Supporting Information

A Very Simple, Highly Stereoselective and Modular Synthesis of Ferrocene-Based P-Chiral Phosphine Ligands**

Weiping Chen,* William Mbafor, Stanley M. Roberts, John Whittall

(R_c, S_{Fc}, S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-[(2-methoxyphenyl)phenyl phosphino]ferrocene [(R_c,S_{Fc},S_P)-2a]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (3.86 g, 15 mmol) in Et₂O (50 mL) was added 1.7 M t-BuLi solution in pentane (9.7 mL,

16.5 mmol) over 10 min via a syringe at $-78\text{ }^{\circ}\text{C}$. After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to $-78\text{ }^{\circ}\text{C}$ again, and dichlorophenylphosphine (2.24 mL, 16.5 mmol) was added in one portion. After stirring for 10 min at $-78\text{ }^{\circ}\text{C}$, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. The mixture was then cooled to $-78\text{ }^{\circ}\text{C}$ again, and a solution of (2-methoxy)phenyllithium [prepared from 2-bromoanisole (3.32 g, 17.7 mmol) and 1.7 M t-BuLi solution in pentane (20.8 mL, 35.4 mmol) in Et₂O (90 mL) at $-78\text{ }^{\circ}\text{C}$] was added slowly via a cannula. The mixture was warmed to room temperature overnight, and filtered through a pad of Celite. The filtrate was concentrated, and the residue was purified by chromatography (SiO₂, hexane-EtOAc-Et₃N = 85:10:5) to afford the title compound (6.50 g, 92%) as orange crystals. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.29 (d, 3H, J = 6.5 Hz); 1.80 (s, 6H); 3.91 (s, 3H); 3.97 (s, 6H, overlap); 4.11 (m, 1H), 4.25 (t, 1H, J = 2.2 Hz); 4.37 (br. s, 1H); 6.87 (m, 1H); 6.94 (dd, 1H, J = 8.3 and 6.7 Hz); 7.12 ~ 7.23 (m, 6H); 7.31 (m, 1H); ³¹P NMR (CDCl₃, 162 MHz): δ -38.82 . The absolute configuration of (R_c, S_{Fc}, S_P)-**2a** was determined by single-crystal X-ray diffraction analysis.

(R_c, S_{Fc}, S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-[(1-naphthyl)phenylphosphino]ferrocene [(R_c, S_{Fc}, S_P)-2b**]:**

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-**1**] (5.15 g, 20 mmol) in Et₂O (60 mL) was added 1.7 M t-BuLi solution in pentane (12.94 mL, 22 mmol) over 10 min via a syringe at $-78\text{ }^{\circ}\text{C}$. After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to $-78\text{ }^{\circ}\text{C}$ again, and dichlorophenylphosphine (2.99 mL, 22 mmol) was added in one portion. After stirring for 10 min at $-78\text{ }^{\circ}\text{C}$, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. The mixture was then cooled to $-78\text{ }^{\circ}\text{C}$ again, and a solution of 1-naphthyllithium [prepared from 1-bromonaphthalene (5.38 g, 26 mmol) and 1.7 M t-BuLi solution in pentane (30.6 mL, 52 mmol) in Et₂O (120 mL) at $-78\text{ }^{\circ}\text{C}$] was added slowly via a cannula. The mixture

was warmed to room temperature overnight, and filtered through a pad of Celite. The filtrate was concentrated, and the residue was purified by chromatography (SiO₂, hexane-EtOAc-Et₃N = 90:6:4) to afford the title compound (8.75 g, 89%) as orange crystals. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.33 (d, 3H, *J* = 6.8 Hz); 1.91 (s, 6H); 3.59 (s, 5H); 4.00 (m, 1H); 4.17 (m, 1H); 4.26 (t, 1H, *J* = 2.2 Hz); 4.38 (m, 1H); 7.13 ~ 7.2 (m, 5H); 7.39 (t, 1H, *J* = 6.7 Hz); 7.43 ~ 7.54 (m, 2H); 7.60 ~ 7.63 (m, 1H); 7.87 (dd, 2H, *J* = 9.7 and 9.2 Hz), 9.33 (dd, 1H, *J* = 7.6 and 7.0 Hz). ³¹P NMR (CDCl₃, 162 MHz): δ -38.73.

(R_c, S_{Fc}, R_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-[(1-naphthyl)phenylphosphino] ferrocene [(R_c, S_{Fc}, R_P)-2c]:

A solution of (R_c, S_{Fc}, S_P)-2b (491 mg, 1.0 mmol) in hexane (5 mL) was refluxed overnight. After cooling to room temperature, the precipitate was filtered and washed with cold hexane to give the title compound (358 mg, 78%) as orange crystals. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.25 (d, 3H, *J* = 6.8 Hz); 1.60 (s, 6H); 3.88 (br. s, 1H); 4.00 (s, 5H); 4.16 (m, 1H), 4.29 (t, 1H, *J* = 2.2 Hz); 4.42 (br. s, 1H); 7.16 ~ 7.19 (m, 1H); 7.28 ~ 7.29 (m, 5H), 7.32 ~ 7.35 (m, 1H); 7.59 ~ 7.63 (m, 2H); 7.69 (d, *J* = 8.2 Hz); 7.76 (d, *J* = 7.6 Hz); 8.45 (m, 1H). ³¹P NMR (CDCl₃, 162 MHz): δ -31.36. The absolute configuration of (R_c, S_{Fc}, R_P)-2c was determined by single-crystal X-ray diffraction analysis.

(R_c, S_{Fc}, S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-[(2-naphthyl)phenylphosphino] ferrocene [(R_c, S_{Fc}, S_P)-2d]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (2.06 g, 8 mmol) in Et₂O (15 mL) was added 1.5 M *t*-BuLi solution in pentane (6.0 mL, 9 mmol) over 10 min via a syringe at -78 °C. After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to -78 °C again, and dichlorophenylphosphine (1.22 mL, 9 mmol) was added in one portion. After stirring for 10 min at -78 °C, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then

the mixture was cooled to $-78\text{ }^{\circ}\text{C}$ again, and a solution of 2-naphthylmagnesium bromide [prepared from 2-bromonaphthalene (2.20 g, 10.6 mmol) and magnesium (258 mg, 10.6 mmol) in Et_2O (20 mL)] was added via a cannula at $-78\text{ }^{\circ}\text{C}$. The mixture was warmed to room temperature overnight. The reaction was quenched with saturated NH_4Cl solution (20 mL). The organic layer was separated, and the aqueous layer was extracted with Et_2O (20 mL). The combined organic layers were washed with brine (20 mL), dried (MgSO_4), and concentrated. The residue was purified by chromatography (SiO_2 , hexane- EtOAc - Et_3N = 85:10:5) to afford the title compound (3.42 g, 87%) as single diastereomer. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.28 (d, 3H, J = 6.2 Hz); 1.80 (s, 6H); 3.90 (br. s, 1H); 3.92 (s, 5H); 4.20 (m, 1H), 4.22 (t, 1H, J = 2.2 Hz); 4.38 (br. s, 1H); 7.18 ~ 7.26 (m, 5H); 7.48 (m, 2H), 7.58 (ddd, 1H, J = 8.4, 5.6 and 1.6 Hz); 7.79 (d, 1H, J = 8.4 Hz); 7.83 (m, 2H); 8.18 (d, 1H, J = 9.5 Hz);. ^{31}P NMR (CDCl_3 , 162 MHz): δ -20.88 .

(R_c , S_{Fc} , S_P)-2-[(1- N,N -Dimethylamino)ethyl]-1-[(2-biphenyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , S_P)-2e]:

To a solution of (R)- N,N -dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (2.57 g, 10 mmol) in Et_2O (20 mL) was added 1.5 M t-BuLi solution in pentane (7.33 mL, 11 mmol) over 10 min via a syringe at $-78\text{ }^{\circ}\text{C}$. After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to $-78\text{ }^{\circ}\text{C}$ again, and dichlorophenylphosphine (1.50 mL, 11 mmol) was added in one portion. After stirring for 10 min at $-78\text{ }^{\circ}\text{C}$, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then the mixture was cooled to $-78\text{ }^{\circ}\text{C}$ again, and a suspension of 2-biphenyllithium [prepared from 2-bromobiphenyl (2.24 mL, 13 mmol) and 1.5 M t-BuLi solution in pentane (17.3 mL, 26 mmol) in Et_2O (30 mL) at $-78\text{ }^{\circ}\text{C}$] was added via a cannula at $-78\text{ }^{\circ}\text{C}$. The mixture was warmed to room temperature overnight and filtered through a pad of Celite. The filtrate was concentrated, and the residue was purified by chromatography (SiO_2 , hexane- EtOAc - Et_3N = 85:10:5) to afford the title compound (4.87 g, 94%) as single diastereomer. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.25 (d, 3H, J = 6.7Hz); 1.85 (s, 6H); 3.69 (s, 5H); 3.76 (m, 1H), 4.17 (m, 1H), 4.29 (t, 1H, J = 2.4 Hz); 4.32 (m, 1H); 7.10 ~

7.19 (m, 5H); 7.31 (m, 1H), 7.37~7.48 (m, 5H), 7.64 (m, 1H); 7.69 (m, 1H); 7.71 (m, 1H). ^{31}P NMR (CDCl_3 , 162 MHz): δ -32.96

(R_c , S_{Fc} , S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-(cyclohexylphenylphosphino) ferrocene [(R_c , S_{Fc} , R_P)-2f]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (2.57 g, 10 mmol) in Et_2O (20 mL) was added 1.5 M t-BuLi solution in pentane (7.35 mL, 11 mmol) over 10 min via a syringe at -78°C . After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to -78°C again, and dichlorophenylphosphine (1.50 mL, 11 mmol) was added in one portion. After stirring for 10 min at -78°C , the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then the mixture was cooled to -78°C again, and 2.0 M solution of cyclohexymagnesium chloride in Et_2O (6.0 mL, 12 mmol) was added via a syringe at -78°C . The mixture was warmed to room temperature overnight. The reaction was quenched with saturated NH_4Cl solution (20 mL). The organic layer was separated, and the aqueous layer was extracted with Et_2O (20 mL). The combined organic layers were washed with brine (20 mL), dried (MgSO_4), and concentrated. The residue was purified by chromatography (SiO_2 , hexane- $\text{EtOAc-Et}_3\text{N}$ = 90:5:5) to afford the title compound (4.09 g, 92%) as red oil. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.16 (d, 3H, J = 6.7 Hz); 1.19~2.03 (m, 11H); 1.50 (s, 6H); 3.99 (m, 1H), 4.11 (s, 5H); 4.30 (m, 1H), 4.32 (t, 1H, J = 2.5 Hz); 4.37 (m, 1H), 7.12 ~ 7.150 (m, 3H); 7.18~7.23 (m, 2H). ^{31}P NMR (CDCl_3 , 162 MHz): δ -14.86

(R_c , S_{Fc} , S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-(cyclohexylphenylphosphino) ferrocene [(R_c , S_{Fc} , S_P)-2g]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (1.29 g, 5 mmol) in Et_2O (20 mL) was added 1.7 M t-BuLi solution in pentane (3.24 mL, 5.5 mmol) over 10 min via a syringe at -78°C . After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The

resulting red solution was cooled to $-78\text{ }^{\circ}\text{C}$ again, and dichlorocyclohexylphosphine (1.00 g, 5.4 mmol) was added in one portion. After stirring for 10 min at $-78\text{ }^{\circ}\text{C}$, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then the mixture was cooled to $-78\text{ }^{\circ}\text{C}$ again, and 3.0 M solution of phenylmagnesium bromide in Et_2O (1.8 mL, 5.5 mmol) was added via a syringe at $-78\text{ }^{\circ}\text{C}$. The mixture was warmed to room temperature overnight. The reaction was quenched with saturated NH_4Cl solution (20 mL). The organic layer was separated, and the aqueous layer was extracted with Et_2O (20 mL). The combined organic layers were washed with brine (20 mL), dried (MgSO_4), and concentrated. The residue was purified by chromatography (SiO_2 , hexane- $\text{EtOAc-Et}_3\text{N}$ = 90:5:5) to afford the title compound (2.12 g, 95%) as red oil. ^1H NMR (CDCl_3 , 250 MHz): δ 1.33 (d, 3H, J = 6.8Hz); 1.09~1.66 (m, 11H); 2.15 (s, 6H); 3.66 (s, 5H); 4.07(m, 1H), 4.23 (m, 2H), 4.28 (m, 1H);, 7.39 ~ 7.42 (m, 3H); 7.82~7.87 (m, 2H). ^{31}P NMR (CDCl_3 , 101 MHz): δ -20.79 .

