	128.0 (6)	C20—C21—C22—Fe2	−60.2 (7)
P1—C15—C16—C17	−172.2 (6)	C20—C21—C22—C23	−0.8 (11)
P1—C15—C16—C25	0.5 (12)	C21—C20—C24—Fe2	59.3 (7)
P1—C15—C19—Fe2	−128.3 (6)	C21—C20—C24—C23	0.3 (11)
P1—C15—C19—C18	173.0 (6)	C21—C22—C23—Fe2	−59.5 (6)
P1—C34—C39—C38	−177.3 (6)	C21—C22—C23—C24	1.0 (11)
P1—C34—C35—C36	177.3 (6)	C22—C23—C24—Fe2	−60.2 (7)
C1—P1—C15—Fe2	−90.6 (6)	C22—C23—C24—C20	−0.8 (11)
C1—P1—C15—C16	174.8 (7)	C24—C20—C21—Fe2	−59.6 (7)
C1—P1—C15—C19	4.2 (7)	C24—C20—C21—C22	0.3 (11)
C1—P1—C34—C39	103.8 (7)	C25—C16—C17—Fe2	128.3 (9)
C1—P1—C34—C35	−75.7 (6)	C25—C16—C17—C18	−173.2 (8)
C1—C2—C3—Fe1	−58.3 (5)	C34—P1—C1—Fe1	−48.9 (6)
C1—C2—C3—C4	0.5 (8)	C34—P1—C1—C2	−146.3 (7)
C1—C2—C11—O1	−128.7 (8)	C34—P1—C1—C5	39.3 (7)
C1—C2—C11—C14	110.3 (9)	C34—P1—C15—Fe2	161.2 (5)
C2—C1—C5—Fe1	59.6 (5)	C34—P1—C15—C16	66.6 (7)
C2—C1—C5—C4	−0.4 (8)	C34—P1—C15—C19	−103.9 (7)
C2—C3—C4—Fe1	−59.4 (6)	C34—C39—C38—C37	−0.4 (13)
C2—C3—C4—C5	−0.7 (9)	C39—C34—C35—C36	−2.2 (11)
C3—C2—C11—O1	44.6 (9)	C39—C38—C37—C36	−1.5 (13)
C3—C2—C11—C14	−76.4 (10)	C38—C37—C36—C35	1.5 (13)
C3—C4—C5—Fe1	−59.3 (5)	C37—C36—C35—C34	0.4 (12)
C3—C4—C5—C1	0.7 (9)	C35—C34—C39—C38	2.2 (12)

{(2*S*$_p$)-2-[(1*R*)-1-Benzylamino)ethyl]ferrocen-1-yl}[(2*S*$_p$)-2-ethenylferrocen-1-yl]phenyl-(*S*)-phosphane sulfide (9b)

Crystal data

$[Fe_2(C_5H_5)_2(C_{27}H_{26}NPS)]$
M_r = 669.40
Orthorhombic, $P2_12_12_1$
a = 12.3578 (9) Å
b = 14.4342 (10) Å
c = 17.4796 (15) Å
V = 3117.9 (4) Å^3
Z = 4
F(000) = 1392
D_x = 1.426 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9501 reflections
θ = 2.2–26.6°
μ = 1.08 mm^{-1}
T = 130 K
Block, clear orange
0.22 × 0.11 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed xray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.486, T_{max} = 0.746
38997 measured reflections
9160 independent reflections
7062 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 30.1°, θ_{min} = 2.2°
h = −17→16
k = −20→17
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.091
S = 0.98
9160 reflections
384 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack x determined using 2549 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.016 (10)

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups At 1.5 times of: All C(H,H,H) groups 2.a Ternary CH refined with riding coordinates: C25(H25) 2.b Secondary CH2 refined with riding coordinates: C26(H26A,H26B) 2.c Aromatic/amide H refined with riding coordinates: C3(H3), C4(H4), C5(H5), C6(H6), C7(H7), C8(H8), C9(H9), C10(H10), C11(H11), C17(H17), C18(H18), C19(H19), C20(H20), C21(H21), C22(H22), C23(H23), C24(H24), C28(H28), C29(H29), C30(H30), C31(H31), C32(H32), C35(H35), C36(H36), C37(H37), C38(H38), C39(H39) 2.d X=CH2 refined with riding coordinates: C12(H12A,H12B) 2.e Idealised Me refined as rotating group: C33(H33A,H33B,H33C)

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

	x	y	z	U_{iso}*/U_{eq}
Fe1	0.51417 (3)	0.51824 (3)	0.44598 (3)	0.02729 (12)
Fe2	0.49276 (3)	0.50436 (3)	0.09718 (3)	0.03059 (12)
S1	0.48101 (8)	0.71100 (6)	0.26305 (5)	0.0377 (2)
P1	0.41368 (7)	0.58912 (6)	0.27301 (5)	0.02534 (18)
N1	0.1929 (2)	0.6660 (2)	0.13393 (18)	0.0313 (7)
H1	0.184 (3)	0.638 (3)	0.177 (2)	0.060 (14)*
C1	0.4824 (2)	0.5067 (2)	0.33292 (17)	0.0258 (6)
C2	0.5979 (2)	0.4958 (2)	0.34693 (18)	0.0289 (7)
C3	0.6093 (3)	0.4193 (2)	0.3971 (2)	0.0336 (8)
H3	0.676050	0.396826	0.416752	0.040*
C4	0.5060 (3)	0.3813 (2)	0.41360 (18)	0.0340 (8)
H4	0.491864	0.329266	0.445371	0.041*
C5	0.4278 (3)	0.4347 (2)	0.37428 (19)	0.0313 (8)

H5	0.351880	0.424507	0.375110	0.038*
C6	0.5020 (3)	0.6536 (2)	0.4784 (2)	0.0362 (8)
H6	0.495646	0.705091	0.444826	0.043*
C7	0.6001 (3)	0.6139 (3)	0.5061 (2)	0.0433 (10)
H7	0.671095	0.634692	0.494224	0.052*
C8	0.5741 (3)	0.5386 (3)	0.5541 (2)	0.0461 (10)
H8	0.624183	0.499956	0.580145	0.055*
C9	0.4597 (3)	0.5308 (3)	0.5564 (2)	0.0400 (9)
H9	0.419534	0.485660	0.584004	0.048*
C10	0.4162 (3)	0.6020 (3)	0.5104 (2)	0.0338 (8)
H10	0.341391	0.613355	0.502286	0.041*
C11	0.6860 (3)	0.5532 (3)	0.3191 (2)	0.0372 (9)
H11	0.669330	0.615155	0.304948	0.045*
C12	0.7875 (3)	0.5258 (3)	0.3120 (2)	0.0468 (10)
H12A	0.807253	0.464396	0.325579	0.056*
H12B	0.840713	0.567579	0.293300	0.056*
C15	0.3901 (2)	0.5270 (2)	0.18474 (18)	0.0243 (7)
C16	0.3439 (2)	0.5629 (2)	0.11501 (19)	0.0258 (7)
C17	0.3356 (2)	0.4871 (3)	0.0635 (2)	0.0311 (8)
H17	0.308584	0.490242	0.012721	0.037*
C18	0.3742 (3)	0.4056 (3)	0.1005 (2)	0.0334 (8)
H18	0.377109	0.345339	0.078782	0.040*
C19	0.4076 (2)	0.4301 (2)	0.1753 (2)	0.0284 (7)
H19	0.436519	0.389158	0.212655	0.034*
C20	0.6375 (3)	0.5637 (3)	0.1238 (2)	0.0486 (11)
H20	0.654219	0.596179	0.169639	0.058*
C21	0.5948 (3)	0.6037 (3)	0.0558 (2)	0.0473 (10)
H21	0.577820	0.667188	0.048183	0.057*
C22	0.5822 (3)	0.5320 (3)	0.0016 (2)	0.0481 (11)
H22	0.555074	0.538751	−0.048898	0.058*
C23	0.6172 (3)	0.4478 (3)	0.0359 (3)	0.0511 (12)
H23	0.618086	0.388488	0.012367	0.061*
C24	0.6507 (3)	0.4688 (4)	0.1119 (3)	0.0560 (12)
H24	0.677411	0.425565	0.148199	0.067*
C25	0.3034 (2)	0.6599 (2)	0.10146 (19)	0.0285 (7)
H25	0.351659	0.704876	0.128471	0.034*
C26	0.1612 (3)	0.7610 (3)	0.1533 (2)	0.0360 (9)
H26A	0.166909	0.800523	0.107220	0.043*
H26B	0.211259	0.785864	0.192468	0.043*
C27	0.0461 (3)	0.7647 (2)	0.1837 (2)	0.0310 (8)
C28	0.0208 (3)	0.8118 (3)	0.2500 (2)	0.0403 (8)
H28	0.076341	0.842763	0.277464	0.048*
C29	−0.0843 (4)	0.8144 (3)	0.2769 (2)	0.0494 (11)
H29	−0.100011	0.845362	0.323587	0.059*
C30	−0.1662 (3)	0.7725 (3)	0.2365 (2)	0.0455 (10)
H30	−0.238792	0.775936	0.254158	0.055*
C31	−0.1420 (3)	0.7255 (3)	0.1700 (2)	0.0439 (10)
H31	−0.198078	0.696254	0.141809	0.053*