(R_c , S_{Fc} , S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-(methylphenylphosphino)ferrocene [(R_c , S_{Fc} , R_P)-2h]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (2.57 g, 10 mmol) in Et_2O (20 mL) was added 1.5 M t-BuLi solution in pentane (7.33 mL, 11 mmol) over 10 min via a syringe at $-78\text{ }^{\circ}\text{C}$. After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to $-78\text{ }^{\circ}\text{C}$ again, and dichlorophenylphosphine (1.50 mL, 11 mmol) was added in one portion. After stirring for 10 min at $-78\text{ }^{\circ}\text{C}$, the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then the mixture was cooled to $-78\text{ }^{\circ}\text{C}$ again, and 3.0 M solution of MeMgBr in Et_2O (4.0 mL, 12 mmol) was added via a syringe at $-78\text{ }^{\circ}\text{C}$. The mixture was warmed to room temperature overnight. The reaction was quenched with saturated NH_4Cl solution (20 mL). The organic layer was separated, and the aqueous layer was extracted with Et_2O (20 mL). The combined organic layers were washed with brine (20 mL), dried (MgSO_4), and concentrated. The residue was purified by chromatography (SiO_2 , hexane- $\text{EtOAc-Et}_3\text{N}$ = 85:10:5) to afford the title compound (3.36 g, 89%) as red oil. ^1H NMR (CDCl_3 , 400.13

MHz): δ 1.24 (d, 3H, J = 6.7Hz); 1.56 (d, 3H, J = 4.4 Hz); 1.72 (s, 6H); 4.07 (m, 1H), 4.13 (s, 5H); 4.30 (m, 1H), 4.34 (m, 2H); 7.14 ~ 7.20 (m, 3H); 7.30~7.37 (m, 2H). ^{31}P NMR (CDCl_3 , 162 MHz): δ -43.47

(R_c , S_{Fc} , S_P)-2-[(1-N,N-Dimethylamino)ethyl]-1-[methyl(*tert*-butyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , R_P)-2i]:

To a solution of (R)-N,N-dimethyl-1-ferrocenylethylamine [(R)-Ugi's amine, (R)-1] (1.29 g, 5 mmol) in Et_2O (15 mL) was added 1.5 M *t*-BuLi solution in pentane (3.7mL, 5.5 mmol) over 10 min via a syringe at -78°C . After addition was completed, the mixture was warmed to room temperature, and stirred for 1.5 h at room temperature. The resulting red solution was cooled to -78°C again, and *tert*-butyldichlorophosphine (875 mg, 5.5 mmol) was added in one portion. After stirring for 10 min at -78°C , the mixture was slowly warmed to room temperature, and stirred for 1.5 h at room temperature. Then to the mixture a 1.6 M solution of methyllithium in Et_2O (3.75 mL, 6.0 mmol) was added via a syringe at -78°C . The mixture was warmed to room temperature overnight and filtered through a pad of Celite. The filtrate was concentrated, and the residue was purified by chromatography (SiO_2 , hexane-EtOAc- Et_3N = 90:5:5) to afford the title compound (1.54 g, 86%) as red oil. ^1H NMR (CDCl_3 , 250.13 MHz): δ 1.09 (d, 9H, J = 12.0 Hz), 1.27 (d, 3H, J = 6.7Hz); 1.45 (d, 3H, J = 3.3 Hz); 2.08 (s, 6H); 3.92 (m, 1H), 4.10 (s, 5H);, 4.28 (m, 3H). ^{31}P NMR (CDCl_3 , 101 MHz): δ -6.47.

(R_c , S_{Fc} , S_P)-2-(1-Acetoxyethyl)-1-[(2-methoxyphenyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , S_P)-7a]:

A solution of (R_c , S_{Fc} , S_P)-2a (1.18 g, 2.5 mmol) in acetic anhydride (10 mL) was stirred for 60 h at room temperature. The excess acetic anhydride was removed under reduced pressure (<1 Torr, <30 $^\circ\text{C}$) to give the title compound (1.21 g, 100%) as yellow solid, which is pure enough for the use in the next reaction. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.19 (s, 3H); 1.64 (d, 3H, J = 6.5 Hz); 3.90 (s, 3H); 3.92 (m, 1H); 4.07 (s, 5H); 4.34 (t,

1H, $J = 2.6$ Hz); 5.55 (m, 1H); 6.15 (m, 1H); 6.87 (td, 1H, $J = 7.4$ and 0.9 Hz); 6.95 (q, 1H, $J = 4.8$ Hz); 7.08 ~ 7.21 (m, 6H); 7.35 (m, 1H); ^{31}P NMR (CDCl_3 , 162 MHz): δ – 39.30.

(R_c , S_{Fc} , S_P)-2-(1-Acetoxyethyl)-1-[(1-naphthyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , S_P)-7b]:

A solution of (R_c , S_{Fc} , S_P)-**2b** (1.47 g, 3.0 mmol) in acetic anhydride (20 mL) was stirred for 60 h at room temperature. The excess acetic anhydride was removed under reduced pressure (<1 Torr, <30 °C) to give the title compound (1.52 g, 100%) as yellow solid, which is pure enough for the use in the next reaction. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.29 (s, 3H); 1.67 (d, 3H, $J = 6.5$ Hz); 3.72 (s, 5H); 3.94 (m, 1H); 4.35 (t, 1H, $J = 2.6$ Hz); 4.57 (m, 1H); 6.28 (m, 1H); 7.13 ~ 7.22 (m, 5H); 7.38~7.43 (m, 2H), 7.53 (ddd, 1H, $J = 8.0, 6.7$ and 1.1 Hz), 7.64(ddd, 1H, $J = 8.4, 6.8$ and 1.4 Hz), 7.89 (t, 2H, $J = 7.0$ Hz); 9.28 (t, 1H, $J = 7.0$ Hz); ^{31}P NMR (CDCl_3 , 162 MHz): δ –39.81.

(R_c , S_{Fc} , R_P)-2-(1-Acetoxyethyl)-1-[(1-naphthyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , R_P)-7c]:

A solution of (R_c , S_{Fc} , R_P)-**2c** (1.47 g, 3.0 mmol) in acetic anhydride (20 mL) was stirred for 60 h at room temperature. The excess acetic anhydride was removed under reduced pressure (<1 Torr, <30 °C) to give the title compound (1.52 g, 100%) as yellow solid, which is pure enough for the use in the next reaction. ^1H NMR (CDCl_3 , 400.13 MHz): δ 0.83 (s, 3H); 1.62 (d, 3H, $J = 6.5$ Hz); 3.83 (m, 1H); 4.10 (s, 5H); 4.40 (t, 1H, $J = 2.6$ Hz); 5.61 (m, 1H); 6.21 (m, 1H); 7.11 (ddd, 1H, $J = 7.0, 4.6$ and 1.1 Hz), 7.28 ~ 7.41(m, 6H); 7.55~7.43 (m, 2H), 7.75 (m, 2H), 8.29 (m, 1H); ^{31}P NMR (CDCl_3 , 162 MHz): δ – 31.33.

(R_c , S_{Fc} , S_P)-2-(1-Acetoxyethyl)-1-[(2-naphthyl)phenylphosphino]ferrocene [(R_c , S_{Fc} , S_P)-7d]:

A solution of (R_c , S_{Fe} , S_P)-**2d** (1.47 g, 3.0 mmol) in acetic anhydride (20 mL) was stirred for 60 h at room temperature. The excess acetic anhydride was removed under reduced pressure (<1 Torr, <30 °C) to give the title compound (1.52 g, 100%) as yellow solid, which is pure enough for the use in the next reaction. 1H NMR ($CDCl_3$, 400.13 MHz): δ 1.21 (s, 3H); 1.65 (d, 3H, J = 6.5 Hz); 3.83 (m, 1H); 4.03 (s, 5H); 4.33 (t, 1H, J = 2.6 Hz); 4.57 (m, 1H); 6.24 (m, 1H); 7.19 ~ 7.27(m, 5H); 7.46~7.51 (m, 3H), 7.81 (m, 3H), 8.11 (d, 1H, J = 10.4 Hz); ^{31}P NMR ($CDCl_3$, 162 MHz): δ -22.89.

(R_c , S_{Fe} , S_P)-2-(1-Acetoxyethyl)-1-[(2-biphenyl)phenylphosphino]ferrocene [(R_c , S_{Fe} , S_P)-7e**]:**

A solution of (R_c , S_{Fe} , S_P)-**2e** (1.47 g, 3.0 mmol) in acetic anhydride (20 mL) was stirred for 60 h at room temperature. The excess acetic anhydride was removed under reduced pressure (<1 Torr, <30 °C) to give the title compound (1.52 g, 100%) as yellow solid, which is pure enough for the use in the next reaction. 1H NMR ($CDCl_3$, 400.13 MHz): δ 1.25 (s, 3H); 1.52 (d, 3H, J = 6.5 Hz); 3.73 (s, 5H); 3.96 (m, 1H); 4.33 (t, 1H, J = 2.6 Hz); 4.48 (m, 1H); 5.81 (m, 1H); 7.16 ~ 7.27(m, 6H); 7.38~7.51 (m, 6H), 7.70~7.73 (m, 2H). ^{31}P NMR ($CDCl_3$, 162 MHz): δ -35.03.

(R_c , S_{Fe} , S_P)-2-[(1- N-Methylamino)ethyl]-1-[(2-methoxyphenyl)phenylphosphino]ferrocene [(R_c , S_{Fe} , S_P)-8a**]:**

A solution of (R_c , S_{Fe} , S_P)-**7a** (1.21 g, 2.5 mmol) and 40% methylamine aqueous solution (6.0 mL) in THF (20 mL) and MeOH (5 mL) was stirred for 3 days at 40 °C, and concentrated. The residue was dissolved in Et_2O (20 mL), washed with brine (10 mL), dried (Na_2SO_4), and evaporated under reduced pressure. The crude product was purified by chromatography (SiO_2 , hexane- $EtOAc$ - Et_3N = 80:15:5) to give the title compound

(1.07 g, 94%) as orange crystals. ^1H NMR (CDCl_3 , 250.13 MHz): δ 1.44 (d, 3H, $J = 6.5$ Hz); 1.94 (s, 3H); 3.91 (m, 2H); 3.95 (s, 3H); 4.05 (s, 5H); 4.29 (t, 1H, $J = 2.5$ Hz); 4.46 (m, 1H); 7.90 (dt, 1H, $J = 7.3$ and 1.0 Hz), 6.97 (ddd, 1H, $J = 8.3$, 5.0 and 1.0 Hz), 7.15 (ddd, 1H, $J = 7.3$, 5.5 and 1.8 Hz), 7.23 (m, 5H); 7.36 (ddd, 1H, $J = 8.3$, 7.3 and 1.8 Hz),. ^{31}P NMR (CDCl_3 , 101 MHz): δ -41.43.

(R_c , S_{Fc} , S_P)-2-[(1-N-Methylamino)ethyl]-1-[(1-naphthyl)phenylphosphino] ferrocene[(R_c , S_{Fc} , S_P)-8b]:

A solution of (R_c , S_{Fc} , S_P)-**7b** (633 mg, 1.25 mmol) and 40% methylamine aqueous solution (3.0 mL) in THF (10 mL) and MeOH (2.5 mL) was stirred for 3 days at 40 °C, and concentrated. The residue was dissolved in Et_2O (20 mL), washed with brine (10 mL), dried (Na_2SO_4), and evaporated under reduced pressure. The crude product was purified by chromatography (SiO_2 , hexane-EtOAc- $\text{Et}_3\text{N} = 85:10:5$) to give the title compound (549 mg, 92%) as orange crystals. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.49 (d, 3H, $J = 6.6$ Hz); 2.07 (s, 3H); 3.69 (s, 5H); 3.95 (m, 1H); 4.01 (m, 1H); 4.31 (t, 1H, $J = 2.5$ Hz); 4.48 (m, 1H); 7.23 (m, 5H); 7.39 ~ 7.47 (m, 2H); 7.54 (m, 1H); 7.66 (m, 1H); 7.90 (t, 2H, $J = 7.9$ Hz), 9.25 (dd, 1H, $J = 7.9$ and 6.7 Hz). ^{31}P NMR (CDCl_3 , 162 MHz): δ -39.91.

(R_c , S_{Fc} , R_P)-2-[(1-N-Methylamino)ethyl]-1-[(1-naphthyl)phenylphosphino] ferrocene [(R_c , S_{Fc} , R_P)-8c]:

A solution of (R_c , S_{Fc} , R_P)-**7c** (633 mg, 1.25 mmol) and 40% methylamine aqueous solution (3.0 mL) in THF (10 mL) and MeOH (2.5 mL) was stirred for 3 days at 40 °C, and concentrated. The residue was dissolved in Et_2O (20 mL), washed with brine (10 mL), dried (Na_2SO_4), and evaporated under reduced pressure. The crude product was purified by chromatography (SiO_2 , hexane-EtOAc- $\text{Et}_3\text{N} = 85:10:5$) to give the title compound (537 mg, 90%) as orange crystals. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.45 (d, 3H, $J = 6.5$ Hz); 1.83 (s, 3H); 3.82 (m, 1H); 3.97 (m, 1H); 4.07 (s, 5H); 3 4.35 (t, 1H, $J =$

2.5 Hz); 4.53 (m, 1H); 7.20 (m, 1H); 7.30 ~ 7.36 (m, 5H); 7.40 (m, 1H); 7.56 ~ 7.61 (m, 2H); 7.78 (t, 2H, $J = 8.2$ Hz), 8.38 (m, 1H). ^{31}P NMR (CDCl_3 , 162 MHz): $\delta -32.25$.

(R_c, S_{Fe}, S_P)-2-[(1-N-Methylamino)ethyl]-1-[(2-naphthyl)phenylphosphino] ferrocene [(R_c, S_{Fe}, S_P)-8d]:

A solution of (R_c, S_{Fe}, S_P)-**7d** (633 mg, 1.25 mmol) and 40% methylamine aqueous solution (3.0 mL) in THF (10 mL) and MeOH (2.5 mL) was stirred for 3 days at 40 °C, and concentrated. The residue was dissolved in Et₂O (20 mL), washed with brine (10 mL), dried (Na_2SO_4), and evaporated under reduced pressure. The crude product was purified by chromatography (SiO_2 , hexane-EtOAc-Et₃N = 85:10:5) to give the title compound (513 mg, 86%) as orange crystals. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.47 (d, 3H, $J = 6.7$ Hz); 1.98 (s, 3H); 3.82 (m, 1H); 3.98 (m, 1H); 4.02 (s, 5H); 4.27 (t, 1H, $J = 2.5$ Hz); 4.47 (m, 1H); 7.27~7.34 (m, 5H); 7.50 (m, 2H); 7.55 (m, 1H); 7.83 (m, 3H); 8.12 (d, 1H, $J = 10.0$ Hz). ^{31}P NMR (CDCl_3 , 162 MHz): $\delta -22.68$.