C32	−0.0363 (3)	0.7208 (3)	0.1443 (2)	0.0371 (8)
H32	−0.020110	0.686947	0.099091	0.045*
C33	0.2996 (3)	0.6840 (3)	0.0164 (2)	0.0393 (9)
H33A	0.246891	0.643902	−0.009349	0.059*
H33B	0.371270	0.674540	−0.006238	0.059*
H33C	0.278049	0.748884	0.010187	0.059*
C34	0.2781 (3)	0.5969 (2)	0.31390 (19)	0.0282 (7)
C35	0.2483 (3)	0.6744 (3)	0.3560 (2)	0.0355 (8)
H35	0.299204	0.722567	0.364829	0.043*
C36	0.1443 (3)	0.6813 (3)	0.3852 (2)	0.0447 (10)
H36	0.124415	0.733674	0.414952	0.054*
C37	0.0706 (3)	0.6131 (3)	0.3711 (2)	0.0474 (10)
H37	−0.001096	0.619178	0.390135	0.057*
C38	0.0984 (3)	0.5360 (3)	0.3299 (2)	0.0416 (9)
H38	0.046658	0.488446	0.321133	0.050*
C39	0.2026 (3)	0.5277 (3)	0.3009 (2)	0.0321 (8)
H39	0.222188	0.474427	0.272187	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0245 (2)	0.0255 (2)	0.0319 (2)	0.0007 (2)	−0.00393 (19)	−0.00231 (19)
Fe2	0.0203 (2)	0.0359 (3)	0.0356 (2)	0.0005 (2)	0.00347 (18)	−0.0043 (2)
S1	0.0400 (5)	0.0212 (4)	0.0519 (5)	−0.0088 (4)	−0.0131 (4)	0.0047 (4)
P1	0.0242 (4)	0.0192 (4)	0.0326 (4)	−0.0014 (3)	−0.0036 (3)	−0.0008 (4)
N1	0.0276 (14)	0.0259 (17)	0.0403 (18)	0.0052 (13)	0.0000 (13)	0.0024 (14)
C1	0.0272 (14)	0.0196 (15)	0.0305 (15)	−0.0003 (15)	−0.0023 (12)	−0.0002 (12)
C2	0.0272 (14)	0.0250 (18)	0.0343 (17)	0.0025 (15)	0.0000 (13)	0.0010 (14)
C3	0.0353 (18)	0.0278 (19)	0.0376 (19)	0.0075 (16)	0.0001 (15)	0.0034 (16)
C4	0.047 (2)	0.0213 (16)	0.0339 (17)	0.0035 (17)	−0.0012 (17)	0.0012 (13)
C5	0.0333 (18)	0.0286 (19)	0.0320 (18)	−0.0049 (15)	−0.0033 (14)	−0.0030 (15)
C6	0.0340 (19)	0.0281 (18)	0.0464 (19)	0.0004 (17)	−0.0032 (17)	−0.0108 (15)
C7	0.0292 (18)	0.043 (2)	0.058 (3)	−0.0043 (19)	−0.0082 (17)	−0.016 (2)
C8	0.047 (2)	0.053 (3)	0.039 (2)	0.012 (2)	−0.0177 (18)	−0.013 (2)
C9	0.043 (2)	0.044 (2)	0.0329 (18)	0.0008 (18)	−0.0030 (16)	−0.0030 (18)
C10	0.0275 (16)	0.036 (2)	0.0383 (19)	0.0049 (17)	−0.0012 (15)	−0.0118 (16)
C11	0.0309 (18)	0.040 (2)	0.040 (2)	0.0012 (17)	−0.0055 (16)	0.0067 (17)
C12	0.0333 (18)	0.051 (3)	0.057 (2)	0.0004 (19)	0.0001 (17)	0.015 (2)
C15	0.0158 (13)	0.0224 (17)	0.0347 (17)	−0.0013 (13)	0.0016 (12)	−0.0009 (14)
C16	0.0193 (14)	0.0256 (18)	0.0325 (18)	−0.0012 (13)	0.0009 (13)	−0.0015 (15)
C17	0.0201 (13)	0.038 (2)	0.0350 (18)	−0.0026 (15)	−0.0005 (12)	−0.0083 (17)
C18	0.0253 (15)	0.031 (2)	0.044 (2)	−0.0024 (15)	0.0028 (15)	−0.0128 (17)
C19	0.0230 (15)	0.0226 (18)	0.0396 (19)	0.0046 (14)	0.0010 (14)	−0.0018 (14)
C20	0.0262 (19)	0.070 (3)	0.049 (3)	−0.016 (2)	0.0054 (17)	−0.010 (2)
C21	0.0307 (19)	0.055 (3)	0.056 (2)	−0.0146 (19)	0.0130 (19)	−0.005 (2)
C22	0.0316 (18)	0.070 (3)	0.042 (2)	−0.005 (2)	0.0108 (16)	−0.002 (2)
C23	0.0279 (18)	0.065 (3)	0.061 (3)	0.008 (2)	0.0154 (18)	−0.016 (2)
C24	0.0203 (16)	0.087 (4)	0.061 (3)	0.011 (2)	0.0045 (17)	0.007 (3)