(R_c, S_{Fe}, S_P)-2-[(1-N-Methylamino)ethyl]-1-[(2-biphenyl)phenylphosphino] ferrocene [(R_c, S_{Fe}, S_P)-8e]:

A solution of (R_c, S_{Fe}, S_P)-**7e** (1.063 g, 2 mmol) and 40% methylamine aqueous solution (5.0 mL) in THF (10 mL) and MeOH (2.5 mL) was stirred for 2 days at 40 °C, and concentrated. The residue was dissolved in Et₂O (20 mL), washed with brine (10 mL), dried (Na_2SO_4), and evaporated under reduced pressure. The residue was recrystallized from hexane to give the title compound (621 mg, 62%) as orange crystals. ^1H NMR (CDCl_3 , 400.13 MHz): δ 1.34 (d, 3H, $J = 6.6$ Hz); 1.93 (s, 3H); 3.60 (m, 1H); 3.74 (s, 5H); 4.08 (m, 1H); 4.30 (t, 1H, $J = 2.5$ Hz); 4.39 (m, 1H); 7.19~7.24 (m, 5H); 7.31 (m, 1H); 7.38~7.50 (m, 5H), 7.59 (ddt, 1H, $J = 7.6, 3.5$ and 1.0 Hz); 7.67 (m, 2H). ^{31}P NMR (CDCl_3 , 162 MHz): $\delta -34.29$.

(R_c, S_{Fc}, S_P)-2-[1-[(N-Methyl-N-diphenylphosphino)amino]ethyl]-1-[(2-methoxyphenyl)phenylphosphino]ferrocene [(R_c, S_{Fc}, S_P)-4a]:

To a solution of (R_c, S_{Fc}, S_P)-**8a** (457 mg, 1.0 mmol) and Et₃N (0.28 mL, 2.0 mmol) in toluene (2.5 mL) was added dropwise chlorodiphenylphosphine (188 uL, 1.05 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (570 mg, 89%) as orange foam. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.55 (d, 3H, *J* = 6.9 Hz); 2.17 (d, 3H, *J* = 3.4 Hz); 3.87 (s, 8H, overlap); 4.24 (m, 1H); 4.38 (t, 1H, *J* = 2.4 Hz); 4.53 (m, 1H); 4.88 (m, 1H); 6.88 ~ 6.96 (m, 6H); 7.03 ~ 7.14 (m, 6H); 7.20 ~ 7.37 (m, 7H). ³¹P NMR (CDCl₃, 162 MHz): δ 56.93, -38.64.

(R_c, S_{Fc}, S_P)-2-[1-[(N-Methyl-N-diphenylphosphino)amino]ethyl]-1-[(1-naphthyl)phenylphosphino]ferrocene [(R_c, S_{Fc}, S_P)-4b]:

To a solution of (R_c, S_{Fc}, S_P)-**8b** (477 mg, 1.0 mmol) and Et₃N (0.28 mL, 2.0 mmol) in toluene (2.5 mL) was added dropwise chlorodiphenylphosphine (188 uL, 1.05 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (595 mg, 90%) as orange foam. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.53 (d, 3H, *J* = 6.8 Hz); 2.22 (d, 3H, *J* = 3.3 Hz); 3.44 (s, 5H); 4.26 (m, 1H); 4.39 (t, 1H, *J* = 2.4 Hz); 4.50 (m, 1H); 5.03 (m, 1H); 6.85 ~ 6.94 (m, 4H); 7.04 (tt, 1H, *J* = 7.2 and 1.4 Hz); 7.09 ~ 7.19 (m, 4H); 7.27 ~ 7.31 (m, 4H); 7.37 ~ 7.43 (m, 3H); 7.48 ~ 7.56 (m, 2H); 7.68 (m, 1H); 7.89 (dd, 2H, *J* = 8.1 and 4.8 Hz); 9.44 (t, 1H, *J* = 7.6 Hz). ³¹P NMR (CDCl₃, 162 MHz): δ 59.59, -41.03.

(R_c, S_{Fc}, R_P)-2-[1-[(N-Methyl-N-diphenylphosphino)amino]ethyl]-1-[(1-naphthyl)phenylphosphino]ferrocene [(R_c, S_{Fc}, R_P)-4c]:

To a solution of (*R_c*, *S_{Fe}*, *R_P*)-**8c** (239 mg, 0.5 mmol) and Et₃N (0.14 mL, 1.0 mmol) in toluene (2.0 mL) was added dropwise chlorodiphenylphosphine (89 uL, 0.50 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (304 mg, 92%) as orange foam. ¹H NMR (CDCl₃, 400.13 MHz): δ 1.51 (d, 3H, *J* = 6.8 Hz); 2.08 (d, 3H, *J* = 3.5 Hz); 3.90 (s, 5H); 4.15 (m, 1H); 4.44 (t, 1H, *J* = 2.4 Hz); 4.58 (m, 1H); 5.02 (m, 1H); 6.44 (td, 2H, *J* = 8.0 and 1.8 Hz); 6.62 (td, 2H, *J* = 8.0 and 1.2 Hz); 6.80 (tt, 1H, *J* = 7.4 and 1.2 Hz); 7.20 (m, 1H); 7.15 ~ 7.30 (m, H); 7.58 ~ 7.64 (m, H); 7.70 (dd, 1H, *J* = 6.8 and 1.8 Hz); 7.79 (d, 1H, *J* = 8.0 Hz); 8.20 (dd, 1H, *J* = 8.2 and 2.4 Hz). ³¹P NMR (CDCl₃, 162 MHz): δ 58.81, -31.16.

(*R_c*, *S_{Fe}*, *S_P*)-2-[1-[(*N*-Methyl-*N*-diphenylphosphino)amino]ethyl]-1-[(2-biphenyl)phenylphosphino]ferrocene [(*R_c*, *S_{Fe}*, *S_P*)-4e**]:**

To a solution of (*R_c*, *S_{Fe}*, *S_P*)-**8e** (503 mg, 1.0 mmol) and Et₃N (0.28 mL, 2.0 mmol) in toluene (2.5 mL) was added dropwise chlorodiphenylphosphine (188 uL, 1.05 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (646 mg, 94%) as orange foam. ¹H NMR (CDCl₃, 250 MHz): δ 1.50 (d, 3H, *J* = 6.6 Hz); 2.16 (d, 3H, *J* = 3.0 Hz); 3.68 (s, 5H); 4.08 (m, 1H); 4.33 (m, 1H); 4.42 (m, 2H); 4.56 (m, 1H); 6.98~7.75 (m, 24H). ³¹P NMR (CDCl₃, 101 MHz): δ 50.70, -35.51.

(*R_c*, *S_{Fe}*, *S_P*, *R_a*)-5a**:**

To a solution of (*R_c*, *S_{Fe}*, *S_P*)-**8a** (229 mg, 0.5 mmol) and Et₃N (209 uL, 1.5 mmol) in toluene (4 mL) was added (*R*)-4-chloro-3,5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']binaphthalene (175 mg, 0.5 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title

compound (359 mg, 93%) as orange foam. ^1H NMR (CDCl_3 , 250 MHz): δ 1.73 (d, 3H, J = 3.5 Hz); 1.79 (d, 3H, J = 7.0 Hz); 3.71 (s, 3H), 3.80 (m, 1H); 4.00 (s, 5H); 4.31 (t, 1H, J = 2.3 Hz); 4.46 (m, 1H); 5.34 (m, 1H); 6.60 (ddd, 1H, J = 7.5, 4.5 and 1.8 Hz), 6.72 (t, 1H, J = 7.5 Hz), 6.82 (dd, 1H, J = 8.8 and 0.8 Hz), 6.91 (ddd, 1H, J = 8.8, 4.5 and 0.8 Hz), 7.15~7.38 (m, 11H), 7.58 (m, 2H), 7.77~7.87 (m, 4H). ^{31}P NMR (CDCl_3 , 101 MHz): δ 148.51 (d, J = 53.4 Hz); -35.37 (d, J = 53.4 Hz).

(R_c , S_{Fc} , S_P , R_a)-5b:

To a solution of (R_c , S_{Fc} , S_P)-**8b** (239 mg, 0.5 mmol) and Et_3N (209 μL , 1.5 mmol) in toluene (4 mL) was added (R)-4-chloro-3,5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']binaphthalene (175 mg, 0.5 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (376 mg, 95%) as orange foam. ^1H NMR (CDCl_3 , 250 MHz): δ 0.87 (d, 3H, J = 7.0 Hz); 1.82 (d, 3H, J = 3.5 Hz); 3.62 (s, 5H); 4.06 (m, 1H); 4.33 (t, 1H, J = 2.3 Hz); 4.46 (m, 1H); 5.43 (m, 1H); 6.69 (dd, 1H, J = 8.8 and 0.8 Hz), 7.07~7.93 (m, 22H), 9.39 (m, 1H). ^{31}P NMR (CDCl_3 , 101 MHz): δ 148.37 (d, J = 61.8 Hz); -41.59 (d, J = 61.8 Hz).

(R_c , S_{Fc} , R_P , R_a)-5c:

To a solution of (R_c , S_{Fc} , R_P)-**8c** (239 mg, 0.5 mmol) and Et_3N (209 μL , 1.5 mmol) in toluene (4 mL) was added (R)-4-chloro-3,5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']binaphthalene (175 mg, 0.5 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (371 mg, 95%) as orange foam. ^1H NMR (CDCl_3 , 250 MHz): δ 1.64 (d, 3H, J = 3.5 Hz); 1.79 (d, 3H, J = 7.0 Hz); 4.88 (m, 1H); 4.07 (s, 5H); 4.38 (t, 1H, J = 2.3 Hz); 4.52 (m, 1H); 4.91 (dd, 1H, J = 8.5 and 0.8 Hz), 5.37 (m, 1H); 6.91 (m, 1H); 7.10~7.90

(m, 21H), 8.44 (m, 1H). ^{31}P NMR (CDCl_3 , 101 MHz): δ 148.18 (d, $J = 54.5$ Hz); -32.43 (d, $J = 54.5$ Hz).

(R_c , S_{Fc} , S_P , R_a)-5e:

To a solution of (R_c , S_{Fc} , S_P)-**8e** (252 mg, 0.5 mmol) and Et_3N (209 μL , 1.5 mmol) in toluene (4 mL) was added (R)-4-chloro-3,5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']binaphthalene (175 mg, 0.5 mmol) at 0 °C. Then the mixture was warmed to room temperature, and stirred overnight (16 h) at room temperature, and filtered through a pad of neutral aluminium oxide and eluted with hexane-EtOAc (9:1) to afford the title compound (392 mg, 96%) as orange foam. ^1H NMR (CDCl_3 , 250 MHz): δ 1.63 (d, 3H, $J = 7.0$ Hz); 1.76 (d, 3H, $J = 3.5$ Hz); 3.69 (s, 5H); 4.09 (m, 1H); 4.30 (t, 1H, $J = 2.3$ Hz); 4.34 (m, 1H); 4.89 (m, 1H); 6.71 (dd, 1H, $J = 8.5$ and 0.8 Hz), 7.07~7.84 (m, 25 H). ^{31}P NMR (CDCl_3 , 101 MHz): δ 149.07 (d, $J = 60.5$ Hz); -36.59 (d, $J = 60.5$ Hz).

(R_c , S_{Fc} , S_P)-2-(1-Dicyclohexylphosphino)ethyl]-1-[(2-methoxyphenyl)phenyl phosphino]ferrocene [(R_c , S_{Fc} , S_P)-6a]:

A solution of (R_c , S_{Fc} , S_P)-**7a** (486 mg, 1.0 mmol) and dicyclohexylphosphine (243 μL , 1.2 mmol) in acetic acid (3 mL) was stirred overnight at room temperature, and poured into 10% K_2CO_3 aqueous solution (60 mL) with stirring, extracted with Et_2O (2 $\times$ 25 mL). The combined ether layers were dried (MgSO_4) and concentrated. The residue was purified by chromatography (SiO_2 , hexane-EtOAc = 9:1) to afford the title compound (601 mg, 96%) as orange crystals. ^1H NMR (CDCl_3 , 250.13 MHz): δ 1.08~1.68 (m, 25 H), 3.12 (m, 1H), 3.91 (s, 5H), 4.07 (m, 1H), 4.29 (t, 1H, $J = 2.3$ Hz); 4.38 (m, 1H), 6.87~6.98 (m, 2H), 7.15~7.25 (m, 6 H), 7.35 (t, 1 H, $J = 7.3$ Hz); ^{31}P NMR (CDCl_3 , 101.25 MHz): δ 15.58 (d, $J = 23.2$ Hz); -42.23 (d, $J = 23.2$ Hz).

(R_c , S_{Fc} , S_P)-2-(1-Dicyclohexylphosphino)ethyl]-1-[(1-naphthyl)phenylphosphino] ferrocene [(R_c , S_{Fc} , S_P)-6b]:

A solution of (R_c , S_{Fc} , S_P)-**7b** (506 mg, 1.0 mmol) and dicyclohexylphosphine (243 μ L, 1.2 mmol) in acetic acid (3 mL) was stirred overnight at room temperature, and poured into 10% K_2CO_3 aqueous solution (60 mL) with stirring, extracted with Et_2O (2 $\times$ 25 mL). The combined ether layers were dried ($MgSO_4$) and concentrated. The residue was purified by chromatography (SiO_2 , hexane- $EtOAc$ = 9:1) to afford the title compound (613 mg, 95%) as orange crystals. 1H NMR ($CDCl_3$, 400.13 MHz): δ 1.14 ~1.57 (m, 25 H); 3.22 (m, 1H); 3.40 (s, 5H); 4.08 (m, 1H); 4.23 (t, 1H, J = 2.4 Hz); 4.31 (m, 1H); 7.16 ~ 7.22 (m, 5H); 7.36 (dd, 1H, J = 8.0 and 7.2 Hz); 7.45 ~ 7.49 (m, 2H); 7.60 (ddd, 1H, J = 8.5, 6.8 and 1.4 Hz); 7.82 (t, 2H, J = 8.1 Hz); 9.28 (dd, 1H, J = 7.6 and 6.8 Hz). ^{31}P NMR ($CDCl_3$, 162 MHz): δ 17.46 (d, J = 27.7 Hz); -42.43 (d, J = 27.7 Hz).