C25	0.0257 (15)	0.0284 (18)	0.0313 (17)	0.0000 (14)	−0.0020 (14)	0.0015 (14)
C26	0.0325 (18)	0.029 (2)	0.047 (2)	0.0037 (16)	−0.0019 (16)	0.0004 (17)
C27	0.0322 (17)	0.0251 (18)	0.0358 (18)	0.0075 (15)	−0.0035 (15)	0.0037 (15)
C28	0.048 (2)	0.0313 (19)	0.0417 (19)	0.0061 (19)	−0.0051 (18)	−0.0029 (15)
C29	0.068 (3)	0.041 (2)	0.039 (2)	0.015 (2)	0.013 (2)	0.0002 (19)
C30	0.043 (2)	0.036 (2)	0.057 (3)	0.0111 (19)	0.016 (2)	0.010 (2)
C31	0.036 (2)	0.043 (3)	0.053 (3)	−0.0037 (18)	0.0004 (18)	0.005 (2)
C32	0.0368 (18)	0.038 (2)	0.0362 (18)	0.0001 (17)	0.0009 (15)	0.0016 (16)
C33	0.044 (2)	0.040 (2)	0.034 (2)	0.0032 (19)	−0.0003 (17)	0.0050 (17)
C34	0.0274 (16)	0.0282 (18)	0.0290 (16)	0.0091 (15)	−0.0038 (13)	−0.0037 (14)
C35	0.0398 (19)	0.0301 (19)	0.0366 (19)	0.0072 (17)	−0.0090 (16)	−0.0061 (15)
C36	0.050 (2)	0.041 (2)	0.042 (2)	0.024 (2)	0.0029 (18)	−0.0110 (18)
C37	0.036 (2)	0.059 (3)	0.047 (2)	0.016 (2)	0.0116 (18)	−0.001 (2)
C38	0.0312 (18)	0.049 (3)	0.045 (2)	0.0029 (19)	0.0069 (16)	0.0023 (18)
C39	0.0302 (16)	0.029 (2)	0.0368 (19)	0.0034 (16)	0.0035 (14)	−0.0016 (15)

Geometric parameters (Å, º)

Fe1—C1	2.022 (3)	C15—C16	1.442 (5)
Fe1—C2	2.043 (3)	C15—C19	1.425 (4)
Fe1—C3	2.038 (3)	C16—C17	1.420 (5)
Fe1—C4	2.059 (3)	C16—C25	1.506 (5)
Fe1—C5	2.041 (3)	C17—H17	0.9500
Fe1—C6	2.040 (3)	C17—C18	1.425 (5)
Fe1—C7	2.034 (4)	C18—H18	0.9500
Fe1—C8	2.050 (4)	C18—C19	1.416 (5)
Fe1—C9	2.052 (4)	C19—H19	0.9500
Fe1—C10	2.048 (3)	C20—H20	0.9500
Fe2—C15	2.015 (3)	C20—C21	1.423 (6)
Fe2—C16	2.048 (3)	C20—C24	1.396 (6)
Fe2—C17	2.045 (3)	C21—H21	0.9500
Fe2—C18	2.045 (3)	C21—C22	1.411 (6)
Fe2—C19	2.031 (3)	C22—H22	0.9500
Fe2—C20	2.038 (4)	C22—C23	1.421 (6)
Fe2—C21	2.042 (4)	C23—H23	0.9500
Fe2—C22	2.042 (4)	C23—C24	1.424 (6)
Fe2—C23	2.044 (4)	C24—H24	0.9500
Fe2—C24	2.034 (4)	C25—H25	1.0000
S1—P1	1.9538 (12)	C25—C33	1.528 (5)
P1—C1	1.798 (3)	C26—H26A	0.9900
P1—C15	1.808 (3)	C26—H26B	0.9900
P1—C34	1.826 (3)	C26—C27	1.518 (5)
N1—H1	0.87 (4)	C27—C28	1.379 (5)
N1—C25	1.481 (4)	C27—C32	1.383 (5)
N1—C26	1.466 (4)	C28—H28	0.9500
C1—C2	1.458 (4)	C28—C29	1.382 (5)
C1—C5	1.435 (4)	C29—H29	0.9500
C2—C3	1.417 (5)	C29—C30	1.375 (6)

C2—C11	1.452 (5)	C30—H30	0.9500
C3—H3	0.9500	C30—C31	1.378 (6)
C3—C4	1.420 (5)	C31—H31	0.9500
C4—H4	0.9500	C31—C32	1.383 (5)
C4—C5	1.414 (5)	C32—H32	0.9500
C5—H5	0.9500	C33—H33A	0.9800
C6—H6	0.9500	C33—H33B	0.9800
C6—C7	1.425 (5)	C33—H33C	0.9800
C6—C10	1.412 (5)	C34—C35	1.388 (5)
C7—H7	0.9500	C34—C39	1.385 (5)
C7—C8	1.410 (6)	C35—H35	0.9500
C8—H8	0.9500	C35—C36	1.386 (5)
C8—C9	1.418 (5)	C36—H36	0.9500
C9—H9	0.9500	C36—C37	1.365 (6)
C9—C10	1.412 (5)	C37—H37	0.9500
C10—H10	0.9500	C37—C38	1.370 (5)
C11—H11	0.9500	C38—H38	0.9500
C11—C12	1.321 (5)	C38—C39	1.389 (5)
C12—H12A	0.9500	C39—H39	0.9500
C12—H12B	0.9500		