(R_c , S_{Fc} , R_P)-2-(1-Dicyclohexylphosphino)ethyl]-1-[(1-naphthyl)phenyl phosphino]ferrocene [(R_c , S_{Fc} , R_P)-6c**]:**

A solution of (R_c , S_{Fc} , S_P)-**7c** (506 mg, 1.0 mmol) and dicyclohexylphosphine (243 μ L, 1.2 mmol) in acetic acid (3 mL) was stirred overnight at room temperature, and poured into 10% K_2CO_3 aqueous solution (60 mL) with stirring, extracted with Et_2O (2 $\times$ 25 mL). The combined ether layers were dried ($MgSO_4$) and concentrated. The residue was purified by chromatography (SiO_2 , hexane- $EtOAc$ = 9:1) to afford the title compound (618 mg, 95%) as orange crystals. 1H NMR ($CDCl_3$, 250.13 MHz): δ 0.84~1.85 (m, 25 H), 3.16 (m, 1H), 3.96 (s, 5H), 4.00 (m, 1H), 4.35 (t, 1H, J = 2.3 Hz); 4.41 (m, 1H), 7.29~7.40 (m, 7H), 7.62~7.79 (m, 4 H), 8.33 (m, 1H); ^{31}P NMR ($CDCl_3$, 101.25 MHz): δ 14.93 (d, J = 22.8 Hz); -34.80 (d, J = 22.8 Hz).

(R_c , S_{Fc} , S_P)-2-(1-Dicyclohexylphosphino)ethyl]-1-[(2-naphthyl)phenyl phosphino]ferrocene [(R_c , S_{Fc} , S_P)-6d**]:**

A solution of (R_c , S_{Fc} , S_P)-**7d** (506 mg, 1.0 mmol) and dicyclohexylphosphine (243 μ L, 1.2 mmol) in acetic acid (3 mL) was stirred overnight at room temperature, and poured

into 10% K₂CO₃ aqueous solution (60 mL) with stirring, extracted with Et₂O (2×25 mL). The combined ether layers were dried (MgSO₄) and concentrated. The residue was purified by chromatography (SiO₂, hexane-EtOAc = 9:1) to afford the title compound (599 mg, 93%) as orange crystals. ¹H NMR (CDCl₃, 250.13 MHz): δ 1.15~1.71 (m, 25 H), 3.26 (m, 1H), 3.79 (s, 5H), 4.10 (m, 1H), 4.29 (t, 1H, *J* = 2.3 Hz); 4.37 (m, 1H), 7.17~7.24 (m, 5H), 7.34 (m, 1 H), 7.50 (d, 1H, *J* = 9.5 Hz); 7.50 (dd, 1H, *J* = 3.0 and 1.5 Hz); 7.57 (ddd, 1H, *J* = 8.3, 5.0 and 1.5 Hz); 7.81 (d, 1H, *J* = 8.5 Hz); 7.87 (m, 1H), 8.31 (d, 1H, *J* = 9.5 Hz); ³¹P NMR (CDCl₃, 101.25 MHz): δ 15.67 (d, *J* = 30.9 Hz); -34.20 (d, *J* = 30.9Hz).

(R_c, S_{Fc}, S_P)-2-(1-Dicyclohexylphosphino)ethyl]-1-[(2-biphenyl)phenylphosphino] ferrocene [(R_c, S_{Fc}, S_P)-6e]:

A solution of (R_c, S_{Fc}, S_P)-**7e** (531 mg, 1.0 mmol) and dicyclohexylphosphine (243 uL, 1.2 mmol) in acetic acid (3 mL) was stirred overnight at room temperature, and poured into 10% K₂CO₃ aqueous solution (60 mL) with stirring, extracted with Et₂O (2×25 mL). The combined ether layers were dried (MgSO₄) and concentrated. The residue was purified by chromatography (SiO₂, hexane-EtOAc = 9:1) to afford the title compound (650 mg, 97%) as orange crystals. ¹H NMR (CDCl₃, 250.13 MHz): δ 1.02~1.72 (m, 25 H), 2.93 (m, 1H), 3.66 (s, 5H), 3.76 (m, 1H), 4.29 (t, 1H, *J* = 2.3 Hz); 4.32 (m, 1H), 7.14~7.69 (m, 14 H); ³¹P NMR (CDCl₃, 101.25 MHz): δ 18.44 (d, *J* = 36.7 Hz); -37.67 (d, *J* = 36.7 Hz).

Asymmetric Hydrogenation-General Procedure:

Bis(1,5-cyclooctadiene)rhodium trifluoromethanesulfonate [Rh(COD)₂TfO] (2.3 mg, 5 umol) and the desired ligand (6 umol)) were placed in a vessel. The desired solvent (5.0 mL) was added to the reaction vessel via syringe. This solution was stirred at 25 °C.under argon for 15 minutes. The desired substrate (1.0 mmol) was then added to the catalyst solution. The solution was then purged five times with argon and pressurized with

hydrogen to the desired pressure and stirred at room temperature. The reactions were run for the desired time at the desired pressure, and then depressurized. Samples were taken and analyzed for conversion and enantiomeric excess using standard analytical techniques.

X-Ray crystal structure data for compound (R_C,S_{Fe},S_P)-2a

Table 1. Crystal data and structure refinement for (R_C,S_{Fe},S_P)-2a Identification code

	(R _C ,S _{Fe} ,S _P)-2a	
Empirical formula	C ₂₇ H ₃₀ Fe N O P	
Formula weight	471.34	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 11.6455(8) Å	α = 90°.
	b = 12.1775(8) Å	β = 90°.
	c = 16.1295(11) Å	γ = 90°.
Volume	2287.4(3) Å ³	
Z	4	
Density (calculated)	1.369 Mg/m ³	
Absorption coefficient	0.749 mm ⁻¹	
F(000)	992	
Theta range for data collection	2.10 to 28.27°.	
Index ranges	-11 ≤ h ≤ 15, -16 ≤ k ≤ 13, -21 ≤ l ≤ 21	
Reflections collected	14381	
Independent reflections	5316 [R(int) = 0.0373]	
Completeness to theta = 28.27°	96.3 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5316 / 0 / 284	
Goodness-of-fit on F ²	1.016	
Final R indices [I > 2σ(I)]	R1 = 0.0256, wR2 = 0.0639	
R indices (all data)	R1 = 0.0270, wR2 = 0.0644	
Absolute structure parameter	-0.008(10)	

Largest diff. peak and hole

0.376 and -0.183 e.Å⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (R_C, S_{Fe}, S_P)-**2a**. $U(eq)$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8783(2)	6679(1)	782(1)	22(1)
C(2)	9762(2)	6246(1)	1191(1)	25(1)
C(3)	10713(2)	6298(1)	649(1)	27(1)
C(4)	10322(2)	6766(1)	-113(1)	24(1)
C(5)	9130(2)	6998(1)	-32(1)	21(1)
C(6)	9347(1)	9216(1)	1338(1)	17(1)
C(7)	10182(1)	8771(1)	1889(1)	21(1)
C(8)	11257(2)	8728(1)	1469(1)	22(1)
C(9)	11099(1)	9164(1)	660(1)	19(1)
C(10)	9918(1)	9468(1)	569(1)	16(1)
C(11)	8079(1)	9399(1)	1492(1)	18(1)
C(12)	7703(2)	8976(1)	2343(1)	27(1)
C(13)	8241(2)	11311(1)	1957(1)	25(1)
C(14)	6610(2)	10752(2)	1149(1)	28(1)
C(15)	9229(2)	11492(1)	-170(1)	19(1)
C(16)	9965(2)	12023(1)	379(1)	23(1)
C(17)	9905(2)	13150(1)	484(1)	27(1)
C(18)	9116(2)	13772(1)	48(1)	27(1)
C(19)	8369(2)	13252(1)	-496(1)	28(1)
C(20)	8420(2)	12121(1)	-606(1)	23(1)
C(21)	10348(1)	9854(1)	-1122(1)	18(1)
C(22)	11295(2)	10546(1)	-1142(1)	19(1)
C(23)	12174(2)	10426(1)	-1720(1)	21(1)
C(24)	12097(2)	9601(1)	-2308(1)	22(1)
C(25)	11165(2)	8893(1)	-2308(1)	21(1)
C(26)	10300(1)	9005(1)	-1716(1)	19(1)
C(27)	9425(2)	7352(1)	-2189(1)	27(1)
Fe(1)	10057(1)	7834(1)	843(1)	17(1)
N(1)	7813(1)	10561(1)	1329(1)	19(1)
O(1)	9383(1)	8315(1)	-1682(1)	24(1)
P(1)	9177(1)	9999(1)	-346(1)	16(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $(\text{R}_\text{C}, \text{S}_\text{Fc}, \text{S}_\text{P})$ -**2a**.

C(1)-C(2)	1.420(2)
C(1)-C(5)	1.427(2)
C(1)-Fe(1)	2.0470(16)
C(2)-C(3)	1.413(3)
C(2)-Fe(1)	2.0433(16)
C(3)-C(4)	1.428(2)
C(3)-Fe(1)	2.0448(16)
C(4)-C(5)	1.422(3)
C(4)-Fe(1)	2.0408(16)
C(5)-Fe(1)	2.0475(16)
C(6)-C(7)	1.425(2)
C(6)-C(10)	1.441(2)
C(6)-C(11)	1.513(2)
C(6)-Fe(1)	2.0377(15)
C(7)-C(8)	1.424(2)
C(7)-Fe(1)	2.0413(15)
C(8)-C(9)	1.421(2)
C(8)-Fe(1)	2.0387(16)
C(9)-C(10)	1.433(2)
C(9)-Fe(1)	2.0453(16)
C(10)-P(1)	1.8272(15)
C(10)-Fe(1)	2.0441(14)
C(11)-N(1)	1.4718(19)
C(11)-C(12)	1.529(2)
C(13)-N(1)	1.452(2)
C(14)-N(1)	1.450(2)
C(15)-C(16)	1.391(2)
C(15)-C(20)	1.403(2)
C(15)-P(1)	1.8406(15)
C(16)-C(17)	1.385(2)
C(17)-C(18)	1.382(3)
C(18)-C(19)	1.388(3)

C(19)-C(20)	1.390(2)
C(21)-C(22)	1.388(2)
C(21)-C(26)	1.410(2)
C(21)-P(1)	1.8593(16)
C(22)-C(23)	1.393(2)
C(23)-C(24)	1.384(2)
C(24)-C(25)	1.386(2)
C(25)-C(26)	1.396(2)
C(26)-O(1)	1.361(2)
C(27)-O(1)	1.4296(19)

C(2)-C(1)-C(5)	107.54(15)
C(2)-C(1)-Fe(1)	69.55(10)
C(5)-C(1)-Fe(1)	69.63(9)
C(3)-C(2)-C(1)	108.96(15)
C(3)-C(2)-Fe(1)	69.84(9)
C(1)-C(2)-Fe(1)	69.84(9)
C(2)-C(3)-C(4)	107.48(16)
C(2)-C(3)-Fe(1)	69.73(9)
C(4)-C(3)-Fe(1)	69.39(9)
C(5)-C(4)-C(3)	108.16(16)
C(5)-C(4)-Fe(1)	69.89(9)
C(3)-C(4)-Fe(1)	69.69(9)
C(4)-C(5)-C(1)	107.85(15)
C(4)-C(5)-Fe(1)	69.38(10)
C(1)-C(5)-Fe(1)	69.59(9)
C(7)-C(6)-C(10)	107.65(13)
C(7)-C(6)-C(11)	128.28(14)
C(10)-C(6)-C(11)	124.07(14)
C(7)-C(6)-Fe(1)	69.69(9)
C(10)-C(6)-Fe(1)	69.57(8)
C(11)-C(6)-Fe(1)	125.56(11)
C(8)-C(7)-C(6)	108.50(14)
C(8)-C(7)-Fe(1)	69.48(9)
C(6)-C(7)-Fe(1)	69.42(9)
C(9)-C(8)-C(7)	108.07(14)

C(9)-C(8)-Fe(1)	69.89(9)
C(7)-C(8)-Fe(1)	69.67(9)
C(8)-C(9)-C(10)	108.32(14)
C(8)-C(9)-Fe(1)	69.39(9)
C(10)-C(9)-Fe(1)	69.45(9)
C(9)-C(10)-C(6)	107.46(13)
C(9)-C(10)-P(1)	128.86(12)
C(6)-C(10)-P(1)	123.58(12)
C(9)-C(10)-Fe(1)	69.54(9)
C(6)-C(10)-Fe(1)	69.09(8)
P(1)-C(10)-Fe(1)	123.83(8)
N(1)-C(11)-C(6)	108.52(13)
N(1)-C(11)-C(12)	115.09(14)
C(6)-C(11)-C(12)	112.17(14)
C(16)-C(15)-C(20)	118.56(15)
C(16)-C(15)-P(1)	125.28(12)
C(20)-C(15)-P(1)	116.10(13)
C(17)-C(16)-C(15)	120.52(17)
C(18)-C(17)-C(16)	120.91(17)
C(17)-C(18)-C(19)	119.24(16)
C(18)-C(19)-C(20)	120.34(17)
C(19)-C(20)-C(15)	120.43(17)
C(22)-C(21)-C(26)	117.40(14)
C(22)-C(21)-P(1)	122.74(12)
C(26)-C(21)-P(1)	119.85(12)
C(21)-C(22)-C(23)	122.42(15)
C(24)-C(23)-C(22)	119.15(16)
C(23)-C(24)-C(25)	120.17(16)
C(24)-C(25)-C(26)	120.26(15)
O(1)-C(26)-C(25)	122.23(14)
O(1)-C(26)-C(21)	117.20(14)
C(25)-C(26)-C(21)	120.57(15)
C(6)-Fe(1)-C(8)	69.09(7)
C(6)-Fe(1)-C(4)	152.11(7)
C(8)-Fe(1)-C(4)	127.65(7)
C(6)-Fe(1)-C(7)	40.89(6)