C1—Fe1—C2	42.02 (12)	C8—C7—H7	125.7
C1—Fe1—C3	69.20 (13)	Fe1—C8—H8	126.4
C1—Fe1—C4	69.07 (12)	C7—C8—Fe1	69.2 (2)
C1—Fe1—C5	41.37 (12)	C7—C8—H8	126.1
C1—Fe1—C6	109.64 (14)	C7—C8—C9	107.8 (4)
C1—Fe1—C7	131.46 (16)	C9—C8—Fe1	69.9 (2)
C1—Fe1—C8	169.32 (15)	C9—C8—H8	126.1
C1—Fe1—C9	149.64 (13)	Fe1—C9—H9	126.1
C1—Fe1—C10	118.11 (13)	C8—C9—Fe1	69.7 (2)
C2—Fe1—C4	68.88 (13)	C8—C9—H9	126.1
C2—Fe1—C8	128.36 (14)	C10—C9—Fe1	69.7 (2)
C2—Fe1—C9	167.74 (13)	C10—C9—C8	107.7 (4)
C2—Fe1—C10	149.20 (14)	C10—C9—H9	126.1
C3—Fe1—C2	40.65 (13)	Fe1—C10—H10	126.5
C3—Fe1—C4	40.54 (13)	C6—C10—Fe1	69.51 (19)
C3—Fe1—C5	68.28 (14)	C6—C10—C9	108.9 (3)
C3—Fe1—C6	146.12 (14)	C6—C10—H10	125.5
C3—Fe1—C8	106.16 (15)	C9—C10—Fe1	70.0 (2)
C3—Fe1—C9	130.18 (15)	C9—C10—H10	125.5
C3—Fe1—C10	170.14 (15)	C2—C11—H11	117.6
C5—Fe1—C2	69.56 (13)	C12—C11—C2	124.9 (4)
C5—Fe1—C4	40.34 (13)	C12—C11—H11	117.6
C5—Fe1—C8	147.07 (17)	C11—C12—H12A	120.0
C5—Fe1—C9	117.27 (14)	C11—C12—H12B	120.0
C5—Fe1—C10	112.19 (14)	H12A—C12—H12B	120.0
C6—Fe1—C2	115.12 (14)	P1—C15—Fe2	128.81 (15)
C6—Fe1—C4	172.97 (14)	C16—C15—Fe2	70.45 (18)