C(8)-Fe(1)-C(7)	40.84(7)
C(4)-Fe(1)-C(7)	165.82(7)
C(6)-Fe(1)-C(2)	127.31(7)
C(8)-Fe(1)-C(2)	118.97(7)
C(4)-Fe(1)-C(2)	68.24(7)
C(7)-Fe(1)-C(2)	108.29(7)
C(6)-Fe(1)-C(10)	41.34(6)
C(8)-Fe(1)-C(10)	69.03(6)
C(4)-Fe(1)-C(10)	117.96(6)
C(7)-Fe(1)-C(10)	68.97(6)
C(2)-Fe(1)-C(10)	165.34(7)
C(6)-Fe(1)-C(3)	165.26(7)
C(8)-Fe(1)-C(3)	107.94(7)
C(4)-Fe(1)-C(3)	40.92(7)
C(7)-Fe(1)-C(3)	127.65(7)
C(2)-Fe(1)-C(3)	40.43(7)
C(10)-Fe(1)-C(3)	152.44(7)
C(6)-Fe(1)-C(9)	69.13(6)
C(8)-Fe(1)-C(9)	40.73(7)
C(4)-Fe(1)-C(9)	107.80(7)
C(7)-Fe(1)-C(9)	68.59(6)
C(2)-Fe(1)-C(9)	152.73(7)
C(10)-Fe(1)-C(9)	41.01(6)
C(3)-Fe(1)-C(9)	118.69(7)
C(6)-Fe(1)-C(1)	107.02(7)
C(8)-Fe(1)-C(1)	152.57(7)
C(4)-Fe(1)-C(1)	68.58(7)
C(7)-Fe(1)-C(1)	118.41(7)
C(2)-Fe(1)-C(1)	40.61(7)
C(10)-Fe(1)-C(1)	126.94(7)
C(3)-Fe(1)-C(1)	68.57(7)
C(9)-Fe(1)-C(1)	165.32(7)
C(6)-Fe(1)-C(5)	117.83(6)
C(8)-Fe(1)-C(5)	165.47(7)
C(4)-Fe(1)-C(5)	40.72(7)
C(7)-Fe(1)-C(5)	152.25(7)

C(2)-Fe(1)-C(5)	68.28(7)
C(10)-Fe(1)-C(5)	107.03(6)
C(3)-Fe(1)-C(5)	68.68(7)
C(9)-Fe(1)-C(5)	127.37(7)
C(1)-Fe(1)-C(5)	40.79(7)
C(14)-N(1)-C(13)	111.69(13)
C(14)-N(1)-C(11)	113.22(14)
C(13)-N(1)-C(11)	114.04(13)
C(26)-O(1)-C(27)	117.20(13)
C(10)-P(1)-C(15)	102.10(7)
C(10)-P(1)-C(21)	99.42(7)
C(15)-P(1)-C(21)	99.98(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (R_C, S_{FC}, S_P) -**2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(1)	16(1)	23(1)	-1(1)	-1(1)	-4(1)
C(2)	35(1)	18(1)	23(1)	2(1)	-6(1)	0(1)
C(3)	30(1)	17(1)	34(1)	-4(1)	-6(1)	6(1)
C(4)	30(1)	18(1)	24(1)	-6(1)	1(1)	2(1)
C(5)	27(1)	15(1)	22(1)	-3(1)	-4(1)	-1(1)
C(6)	20(1)	13(1)	18(1)	-3(1)	-1(1)	-1(1)
C(7)	23(1)	21(1)	19(1)	-3(1)	-3(1)	-1(1)
C(8)	17(1)	24(1)	25(1)	-4(1)	-6(1)	1(1)
C(9)	17(1)	18(1)	22(1)	-3(1)	0(1)	-2(1)
C(10)	18(1)	14(1)	18(1)	-2(1)	-2(1)	-1(1)
C(11)	19(1)	18(1)	18(1)	-4(1)	0(1)	-1(1)
C(12)	28(1)	27(1)	27(1)	3(1)	7(1)	0(1)
C(13)	23(1)	22(1)	29(1)	-6(1)	-3(1)	0(1)
C(14)	22(1)	30(1)	32(1)	-7(1)	-4(1)	5(1)
C(15)	23(1)	17(1)	17(1)	-1(1)	6(1)	1(1)
C(16)	25(1)	23(1)	22(1)	-2(1)	3(1)	-2(1)

C(17)	31(1)	23(1)	27(1)	-7(1)	6(1)	-7(1)
C(18)	34(1)	17(1)	29(1)	-2(1)	14(1)	-1(1)
C(19)	33(1)	24(1)	27(1)	4(1)	8(1)	8(1)
C(20)	27(1)	22(1)	20(1)	-1(1)	1(1)	3(1)
C(21)	21(1)	17(1)	15(1)	0(1)	-1(1)	1(1)
C(22)	23(1)	18(1)	17(1)	1(1)	-1(1)	1(1)
C(23)	21(1)	19(1)	22(1)	4(1)	0(1)	-3(1)
C(24)	25(1)	21(1)	18(1)	3(1)	4(1)	2(1)
C(25)	28(1)	21(1)	14(1)	-1(1)	-1(1)	2(1)
C(26)	22(1)	18(1)	17(1)	1(1)	-3(1)	-1(1)
C(27)	27(1)	25(1)	30(1)	-10(1)	0(1)	-5(1)
Fe(1)	18(1)	15(1)	17(1)	-1(1)	-2(1)	1(1)
N(1)	18(1)	20(1)	19(1)	-3(1)	-1(1)	1(1)
O(1)	24(1)	24(1)	25(1)	-8(1)	2(1)	-5(1)
P(1)	17(1)	15(1)	17(1)	-1(1)	-1(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for (R_C,S_{Fe},S_P)-**2a**.

	x	y	z	U(eq)
H(1)	7993	6747	1020	26
H(2)	9779	5963	1773	30
H(3)	11513	6052	775	32
H(4)	10803	6908	-615	28
H(5)	8626	7333	-466	25
H(7)	10034	8513	2468	25
H(8)	11993	8440	1703	26
H(9)	11706	9231	224	23
H(11)	7655	8958	1068	22
H(12A)	8147	9346	2776	41
H(12B)	7836	8182	2374	41
H(12C)	6884	9128	2422	41
H(13A)	8078	12069	1789	37

H(13B)	9072	11213	2019	37
H(13C)	7861	11157	2487	37
H(14A)	6148	10572	1638	42
H(14B)	6372	10289	683	42
H(14C)	6496	11526	1004	42
H(16)	10512	11609	684	28
H(17)	10414	13501	860	32
H(18)	9086	14545	120	32
H(19)	7819	13671	-794	33
H(20)	7905	11772	-978	27
H(22)	11345	11123	-747	23
H(23)	12818	10904	-1712	25
H(24)	12685	9519	-2712	26
H(25)	11115	8329	-2714	25
H(27A)	9408	7565	-2774	41
H(27B)	8762	6885	-2065	41
H(27C)	10134	6947	-2073	41

Table 6. Torsion angles [°] for (R_C,S_{Fe},S_P)-**2a**.

C(5)-C(1)-C(2)-C(3)	0.45(19)
Fe(1)-C(1)-C(2)-C(3)	-59.05(12)
C(5)-C(1)-C(2)-Fe(1)	59.50(11)
C(1)-C(2)-C(3)-C(4)	-0.30(18)
Fe(1)-C(2)-C(3)-C(4)	-59.35(11)
C(1)-C(2)-C(3)-Fe(1)	59.05(11)
C(2)-C(3)-C(4)-C(5)	0.04(18)
Fe(1)-C(3)-C(4)-C(5)	-59.52(11)
C(2)-C(3)-C(4)-Fe(1)	59.56(11)
C(3)-C(4)-C(5)-C(1)	0.24(17)
Fe(1)-C(4)-C(5)-C(1)	-59.16(11)
C(3)-C(4)-C(5)-Fe(1)	59.40(11)
C(2)-C(1)-C(5)-C(4)	-0.42(18)
Fe(1)-C(1)-C(5)-C(4)	59.03(11)
C(2)-C(1)-C(5)-Fe(1)	-59.45(11)

C(10)-C(6)-C(7)-C(8)	-0.80(17)
C(11)-C(6)-C(7)-C(8)	178.50(15)
Fe(1)-C(6)-C(7)-C(8)	58.64(11)
C(10)-C(6)-C(7)-Fe(1)	-59.45(10)
C(11)-C(6)-C(7)-Fe(1)	119.86(16)
C(6)-C(7)-C(8)-C(9)	0.96(18)
Fe(1)-C(7)-C(8)-C(9)	59.56(11)
C(6)-C(7)-C(8)-Fe(1)	-58.60(11)
C(7)-C(8)-C(9)-C(10)	-0.74(18)
Fe(1)-C(8)-C(9)-C(10)	58.69(11)
C(7)-C(8)-C(9)-Fe(1)	-59.43(11)
C(8)-C(9)-C(10)-C(6)	0.24(17)
Fe(1)-C(9)-C(10)-C(6)	58.89(10)
C(8)-C(9)-C(10)-P(1)	-176.21(11)
Fe(1)-C(9)-C(10)-P(1)	-117.55(12)
C(8)-C(9)-C(10)-Fe(1)	-58.65(11)
C(7)-C(6)-C(10)-C(9)	0.35(17)
C(11)-C(6)-C(10)-C(9)	-178.99(14)
Fe(1)-C(6)-C(10)-C(9)	-59.17(10)
C(7)-C(6)-C(10)-P(1)	177.03(10)
C(11)-C(6)-C(10)-P(1)	-2.3(2)
Fe(1)-C(6)-C(10)-P(1)	117.51(11)
C(7)-C(6)-C(10)-Fe(1)	59.52(10)
C(11)-C(6)-C(10)-Fe(1)	-119.82(15)
C(7)-C(6)-C(11)-N(1)	124.80(16)
C(10)-C(6)-C(11)-N(1)	-56.00(19)
Fe(1)-C(6)-C(11)-N(1)	-144.02(11)
C(7)-C(6)-C(11)-C(12)	-3.5(2)
C(10)-C(6)-C(11)-C(12)	175.73(14)
Fe(1)-C(6)-C(11)-C(12)	87.71(16)
C(20)-C(15)-C(16)-C(17)	-0.8(2)
P(1)-C(15)-C(16)-C(17)	-177.81(13)
C(15)-C(16)-C(17)-C(18)	0.1(3)
C(16)-C(17)-C(18)-C(19)	0.6(3)
C(17)-C(18)-C(19)-C(20)	-0.6(2)
C(18)-C(19)-C(20)-C(15)	-0.1(3)

C(16)-C(15)-C(20)-C(19)	0.8(2)
P(1)-C(15)-C(20)-C(19)	178.08(13)
C(26)-C(21)-C(22)-C(23)	0.1(2)
P(1)-C(21)-C(22)-C(23)	179.38(12)
C(21)-C(22)-C(23)-C(24)	1.2(2)
C(22)-C(23)-C(24)-C(25)	-1.1(2)
C(23)-C(24)-C(25)-C(26)	-0.2(2)
C(24)-C(25)-C(26)-O(1)	-178.57(15)
C(24)-C(25)-C(26)-C(21)	1.5(2)
C(22)-C(21)-C(26)-O(1)	178.64(14)
P(1)-C(21)-C(26)-O(1)	-0.7(2)
C(22)-C(21)-C(26)-C(25)	-1.4(2)
P(1)-C(21)-C(26)-C(25)	179.26(12)
C(7)-C(6)-Fe(1)-C(8)	-37.25(9)
C(10)-C(6)-Fe(1)-C(8)	81.62(10)
C(11)-C(6)-Fe(1)-C(8)	-160.45(15)
C(7)-C(6)-Fe(1)-C(4)	-169.79(14)
C(10)-C(6)-Fe(1)-C(4)	-50.92(18)
C(11)-C(6)-Fe(1)-C(4)	67.0(2)
C(10)-C(6)-Fe(1)-C(7)	118.87(13)
C(11)-C(6)-Fe(1)-C(7)	-123.19(17)
C(7)-C(6)-Fe(1)-C(2)	73.90(12)
C(10)-C(6)-Fe(1)-C(2)	-167.23(9)
C(11)-C(6)-Fe(1)-C(2)	-49.30(16)
C(7)-C(6)-Fe(1)-C(10)	-118.87(13)
C(11)-C(6)-Fe(1)-C(10)	117.94(17)
C(7)-C(6)-Fe(1)-C(3)	43.8(3)
C(10)-C(6)-Fe(1)-C(3)	162.6(3)
C(11)-C(6)-Fe(1)-C(3)	-79.4(3)
C(7)-C(6)-Fe(1)-C(9)	-80.99(10)
C(10)-C(6)-Fe(1)-C(9)	37.88(9)
C(11)-C(6)-Fe(1)-C(9)	155.82(15)
C(7)-C(6)-Fe(1)-C(1)	114.00(10)
C(10)-C(6)-Fe(1)-C(1)	-127.13(9)
C(11)-C(6)-Fe(1)-C(1)	-9.20(15)
C(7)-C(6)-Fe(1)-C(5)	156.79(9)

C(10)-C(6)-Fe(1)-C(5)	-84.34(10)
C(11)-C(6)-Fe(1)-C(5)	33.60(15)
C(9)-C(8)-Fe(1)-C(6)	-81.91(10)
C(7)-C(8)-Fe(1)-C(6)	37.29(9)
C(9)-C(8)-Fe(1)-C(4)	72.29(12)
C(7)-C(8)-Fe(1)-C(4)	-168.51(9)
C(9)-C(8)-Fe(1)-C(7)	-119.20(14)
C(9)-C(8)-Fe(1)-C(2)	156.08(10)
C(7)-C(8)-Fe(1)-C(2)	-84.72(11)
C(9)-C(8)-Fe(1)-C(10)	-37.50(9)
C(7)-C(8)-Fe(1)-C(10)	81.70(10)
C(9)-C(8)-Fe(1)-C(3)	113.41(10)
C(7)-C(8)-Fe(1)-C(3)	-127.39(10)
C(7)-C(8)-Fe(1)-C(9)	119.20(14)
C(9)-C(8)-Fe(1)-C(1)	-168.70(13)
C(7)-C(8)-Fe(1)-C(1)	-49.50(18)
C(9)-C(8)-Fe(1)-C(5)	39.3(3)
C(7)-C(8)-Fe(1)-C(5)	158.5(2)
C(5)-C(4)-Fe(1)-C(6)	-48.30(19)
C(3)-C(4)-Fe(1)-C(6)	-167.60(14)
C(5)-C(4)-Fe(1)-C(8)	-167.91(10)
C(3)-C(4)-Fe(1)-C(8)	72.78(13)
C(5)-C(4)-Fe(1)-C(7)	160.0(2)
C(3)-C(4)-Fe(1)-C(7)	40.7(3)
C(5)-C(4)-Fe(1)-C(2)	81.56(11)
C(3)-C(4)-Fe(1)-C(2)	-37.75(11)
C(5)-C(4)-Fe(1)-C(10)	-83.78(11)
C(3)-C(4)-Fe(1)-C(10)	156.92(11)
C(5)-C(4)-Fe(1)-C(3)	119.30(15)
C(5)-C(4)-Fe(1)-C(9)	-127.16(10)
C(3)-C(4)-Fe(1)-C(9)	113.53(11)
C(5)-C(4)-Fe(1)-C(1)	37.73(10)
C(3)-C(4)-Fe(1)-C(1)	-81.58(12)
C(3)-C(4)-Fe(1)-C(5)	-119.30(15)
C(8)-C(7)-Fe(1)-C(6)	-120.15(14)
C(6)-C(7)-Fe(1)-C(8)	120.15(14)

C(8)-C(7)-Fe(1)-C(4)	40.1(3)
C(6)-C(7)-Fe(1)-C(4)	160.2(3)
C(8)-C(7)-Fe(1)-C(2)	113.44(10)
C(6)-C(7)-Fe(1)-C(2)	-126.41(10)
C(8)-C(7)-Fe(1)-C(10)	-81.86(10)
C(6)-C(7)-Fe(1)-C(10)	38.29(9)
C(8)-C(7)-Fe(1)-C(3)	72.69(12)
C(6)-C(7)-Fe(1)-C(3)	-167.16(10)
C(8)-C(7)-Fe(1)-C(9)	-37.72(10)
C(6)-C(7)-Fe(1)-C(9)	82.44(10)
C(8)-C(7)-Fe(1)-C(1)	156.53(10)
C(6)-C(7)-Fe(1)-C(1)	-83.31(11)
C(8)-C(7)-Fe(1)-C(5)	-168.61(13)
C(6)-C(7)-Fe(1)-C(5)	-48.46(17)
C(3)-C(2)-Fe(1)-C(6)	-168.64(10)
C(1)-C(2)-Fe(1)-C(6)	71.13(12)
C(3)-C(2)-Fe(1)-C(8)	-83.86(11)
C(1)-C(2)-Fe(1)-C(8)	155.91(10)
C(3)-C(2)-Fe(1)-C(4)	38.19(10)
C(1)-C(2)-Fe(1)-C(4)	-82.04(11)
C(3)-C(2)-Fe(1)-C(7)	-127.16(10)
C(1)-C(2)-Fe(1)-C(7)	112.61(10)
C(3)-C(2)-Fe(1)-C(10)	156.1(2)
C(1)-C(2)-Fe(1)-C(10)	35.9(3)
C(1)-C(2)-Fe(1)-C(3)	-120.23(14)
C(3)-C(2)-Fe(1)-C(9)	-48.59(18)
C(1)-C(2)-Fe(1)-C(9)	-168.82(14)
C(3)-C(2)-Fe(1)-C(1)	120.23(14)
C(3)-C(2)-Fe(1)-C(5)	82.19(11)
C(1)-C(2)-Fe(1)-C(5)	-38.04(10)
C(9)-C(10)-Fe(1)-C(6)	119.03(13)
P(1)-C(10)-Fe(1)-C(6)	-117.18(14)
C(9)-C(10)-Fe(1)-C(8)	37.25(9)
C(6)-C(10)-Fe(1)-C(8)	-81.79(10)
P(1)-C(10)-Fe(1)-C(8)	161.04(12)
C(9)-C(10)-Fe(1)-C(4)	-85.24(11)

C(6)-C(10)-Fe(1)-C(4)	155.73(9)
P(1)-C(10)-Fe(1)-C(4)	38.55(13)
C(9)-C(10)-Fe(1)-C(7)	81.14(10)
C(6)-C(10)-Fe(1)-C(7)	-37.89(9)
P(1)-C(10)-Fe(1)-C(7)	-155.07(12)
C(9)-C(10)-Fe(1)-C(2)	163.0(2)
C(6)-C(10)-Fe(1)-C(2)	44.0(3)
P(1)-C(10)-Fe(1)-C(2)	-73.2(3)
C(9)-C(10)-Fe(1)-C(3)	-51.52(18)
C(6)-C(10)-Fe(1)-C(3)	-170.56(14)
P(1)-C(10)-Fe(1)-C(3)	72.3(2)
C(6)-C(10)-Fe(1)-C(9)	-119.03(13)
P(1)-C(10)-Fe(1)-C(9)	123.79(14)
C(9)-C(10)-Fe(1)-C(1)	-168.45(10)
C(6)-C(10)-Fe(1)-C(1)	72.52(11)
P(1)-C(10)-Fe(1)-C(1)	-44.66(13)
C(9)-C(10)-Fe(1)-C(5)	-127.95(10)
C(6)-C(10)-Fe(1)-C(5)	113.02(9)
P(1)-C(10)-Fe(1)-C(5)	-4.16(12)
C(2)-C(3)-Fe(1)-C(6)	38.0(3)
C(4)-C(3)-Fe(1)-C(6)	156.7(2)
C(2)-C(3)-Fe(1)-C(8)	113.89(10)
C(4)-C(3)-Fe(1)-C(8)	-127.35(11)
C(2)-C(3)-Fe(1)-C(4)	-118.76(15)
C(2)-C(3)-Fe(1)-C(7)	72.88(12)
C(4)-C(3)-Fe(1)-C(7)	-168.37(10)
C(4)-C(3)-Fe(1)-C(2)	118.76(15)
C(2)-C(3)-Fe(1)-C(10)	-167.22(14)
C(4)-C(3)-Fe(1)-C(10)	-48.5(2)
C(2)-C(3)-Fe(1)-C(9)	156.94(10)
C(4)-C(3)-Fe(1)-C(9)	-84.31(12)
C(2)-C(3)-Fe(1)-C(1)	-37.17(10)
C(4)-C(3)-Fe(1)-C(1)	81.59(11)
C(2)-C(3)-Fe(1)-C(5)	-81.12(11)
C(4)-C(3)-Fe(1)-C(5)	37.64(11)
C(8)-C(9)-Fe(1)-C(6)	81.81(10)

C(10)-C(9)-Fe(1)-C(6)	-38.17(9)
C(10)-C(9)-Fe(1)-C(8)	-119.98(13)
C(8)-C(9)-Fe(1)-C(4)	-127.61(10)
C(10)-C(9)-Fe(1)-C(4)	112.41(9)
C(8)-C(9)-Fe(1)-C(7)	37.82(10)
C(10)-C(9)-Fe(1)-C(7)	-82.15(9)
C(8)-C(9)-Fe(1)-C(2)	-50.74(18)
C(10)-C(9)-Fe(1)-C(2)	-170.71(13)
C(8)-C(9)-Fe(1)-C(10)	119.98(13)
C(8)-C(9)-Fe(1)-C(3)	-84.41(11)
C(10)-C(9)-Fe(1)-C(3)	155.61(9)
C(8)-C(9)-Fe(1)-C(1)	159.1(2)
C(10)-C(9)-Fe(1)-C(1)	39.2(3)
C(8)-C(9)-Fe(1)-C(5)	-168.47(10)
C(10)-C(9)-Fe(1)-C(5)	71.56(11)
C(2)-C(1)-Fe(1)-C(6)	-128.09(10)
C(5)-C(1)-Fe(1)-C(6)	113.12(10)
C(2)-C(1)-Fe(1)-C(8)	-50.82(19)
C(5)-C(1)-Fe(1)-C(8)	-169.61(13)
C(2)-C(1)-Fe(1)-C(4)	81.12(11)
C(5)-C(1)-Fe(1)-C(4)	-37.67(10)
C(2)-C(1)-Fe(1)-C(7)	-85.25(11)
C(5)-C(1)-Fe(1)-C(7)	155.96(9)
C(5)-C(1)-Fe(1)-C(2)	-118.79(14)
C(2)-C(1)-Fe(1)-C(10)	-169.29(9)
C(5)-C(1)-Fe(1)-C(10)	71.92(12)
C(2)-C(1)-Fe(1)-C(3)	37.01(10)
C(5)-C(1)-Fe(1)-C(3)	-81.78(11)
C(2)-C(1)-Fe(1)-C(9)	159.5(2)
C(5)-C(1)-Fe(1)-C(9)	40.7(3)
C(2)-C(1)-Fe(1)-C(5)	118.79(14)
C(4)-C(5)-Fe(1)-C(6)	156.74(10)
C(1)-C(5)-Fe(1)-C(6)	-83.95(11)
C(4)-C(5)-Fe(1)-C(8)	41.4(3)
C(1)-C(5)-Fe(1)-C(8)	160.7(2)
C(1)-C(5)-Fe(1)-C(4)	119.31(14)

C(4)-C(5)-Fe(1)-C(7)	-169.61(13)
C(1)-C(5)-Fe(1)-C(7)	-50.31(17)
C(4)-C(5)-Fe(1)-C(2)	-81.42(11)
C(1)-C(5)-Fe(1)-C(2)	37.88(10)
C(4)-C(5)-Fe(1)-C(10)	113.32(11)
C(1)-C(5)-Fe(1)-C(10)	-127.38(10)
C(4)-C(5)-Fe(1)-C(3)	-37.82(10)
C(1)-C(5)-Fe(1)-C(3)	81.49(11)
C(4)-C(5)-Fe(1)-C(9)	72.69(12)
C(1)-C(5)-Fe(1)-C(9)	-168.00(9)
C(4)-C(5)-Fe(1)-C(1)	-119.31(14)
C(6)-C(11)-N(1)-C(14)	158.06(13)
C(12)-C(11)-N(1)-C(14)	-75.34(18)
C(6)-C(11)-N(1)-C(13)	-72.75(17)
C(12)-C(11)-N(1)-C(13)	53.85(19)
C(25)-C(26)-O(1)-C(27)	10.2(2)
C(21)-C(26)-O(1)-C(27)	-169.83(14)
C(9)-C(10)-P(1)-C(15)	-95.72(14)
C(6)-C(10)-P(1)-C(15)	88.35(13)
Fe(1)-C(10)-P(1)-C(15)	174.30(10)
C(9)-C(10)-P(1)-C(21)	6.71(15)
C(6)-C(10)-P(1)-C(21)	-169.23(12)
Fe(1)-C(10)-P(1)-C(21)	-83.27(11)
C(16)-C(15)-P(1)-C(10)	17.61(16)
C(20)-C(15)-P(1)-C(10)	-159.47(13)
C(16)-C(15)-P(1)-C(21)	-84.38(15)
C(20)-C(15)-P(1)-C(21)	98.54(13)
C(22)-C(21)-P(1)-C(10)	-73.95(14)
C(26)-C(21)-P(1)-C(10)	105.33(13)
C(22)-C(21)-P(1)-C(15)	30.23(15)
C(26)-C(21)-P(1)-C(15)	-150.49(13)

Symmetry transformations used to generate equivalent atoms:

X-Ray crystal structure data for compound (R_C,S_{Fe},R_P)-2c

Table 1. Crystal data and structure refinement for (R_C,S_{Fe},R_P)-2c.