C6—Fe1—C5	134.31 (14)	C16—C15—P1	127.4 (2)
C6—Fe1—C8	68.49 (16)	C19—C15—Fe2	69.98 (19)
C6—Fe1—C9	68.30 (15)	C19—C15—P1	124.1 (3)
C6—Fe1—C10	40.40 (14)	C19—C15—C16	108.4 (3)
C7—Fe1—C2	106.31 (15)	C15—C16—Fe2	67.99 (17)
C7—Fe1—C3	113.02 (15)	C15—C16—C25	126.8 (3)
C7—Fe1—C4	145.02 (15)	C17—C16—Fe2	69.58 (17)
C7—Fe1—C5	172.48 (17)	C17—C16—C15	106.7 (3)
C7—Fe1—C6	40.95 (14)	C17—C16—C25	126.3 (3)
C7—Fe1—C8	40.39 (17)	C25—C16—Fe2	131.2 (2)
C7—Fe1—C9	68.02 (16)	Fe2—C17—H17	126.6
C7—Fe1—C10	67.90 (14)	C16—C17—Fe2	69.82 (17)
C8—Fe1—C4	114.12 (15)	C16—C17—H17	125.5
C8—Fe1—C9	40.46 (15)	C16—C17—C18	108.9 (3)
C9—Fe1—C4	109.09 (15)	C18—C17—Fe2	69.61 (18)
C10—Fe1—C4	133.55 (14)	C18—C17—H17	125.5
C10—Fe1—C8	67.79 (15)	Fe2—C18—H18	126.9
C10—Fe1—C9	40.27 (14)	C17—C18—Fe2	69.62 (19)
C15—Fe2—C16	41.56 (13)	C17—C18—H18	126.0
C15—Fe2—C17	68.88 (13)	C19—C18—Fe2	69.13 (19)
C15—Fe2—C18	68.90 (13)	C19—C18—C17	108.1 (3)
C15—Fe2—C19	41.24 (12)	C19—C18—H18	126.0
C15—Fe2—C20	108.12 (15)	Fe2—C19—H19	126.5
C15—Fe2—C21	122.99 (15)	C15—C19—Fe2	68.79 (19)
C15—Fe2—C22	158.52 (17)	C15—C19—H19	126.1
C15—Fe2—C23	159.51 (16)	C18—C19—Fe2	70.2 (2)
C15—Fe2—C24	123.33 (16)	C18—C19—C15	107.9 (3)
C17—Fe2—C16	40.60 (13)	C18—C19—H19	126.1
C17—Fe2—C18	40.78 (14)	Fe2—C20—H20	126.2
C18—Fe2—C16	68.88 (13)	C21—C20—Fe2	69.7 (2)
C19—Fe2—C16	69.50 (13)	C21—C20—H20	125.8
C19—Fe2—C17	68.69 (14)	C24—C20—Fe2	69.8 (2)
C19—Fe2—C18	40.66 (13)	C24—C20—H20	125.8
C19—Fe2—C20	121.55 (15)	C24—C20—C21	108.4 (4)
C19—Fe2—C21	158.32 (15)	Fe2—C21—H21	126.2
C19—Fe2—C22	159.04 (16)	C20—C21—Fe2	69.4 (2)
C19—Fe2—C23	122.14 (17)	C20—C21—H21	126.1
C19—Fe2—C24	106.22 (17)	C22—C21—Fe2	69.8 (2)
C20—Fe2—C16	125.46 (15)	C22—C21—C20	107.7 (4)
C20—Fe2—C17	161.99 (17)	C22—C21—H21	126.1
C20—Fe2—C18	156.30 (17)	Fe2—C22—H22	126.1
C20—Fe2—C21	40.84 (17)	C21—C22—Fe2	69.8 (2)
C20—Fe2—C22	68.27 (17)	C21—C22—H22	125.9
C20—Fe2—C23	68.13 (17)	C21—C22—C23	108.1 (4)
C21—Fe2—C16	108.60 (15)	C23—C22—Fe2	69.7 (2)
C21—Fe2—C17	124.77 (17)	C23—C22—H22	125.9
C21—Fe2—C18	160.40 (16)	Fe2—C23—H23	126.5
C21—Fe2—C22	40.43 (16)	C22—C23—Fe2	69.6 (2)

C21—Fe2—C23	68.27 (18)	C22—C23—H23	126.3
C22—Fe2—C16	122.02 (16)	C22—C23—C24	107.4 (4)
C22—Fe2—C17	107.63 (15)	C24—C23—Fe2	69.2 (2)
C22—Fe2—C18	123.18 (16)	C24—C23—H23	126.3
C22—Fe2—C23	40.70 (17)	Fe2—C24—H24	125.7
C23—Fe2—C16	156.93 (15)	C20—C24—Fe2	70.1 (2)
C23—Fe2—C17	121.02 (16)	C20—C24—C23	108.4 (4)
C23—Fe2—C18	106.00 (16)	C20—C24—H24	125.8
C24—Fe2—C16	161.19 (17)	C23—C24—Fe2	70.0 (2)
C24—Fe2—C17	156.49 (18)	C23—C24—H24	125.8
C24—Fe2—C18	120.53 (19)	N1—C25—C16	107.5 (3)
C24—Fe2—C20	40.09 (17)	N1—C25—H25	109.3
C24—Fe2—C21	68.24 (19)	N1—C25—C33	109.3 (3)
C24—Fe2—C22	68.47 (18)	C16—C25—H25	109.3
C24—Fe2—C23	40.86 (17)	C16—C25—C33	112.0 (3)
C1—P1—S1	116.52 (11)	C33—C25—H25	109.3
C1—P1—C15	104.19 (15)	N1—C26—H26A	109.4
C1—P1—C34	104.25 (15)	N1—C26—H26B	109.4
C15—P1—S1	116.06 (11)	N1—C26—C27	111.4 (3)
C15—P1—C34	102.49 (14)	H26A—C26—H26B	108.0
C34—P1—S1	111.75 (12)	C27—C26—H26A	109.4
C25—N1—H1	115 (3)	C27—C26—H26B	109.4
C26—N1—H1	102 (3)	C28—C27—C26	121.6 (3)
C26—N1—C25	113.0 (3)	C28—C27—C32	118.5 (3)
P1—C1—Fe1	127.36 (17)	C32—C27—C26	120.0 (3)
C2—C1—Fe1	69.77 (17)	C27—C28—H28	119.6
C2—C1—P1	129.2 (2)	C27—C28—C29	120.9 (4)
C5—C1—Fe1	70.02 (18)	C29—C28—H28	119.6
C5—C1—P1	123.5 (2)	C28—C29—H29	119.9
C5—C1—C2	107.3 (3)	C30—C29—C28	120.3 (4)
C1—C2—Fe1	68.21 (17)	C30—C29—H29	119.9
C3—C2—Fe1	69.48 (19)	C29—C30—H30	120.3
C3—C2—C1	106.6 (3)	C29—C30—C31	119.3 (4)
C3—C2—C11	125.3 (3)	C31—C30—H30	120.3
C11—C2—Fe1	125.0 (3)	C30—C31—H31	119.9
C11—C2—C1	128.0 (3)	C30—C31—C32	120.3 (4)
Fe1—C3—H3	126.1	C32—C31—H31	119.9
C2—C3—Fe1	69.87 (19)	C27—C32—C31	120.7 (4)
C2—C3—H3	125.1	C27—C32—H32	119.6
C2—C3—C4	109.7 (3)	C31—C32—H32	119.6
C4—C3—Fe1	70.52 (19)	C25—C33—H33A	109.5
C4—C3—H3	125.1	C25—C33—H33B	109.5
Fe1—C4—H4	127.4	C25—C33—H33C	109.5
C3—C4—Fe1	68.93 (19)	H33A—C33—H33B	109.5
C3—C4—H4	126.1	H33A—C33—H33C	109.5
C5—C4—Fe1	69.14 (19)	H33B—C33—H33C	109.5
C5—C4—C3	107.8 (3)	C35—C34—P1	120.0 (3)
C5—C4—H4	126.1	C39—C34—P1	120.6 (3)

Fe1—C5—H5	126.8	C39—C34—C35	119.3 (3)
C1—C5—Fe1	68.61 (18)	C34—C35—H35	120.1
C1—C5—H5	125.7	C36—C35—C34	119.9 (4)
C4—C5—Fe1	70.52 (19)	C36—C35—H35	120.1
C4—C5—C1	108.6 (3)	C35—C36—H36	120.0
C4—C5—H5	125.7	C37—C36—C35	120.1 (4)
Fe1—C6—H6	125.7	C37—C36—H36	120.0
C7—C6—Fe1	69.3 (2)	C36—C37—H37	119.5
C7—C6—H6	126.5	C36—C37—C38	120.9 (4)
C10—C6—Fe1	70.1 (2)	C38—C37—H37	119.5
C10—C6—H6	126.5	C37—C38—H38	120.2
C10—C6—C7	107.0 (3)	C37—C38—C39	119.6 (4)
Fe1—C7—H7	125.7	C39—C38—H38	120.2
C6—C7—Fe1	69.8 (2)	C34—C39—C38	120.2 (3)
C6—C7—H7	125.7	C34—C39—H39	119.9
C8—C7—Fe1	70.4 (2)	C38—C39—H39	119.9
C8—C7—C6	108.5 (3)		

Fe1—C1—C2—C3	59.1 (2)	C6—C7—C8—C9	0.1 (5)
Fe1—C1—C2—C11	−118.1 (4)	C7—C6—C10—Fe1	−59.8 (2)
Fe1—C1—C5—C4	−59.3 (2)	C7—C6—C10—C9	−0.7 (4)
Fe1—C2—C3—C4	59.4 (2)	C7—C8—C9—Fe1	59.0 (3)
Fe1—C2—C11—C12	114.7 (4)	C7—C8—C9—C10	−0.6 (5)
Fe1—C3—C4—C5	58.4 (2)	C8—C9—C10—Fe1	59.5 (3)
Fe1—C4—C5—C1	58.2 (2)	C8—C9—C10—C6	0.8 (4)
Fe1—C6—C7—C8	−59.9 (3)	C10—C6—C7—Fe1	60.3 (2)
Fe1—C6—C10—C9	59.1 (3)	C10—C6—C7—C8	0.3 (4)
Fe1—C7—C8—C9	−59.4 (3)	C11—C2—C3—Fe1	119.0 (4)
Fe1—C8—C9—C10	−59.6 (3)	C11—C2—C3—C4	178.4 (3)
Fe1—C9—C10—C6	−58.8 (2)	C15—P1—C1—Fe1	−169.37 (18)
Fe2—C15—C16—C17	59.1 (2)	C15—P1—C1—C2	97.1 (3)
Fe2—C15—C16—C25	−125.8 (3)	C15—P1—C1—C5	−80.0 (3)
Fe2—C15—C19—C18	−59.5 (2)	C15—P1—C34—C35	−146.0 (3)
Fe2—C16—C17—C18	58.8 (2)	C15—P1—C34—C39	31.5 (3)
Fe2—C16—C25—N1	−172.9 (2)	C15—C16—C17—Fe2	−58.0 (2)
Fe2—C16—C25—C33	66.9 (4)	C15—C16—C17—C18	0.7 (3)
Fe2—C17—C18—C19	58.6 (2)	C15—C16—C25—N1	−81.1 (4)
Fe2—C18—C19—C15	58.6 (2)	C15—C16—C25—C33	158.8 (3)
Fe2—C20—C21—C22	−59.5 (2)	C16—C15—C19—Fe2	60.2 (2)
Fe2—C20—C24—C23	59.7 (3)	C16—C15—C19—C18	0.7 (3)
Fe2—C21—C22—C23	−59.4 (3)	C16—C17—C18—Fe2	−58.9 (2)
Fe2—C22—C23—C24	−59.0 (3)	C16—C17—C18—C19	−0.3 (4)
Fe2—C23—C24—C20	−59.8 (3)	C17—C16—C25—N1	93.2 (4)
S1—P1—C1—Fe1	61.4 (2)	C17—C16—C25—C33	−26.9 (4)
S1—P1—C1—C2	−32.1 (3)	C17—C18—C19—Fe2	−58.9 (2)
S1—P1—C1—C5	150.8 (2)	C17—C18—C19—C15	−0.2 (4)
S1—P1—C15—Fe2	48.3 (2)	C19—C15—C16—Fe2	−59.9 (2)
S1—P1—C15—C16	−45.9 (3)	C19—C15—C16—C17	−0.9 (3)