Identification code	(R _C ,S _{Fe} ,R _P)-2c	
Empirical formula	C ₃₀ H ₃₀ Fe N P	
Formula weight	491.37	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.4555(3) Å	α = 90°.
	b = 14.3945(6) Å	β = 107.4650(10)°.
	c = 11.7058(5) Å	γ = 90°.
Volume	1198.33(9) Å ³	
Z	2	
Density (calculated)	1.362 Mg/m ³	
Absorption coefficient	0.715 mm ⁻¹	
F(000)	516	
Theta range for data collection	1.82 to 28.29°.	
Index ranges	-6 ≤ h ≤ 9, -18 ≤ k ≤ 19, -15 ≤ l ≤ 14	
Reflections collected	7539	
Independent reflections	5044 [R(int) = 0.0298]	
Completeness to theta = 28.29°	93.3 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5044 / 1 / 301	
Goodness-of-fit on F ²	1.067	
Final R indices [I > 2σ(I)]	R1 = 0.0252, wR2 = 0.0652	
R indices (all data)	R1 = 0.0254, wR2 = 0.0654	
Absolute structure parameter	0.002(9)	
Largest diff. peak and hole	0.597 and -0.335 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{R}_\text{C}, \text{S}_\text{Fc}, \text{R}_\text{p})\text{-2c}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3411(2)	1705(1)	8062(2)	21(1)
C(2)	2879(2)	1334(1)	6878(2)	20(1)
C(3)	4133(2)	596(1)	6853(2)	22(1)
C(4)	5435(3)	513(1)	8025(2)	23(1)
C(5)	4977(3)	1193(1)	8768(2)	23(1)
C(6)	7622(2)	2783(1)	8076(2)	14(1)
C(7)	8367(2)	2055(1)	7519(2)	16(1)
C(8)	7288(2)	2010(1)	6285(2)	17(1)
C(9)	5885(2)	2714(1)	6064(2)	16(1)
C(10)	6082(2)	3205(1)	7162(1)	13(1)
C(11)	8247(2)	3088(1)	9371(2)	17(1)
C(12)	9700(3)	2427(1)	10165(2)	25(1)
C(13)	8738(4)	4536(2)	10505(2)	35(1)
C(14)	10620(3)	4220(2)	9201(2)	29(1)
C(15)	6102(2)	5163(1)	7092(2)	15(1)
C(16)	7593(2)	5026(1)	6659(2)	17(1)
C(17)	8641(2)	5781(1)	6410(2)	20(1)
C(18)	8177(2)	6671(1)	6603(2)	19(1)
C(19)	6644(2)	6852(1)	7054(1)	16(1)
C(20)	6153(3)	7775(1)	7275(2)	20(1)
C(21)	4674(3)	7949(1)	7705(2)	23(1)
C(22)	3590(3)	7197(1)	7926(2)	22(1)
C(23)	4033(3)	6303(1)	7729(2)	19(1)
C(24)	5587(2)	6092(1)	7303(1)	14(1)
C(25)	2771(2)	4168(1)	6007(1)	14(1)
C(26)	2786(2)	4696(1)	5010(2)	17(1)
C(27)	1274(3)	4673(1)	3962(2)	19(1)
C(28)	-271(2)	4109(1)	3898(2)	18(1)
C(29)	-299(2)	3575(1)	4879(2)	18(1)
C(30)	1203(2)	3613(1)	5932(2)	17(1)
Fe(1)	5596(1)	1814(1)	7357(1)	13(1)

N(1)	8822(2)	4074(1)	9421(1)	22(1)
P(1)	4728(1)	4186(1)	7420(1)	13(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $(\text{R}_\text{C}, \text{S}_\text{Fc}, \text{R}_\text{P})\text{-2c}$.

C(1)-C(5)	1.418(3)
C(1)-C(2)	1.427(3)
C(1)-Fe(1)	2.0413(16)
C(2)-C(3)	1.420(3)
C(2)-Fe(1)	2.0527(16)
C(3)-C(4)	1.428(3)
C(3)-Fe(1)	2.0554(18)
C(4)-C(5)	1.419(3)
C(4)-Fe(1)	2.0471(18)
C(5)-Fe(1)	2.0486(18)
C(6)-C(7)	1.431(2)
C(6)-C(10)	1.447(2)
C(6)-C(11)	1.511(2)
C(6)-Fe(1)	2.0417(16)
C(7)-C(8)	1.428(2)
C(7)-Fe(1)	2.0467(16)
C(8)-C(9)	1.424(2)
C(8)-Fe(1)	2.0489(17)
C(9)-C(10)	1.435(2)
C(9)-Fe(1)	2.0525(16)
C(10)-P(1)	1.8131(17)
C(10)-Fe(1)	2.0584(16)
C(11)-N(1)	1.479(2)
C(11)-C(12)	1.530(2)
C(13)-N(1)	1.450(3)
C(14)-N(1)	1.455(3)
C(15)-C(16)	1.367(2)
C(15)-C(24)	1.433(3)
C(15)-P(1)	1.8466(17)
C(16)-C(17)	1.419(2)

C(17)-C(18)	1.363(3)
C(18)-C(19)	1.419(2)
C(19)-C(20)	1.423(3)
C(19)-C(24)	1.428(2)
C(20)-C(21)	1.366(3)
C(21)-C(22)	1.419(3)
C(22)-C(23)	1.366(3)
C(23)-C(24)	1.424(2)
C(25)-C(26)	1.396(2)
C(25)-C(30)	1.397(2)
C(25)-P(1)	1.8481(16)
C(26)-C(27)	1.394(2)
C(27)-C(28)	1.393(2)
C(28)-C(29)	1.387(3)
C(29)-C(30)	1.395(2)

C(5)-C(1)-C(2)	108.14(17)
C(5)-C(1)-Fe(1)	69.99(10)
C(2)-C(1)-Fe(1)	70.03(9)
C(3)-C(2)-C(1)	107.90(16)
C(3)-C(2)-Fe(1)	69.88(10)
C(1)-C(2)-Fe(1)	69.17(9)
C(2)-C(3)-C(4)	107.79(17)
C(2)-C(3)-Fe(1)	69.67(10)
C(4)-C(3)-Fe(1)	69.32(10)
C(5)-C(4)-C(3)	108.16(16)
C(5)-C(4)-Fe(1)	69.79(10)
C(3)-C(4)-Fe(1)	69.94(10)
C(1)-C(5)-C(4)	108.01(17)
C(1)-C(5)-Fe(1)	69.43(10)
C(4)-C(5)-Fe(1)	69.68(10)
C(7)-C(6)-C(10)	107.53(14)
C(7)-C(6)-C(11)	128.67(15)
C(10)-C(6)-C(11)	123.80(15)
C(7)-C(6)-Fe(1)	69.70(9)
C(10)-C(6)-Fe(1)	69.95(9)

C(11)-C(6)-Fe(1)	125.38(11)
C(8)-C(7)-C(6)	108.42(14)
C(8)-C(7)-Fe(1)	69.68(9)
C(6)-C(7)-Fe(1)	69.33(9)
C(9)-C(8)-C(7)	108.18(14)
C(9)-C(8)-Fe(1)	69.83(9)
C(7)-C(8)-Fe(1)	69.51(9)
C(8)-C(9)-C(10)	108.36(14)
C(8)-C(9)-Fe(1)	69.55(9)
C(10)-C(9)-Fe(1)	69.79(9)
C(9)-C(10)-C(6)	107.50(14)
C(9)-C(10)-P(1)	128.28(12)
C(6)-C(10)-P(1)	124.22(12)
C(9)-C(10)-Fe(1)	69.35(9)
C(6)-C(10)-Fe(1)	68.72(9)
P(1)-C(10)-Fe(1)	127.87(9)
N(1)-C(11)-C(6)	108.52(14)
N(1)-C(11)-C(12)	115.40(15)
C(6)-C(11)-C(12)	112.19(15)
C(16)-C(15)-C(24)	119.24(15)
C(16)-C(15)-P(1)	122.02(13)
C(24)-C(15)-P(1)	118.74(12)
C(15)-C(16)-C(17)	121.61(16)
C(18)-C(17)-C(16)	120.21(16)
C(17)-C(18)-C(19)	120.46(16)
C(18)-C(19)-C(20)	121.26(17)
C(18)-C(19)-C(24)	119.38(17)
C(20)-C(19)-C(24)	119.36(16)
C(21)-C(20)-C(19)	121.19(17)
C(20)-C(21)-C(22)	119.65(18)
C(23)-C(22)-C(21)	120.50(17)
C(22)-C(23)-C(24)	121.55(18)
C(23)-C(24)-C(19)	117.71(17)
C(23)-C(24)-C(15)	123.17(16)
C(19)-C(24)-C(15)	119.10(15)
C(26)-C(25)-C(30)	118.36(15)

C(26)-C(25)-P(1)	122.59(12)
C(30)-C(25)-P(1)	119.04(12)
C(27)-C(26)-C(25)	121.03(16)
C(28)-C(27)-C(26)	119.87(16)
C(29)-C(28)-C(27)	119.75(15)
C(28)-C(29)-C(30)	120.09(16)
C(29)-C(30)-C(25)	120.88(16)
C(1)-Fe(1)-C(6)	117.87(7)
C(1)-Fe(1)-C(7)	151.83(7)
C(6)-Fe(1)-C(7)	40.97(6)
C(1)-Fe(1)-C(4)	68.30(8)
C(6)-Fe(1)-C(4)	126.03(7)
C(7)-Fe(1)-C(4)	107.00(7)
C(1)-Fe(1)-C(5)	40.58(7)
C(6)-Fe(1)-C(5)	106.46(7)
C(7)-Fe(1)-C(5)	117.67(7)
C(4)-Fe(1)-C(5)	40.53(8)
C(1)-Fe(1)-C(8)	166.23(7)
C(6)-Fe(1)-C(8)	69.07(6)
C(7)-Fe(1)-C(8)	40.81(7)
C(4)-Fe(1)-C(8)	118.49(7)
C(5)-Fe(1)-C(8)	152.00(7)
C(1)-Fe(1)-C(9)	128.31(7)
C(6)-Fe(1)-C(9)	69.18(6)
C(7)-Fe(1)-C(9)	68.59(6)
C(4)-Fe(1)-C(9)	152.90(8)
C(5)-Fe(1)-C(9)	165.70(7)
C(8)-Fe(1)-C(9)	40.62(6)
C(1)-Fe(1)-C(2)	40.80(7)
C(6)-Fe(1)-C(2)	152.88(7)
C(7)-Fe(1)-C(2)	165.47(7)
C(4)-Fe(1)-C(2)	68.29(7)
C(5)-Fe(1)-C(2)	68.35(7)
C(8)-Fe(1)-C(2)	128.13(7)
C(9)-Fe(1)-C(2)	108.93(7)
C(1)-Fe(1)-C(3)	68.38(7)

C(6)-Fe(1)-C(3)	164.50(7)
C(7)-Fe(1)-C(3)	127.20(7)
C(4)-Fe(1)-C(3)	40.73(8)
C(5)-Fe(1)-C(3)	68.34(8)
C(8)-Fe(1)-C(3)	108.22(7)
C(9)-Fe(1)-C(3)	119.38(7)
C(2)-Fe(1)-C(3)	40.45(7)
C(1)-Fe(1)-C(10)	107.93(7)
C(6)-Fe(1)-C(10)	41.33(6)
C(7)-Fe(1)-C(10)	68.87(6)
C(4)-Fe(1)-C(10)	164.65(7)
C(5)-Fe(1)-C(10)	127.10(7)
C(8)-Fe(1)-C(10)	68.72(6)
C(9)-Fe(1)-C(10)	40.87(6)
C(2)-Fe(1)-C(10)	119.30(7)
C(3)-Fe(1)-C(10)	153.28(7)
C(13)-N(1)-C(14)	111.88(16)
C(13)-N(1)-C(11)	112.75(15)
C(14)-N(1)-C(11)	113.76(16)
C(10)-P(1)-C(15)	100.82(7)
C(10)-P(1)-C(25)	99.79(7)
C(15)-P(1)-C(25)	99.38(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{R}_\text{C}, \text{S}_\text{Fc}, \text{R}_\text{P})\text{-2c}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	20(1)	18(1)	26(1)	-1(1)	12(1)	-4(1)
C(2)	15(1)	19(1)	25(1)	1(1)	5(1)	-5(1)
C(3)	22(1)	14(1)	32(1)	-3(1)	10(1)	-7(1)
C(4)	22(1)	12(1)	34(1)	7(1)	8(1)	-3(1)
C(5)	24(1)	24(1)	21(1)	4(1)	7(1)	-8(1)
C(6)	13(1)	12(1)	17(1)	0(1)	3(1)	-2(1)
C(7)	14(1)	13(1)	23(1)	2(1)	7(1)	-1(1)
C(8)	19(1)	13(1)	20(1)	-2(1)	8(1)	-1(1)
C(9)	17(1)	14(1)	16(1)	-1(1)	5(1)	-3(1)
C(10)	14(1)	10(1)	15(1)	0(1)	4(1)	0(1)
C(11)	15(1)	17(1)	16(1)	1(1)	2(1)	-3(1)
C(12)	19(1)	29(1)	22(1)	6(1)	1(1)	0(1)
C(13)	50(1)	32(1)	24(1)	-10(1)	13(1)	-12(1)
C(14)	30(1)	31(1)	25(1)	-4(1)	6(1)	-16(1)
C(15)	15(1)	13(1)	15(1)	2(1)	4(1)	-2(1)
C(16)	19(1)	13(1)	18(1)	-1(1)	5(1)	0(1)
C(17)	17(1)	23(1)	22(1)	1(1)	7(1)	-3(1)
C(18)	17(1)	18(1)	21(1)	3(1)	4(1)	-5(1)
C(19)	17(1)	13(1)	15(1)	2(1)	0(1)	-3(1)
C(20)	20(1)	13(1)	22(1)	1(1)	0(1)	-2(1)
C(21)	24(1)	12(1)	27(1)	-2(1)	-1(1)	2(1)
C(22)	19(1)	20(1)	28(1)	-2(1)	8(1)	3(1)
C(23)	19(1)	17(1)	22(1)	-1(1)	7(1)	-1(1)
C(24)	14(1)	14(1)	13(1)	-1(1)	1(1)	-2(1)
C(25)	14(1)	12(1)	16(1)	-1(1)	4(1)	3(1)
C(26)	18(1)	13(1)	21(1)	1(1)	5(1)	-1(1)
C(27)	22(1)	14(1)	19(1)	3(1)	5(1)	2(1)
C(28)	16(1)	16(1)	21(1)	-2(1)	2(1)	2(1)
C(29)	14(1)	16(1)	24(1)	-3(1)	6(1)	-1(1)
C(30)	18(1)	13(1)	22(1)	2(1)	9(1)	2(1)
Fe(1)	13(1)	10(1)	16(1)	0(1)	4(1)	-1(1)