S1—P1—C15—C19	139.1 (2)	C19—C15—C16—C25	174.3 (3)
S1—P1—C34—C35	−21.1 (3)	C20—C21—C22—Fe2	59.3 (2)
S1—P1—C34—C39	156.5 (2)	C20—C21—C22—C23	−0.1 (4)
P1—C1—C2—Fe1	122.3 (3)	C21—C20—C24—Fe2	−59.3 (2)
P1—C1—C2—C3	−178.6 (3)	C21—C20—C24—C23	0.4 (4)
P1—C1—C2—C11	4.2 (5)	C21—C22—C23—Fe2	59.4 (3)
P1—C1—C5—Fe1	−122.3 (2)	C21—C22—C23—C24	0.4 (4)
P1—C1—C5—C4	178.4 (2)	C22—C23—C24—Fe2	59.3 (3)
P1—C15—C16—Fe2	124.4 (2)	C22—C23—C24—C20	−0.5 (4)
P1—C15—C16—C17	−176.5 (2)	C24—C20—C21—Fe2	59.3 (3)
P1—C15—C16—C25	−1.3 (5)	C24—C20—C21—C22	−0.2 (4)
P1—C15—C19—Fe2	−124.0 (2)	C25—N1—C26—C27	177.9 (3)
P1—C15—C19—C18	176.5 (2)	C25—C16—C17—Fe2	126.7 (3)
P1—C34—C35—C36	178.2 (3)	C25—C16—C17—C18	−174.5 (3)
P1—C34—C39—C38	−177.5 (3)	C26—N1—C25—C16	156.5 (3)
N1—C26—C27—C28	131.4 (4)	C26—N1—C25—C33	−81.7 (4)
N1—C26—C27—C32	−49.0 (5)	C26—C27—C28—C29	−179.9 (3)
C1—P1—C15—Fe2	−81.2 (2)	C26—C27—C32—C31	−178.3 (4)
C1—P1—C15—C16	−175.4 (3)	C27—C28—C29—C30	−2.1 (6)
C1—P1—C15—C19	9.6 (3)	C28—C27—C32—C31	1.3 (5)
C1—P1—C34—C35	105.6 (3)	C28—C29—C30—C31	1.9 (6)
C1—P1—C34—C39	−76.9 (3)	C29—C30—C31—C32	−0.1 (6)
C1—C2—C3—Fe1	−58.3 (2)	C30—C31—C32—C27	−1.5 (6)
C1—C2—C3—C4	1.1 (4)	C32—C27—C28—C29	0.5 (6)
C1—C2—C11—C12	−157.0 (4)	C34—P1—C1—Fe1	−62.2 (2)
C2—C1—C5—Fe1	60.1 (2)	C34—P1—C1—C2	−155.8 (3)
C2—C1—C5—C4	0.8 (4)	C34—P1—C1—C5	27.1 (3)
C2—C3—C4—Fe1	−59.0 (2)	C34—P1—C15—Fe2	170.4 (2)
C2—C3—C4—C5	−0.7 (4)	C34—P1—C15—C16	76.2 (3)
C3—C2—C11—C12	26.3 (6)	C34—P1—C15—C19	−98.8 (3)
C3—C4—C5—Fe1	−58.3 (2)	C34—C35—C36—C37	−1.4 (6)
C3—C4—C5—C1	−0.1 (4)	C35—C34—C39—C38	0.0 (5)
C5—C1—C2—Fe1	−60.3 (2)	C35—C36—C37—C38	1.6 (6)
C5—C1—C2—C3	−1.1 (4)	C36—C37—C38—C39	−1.0 (6)
C5—C1—C2—C11	−178.4 (3)	C37—C38—C39—C34	0.2 (6)
C6—C7—C8—Fe1	59.5 (3)	C39—C34—C35—C36	0.6 (5)