N(1)	28(1)	17(1)	18(1)	-3(1)	5(1)	-7(1)
P(1)	14(1)	11(1)	15(1)	1(1)	4(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for ($\text{R}_\text{C}, \text{S}_\text{Fc}, \text{R}_\text{P}$)-**2c**.

	x	y	z	U(eq)
H(1)	2782	2233	8347	25
H(2)	1819	1557	6185	24
H(3)	4114	209	6141	27
H(4)	6488	54	8277	27
H(5)	5650	1298	9636	27
H(7)	9442	1639	7928	20
H(8)	7479	1559	5683	20
H(9)	4916	2840	5279	19
H(11)	7112	3061	9657	20
H(12A)	10822	2413	9894	37
H(12B)	9165	1801	10114	37
H(12C)	10045	2643	10997	37
H(13A)	9721	4286	11193	52
H(13B)	7504	4429	10617	52
H(13C)	8935	5204	10438	52
H(14A)	10783	4883	9068	44
H(14B)	10651	3868	8491	44
H(14C)	11638	4008	9896	44
H(16)	7935	4409	6520	20
H(17)	9670	5666	6109	24
H(18)	8884	7173	6434	23
H(20)	6866	8280	7119	24
H(21)	4372	8569	7856	27
H(22)	2547	7318	8212	27
H(23)	3288	5810	7880	23
H(26)	3842	5077	5045	21
H(27)	1298	5042	3294	23
H(28)	-1302	4090	3186	22
H(29)	-1341	3182	4834	22
H(30)	1159	3257	6606	20

Table 6. Torsion angles [°] for (R_C,S_{Fe},R_P)-**2c**.

C(5)-C(1)-C(2)-C(3)	-0.5(2)
Fe(1)-C(1)-C(2)-C(3)	59.35(12)
C(5)-C(1)-C(2)-Fe(1)	-59.86(12)
C(1)-C(2)-C(3)-C(4)	0.13(19)
Fe(1)-C(2)-C(3)-C(4)	59.05(12)
C(1)-C(2)-C(3)-Fe(1)	-58.91(12)
C(2)-C(3)-C(4)-C(5)	0.29(19)
Fe(1)-C(3)-C(4)-C(5)	59.55(12)
C(2)-C(3)-C(4)-Fe(1)	-59.26(12)
C(2)-C(1)-C(5)-C(4)	0.7(2)
Fe(1)-C(1)-C(5)-C(4)	-59.20(12)
C(2)-C(1)-C(5)-Fe(1)	59.88(12)
C(3)-C(4)-C(5)-C(1)	-0.60(19)
Fe(1)-C(4)-C(5)-C(1)	59.05(12)
C(3)-C(4)-C(5)-Fe(1)	-59.65(12)
C(10)-C(6)-C(7)-C(8)	-1.12(18)
C(11)-C(6)-C(7)-C(8)	178.52(16)
Fe(1)-C(6)-C(7)-C(8)	58.88(11)
C(10)-C(6)-C(7)-Fe(1)	-59.99(11)
C(11)-C(6)-C(7)-Fe(1)	119.65(17)
C(6)-C(7)-C(8)-C(9)	0.66(18)
Fe(1)-C(7)-C(8)-C(9)	59.32(11)
C(6)-C(7)-C(8)-Fe(1)	-58.66(11)
C(7)-C(8)-C(9)-C(10)	0.06(18)
Fe(1)-C(8)-C(9)-C(10)	59.18(11)
C(7)-C(8)-C(9)-Fe(1)	-59.12(11)
C(8)-C(9)-C(10)-C(6)	-0.75(18)
Fe(1)-C(9)-C(10)-C(6)	58.29(11)
C(8)-C(9)-C(10)-P(1)	178.40(12)
Fe(1)-C(9)-C(10)-P(1)	-122.56(14)
C(8)-C(9)-C(10)-Fe(1)	-59.04(11)
C(7)-C(6)-C(10)-C(9)	1.14(18)
C(11)-C(6)-C(10)-C(9)	-178.52(15)
Fe(1)-C(6)-C(10)-C(9)	-58.69(11)

C(7)-C(6)-C(10)-P(1)	-178.05(12)
C(11)-C(6)-C(10)-P(1)	2.3(2)
Fe(1)-C(6)-C(10)-P(1)	122.12(13)
C(7)-C(6)-C(10)-Fe(1)	59.83(11)
C(11)-C(6)-C(10)-Fe(1)	-119.83(15)
C(7)-C(6)-C(11)-N(1)	120.42(18)
C(10)-C(6)-C(11)-N(1)	-60.0(2)
Fe(1)-C(6)-C(11)-N(1)	-148.25(12)
C(7)-C(6)-C(11)-C(12)	-8.3(2)
C(10)-C(6)-C(11)-C(12)	171.31(15)
Fe(1)-C(6)-C(11)-C(12)	83.06(17)
C(24)-C(15)-C(16)-C(17)	-0.1(3)
P(1)-C(15)-C(16)-C(17)	-179.97(13)
C(15)-C(16)-C(17)-C(18)	0.1(3)
C(16)-C(17)-C(18)-C(19)	0.1(3)
C(17)-C(18)-C(19)-C(20)	179.24(16)
C(17)-C(18)-C(19)-C(24)	-0.1(2)
C(18)-C(19)-C(20)-C(21)	179.77(17)
C(24)-C(19)-C(20)-C(21)	-0.8(3)
C(19)-C(20)-C(21)-C(22)	-0.7(3)
C(20)-C(21)-C(22)-C(23)	1.1(3)
C(21)-C(22)-C(23)-C(24)	0.2(3)
C(22)-C(23)-C(24)-C(19)	-1.7(3)
C(22)-C(23)-C(24)-C(15)	179.67(17)
C(18)-C(19)-C(24)-C(23)	-178.60(15)
C(20)-C(19)-C(24)-C(23)	2.0(2)
C(18)-C(19)-C(24)-C(15)	0.1(2)
C(20)-C(19)-C(24)-C(15)	-179.30(15)
C(16)-C(15)-C(24)-C(23)	178.64(16)
P(1)-C(15)-C(24)-C(23)	-1.5(2)
C(16)-C(15)-C(24)-C(19)	0.0(2)
P(1)-C(15)-C(24)-C(19)	179.89(11)
C(30)-C(25)-C(26)-C(27)	0.1(2)
P(1)-C(25)-C(26)-C(27)	-179.29(13)
C(25)-C(26)-C(27)-C(28)	-0.7(3)
C(26)-C(27)-C(28)-C(29)	0.2(3)

C(27)-C(28)-C(29)-C(30)	1.0(3)
C(28)-C(29)-C(30)-C(25)	-1.6(3)
C(26)-C(25)-C(30)-C(29)	1.1(2)
P(1)-C(25)-C(30)-C(29)	-179.52(13)
C(5)-C(1)-Fe(1)-C(6)	-82.84(12)
C(2)-C(1)-Fe(1)-C(6)	158.16(11)
C(5)-C(1)-Fe(1)-C(7)	-48.1(2)
C(2)-C(1)-Fe(1)-C(7)	-167.09(13)
C(5)-C(1)-Fe(1)-C(4)	37.53(12)
C(2)-C(1)-Fe(1)-C(4)	-81.47(12)
C(2)-C(1)-Fe(1)-C(5)	-119.00(16)
C(5)-C(1)-Fe(1)-C(8)	159.7(3)
C(2)-C(1)-Fe(1)-C(8)	40.7(3)
C(5)-C(1)-Fe(1)-C(9)	-167.42(11)
C(2)-C(1)-Fe(1)-C(9)	73.58(13)
C(5)-C(1)-Fe(1)-C(2)	119.00(16)
C(5)-C(1)-Fe(1)-C(3)	81.52(12)
C(2)-C(1)-Fe(1)-C(3)	-37.48(11)
C(5)-C(1)-Fe(1)-C(10)	-126.64(11)
C(2)-C(1)-Fe(1)-C(10)	114.35(11)
C(7)-C(6)-Fe(1)-C(1)	155.77(10)
C(10)-C(6)-Fe(1)-C(1)	-85.76(11)
C(11)-C(6)-Fe(1)-C(1)	32.09(17)
C(10)-C(6)-Fe(1)-C(7)	118.48(13)
C(11)-C(6)-Fe(1)-C(7)	-123.67(18)
C(7)-C(6)-Fe(1)-C(4)	73.38(12)
C(10)-C(6)-Fe(1)-C(4)	-168.14(10)
C(11)-C(6)-Fe(1)-C(4)	-50.29(17)
C(7)-C(6)-Fe(1)-C(5)	113.46(10)
C(10)-C(6)-Fe(1)-C(5)	-128.06(10)
C(11)-C(6)-Fe(1)-C(5)	-10.21(16)
C(7)-C(6)-Fe(1)-C(8)	-37.31(9)
C(10)-C(6)-Fe(1)-C(8)	81.17(10)
C(11)-C(6)-Fe(1)-C(8)	-160.98(16)
C(7)-C(6)-Fe(1)-C(9)	-80.92(10)
C(10)-C(6)-Fe(1)-C(9)	37.56(9)

C(11)-C(6)-Fe(1)-C(9)	155.41(16)
C(7)-C(6)-Fe(1)-C(2)	-172.01(14)
C(10)-C(6)-Fe(1)-C(2)	-53.53(19)
C(11)-C(6)-Fe(1)-C(2)	64.3(2)
C(7)-C(6)-Fe(1)-C(3)	45.4(3)
C(10)-C(6)-Fe(1)-C(3)	163.9(3)
C(11)-C(6)-Fe(1)-C(3)	-78.2(3)
C(7)-C(6)-Fe(1)-C(10)	-118.48(13)
C(11)-C(6)-Fe(1)-C(10)	117.85(18)
C(8)-C(7)-Fe(1)-C(1)	-170.21(14)
C(6)-C(7)-Fe(1)-C(1)	-50.22(19)
C(8)-C(7)-Fe(1)-C(6)	-119.99(13)
C(8)-C(7)-Fe(1)-C(4)	114.14(10)
C(6)-C(7)-Fe(1)-C(4)	-125.87(10)
C(8)-C(7)-Fe(1)-C(5)	156.65(10)
C(6)-C(7)-Fe(1)-C(5)	-83.36(11)
C(6)-C(7)-Fe(1)-C(8)	119.99(13)
C(8)-C(7)-Fe(1)-C(9)	-37.50(9)
C(6)-C(7)-Fe(1)-C(9)	82.49(10)
C(8)-C(7)-Fe(1)-C(2)	45.4(3)
C(6)-C(7)-Fe(1)-C(2)	165.4(3)
C(8)-C(7)-Fe(1)-C(3)	73.85(12)
C(6)-C(7)-Fe(1)-C(3)	-166.17(10)
C(8)-C(7)-Fe(1)-C(10)	-81.50(10)
C(6)-C(7)-Fe(1)-C(10)	38.49(9)
C(5)-C(4)-Fe(1)-C(1)	-37.58(11)
C(3)-C(4)-Fe(1)-C(1)	81.62(11)
C(5)-C(4)-Fe(1)-C(6)	71.86(13)
C(3)-C(4)-Fe(1)-C(6)	-168.94(10)
C(5)-C(4)-Fe(1)-C(7)	112.93(11)
C(3)-C(4)-Fe(1)-C(7)	-127.87(11)
C(3)-C(4)-Fe(1)-C(5)	119.20(15)
C(5)-C(4)-Fe(1)-C(8)	155.66(10)
C(3)-C(4)-Fe(1)-C(8)	-85.13(12)
C(5)-C(4)-Fe(1)-C(9)	-170.99(14)
C(3)-C(4)-Fe(1)-C(9)	-51.8(2)

C(5)-C(4)-Fe(1)-C(2)	-81.65(11)
C(3)-C(4)-Fe(1)-C(2)	37.56(10)
C(5)-C(4)-Fe(1)-C(3)	-119.20(15)
C(5)-C(4)-Fe(1)-C(10)	41.0(3)
C(3)-C(4)-Fe(1)-C(10)	160.2(2)
C(4)-C(5)-Fe(1)-C(1)	119.41(16)
C(1)-C(5)-Fe(1)-C(6)	113.85(11)
C(4)-C(5)-Fe(1)-C(6)	-126.74(11)
C(1)-C(5)-Fe(1)-C(7)	156.63(11)
C(4)-C(5)-Fe(1)-C(7)	-83.96(12)
C(1)-C(5)-Fe(1)-C(4)	-119.41(16)
C(1)-C(5)-Fe(1)-C(8)	-169.89(13)
C(4)-C(5)-Fe(1)-C(8)	-50.48(19)
C(1)-C(5)-Fe(1)-C(9)	43.8(3)
C(4)-C(5)-Fe(1)-C(9)	163.2(3)
C(1)-C(5)-Fe(1)-C(2)	-37.94(11)
C(4)-C(5)-Fe(1)-C(2)	81.47(12)
C(1)-C(5)-Fe(1)-C(3)	-81.61(12)
C(4)-C(5)-Fe(1)-C(3)	37.80(11)
C(1)-C(5)-Fe(1)-C(10)	73.17(13)
C(4)-C(5)-Fe(1)-C(10)	-167.42(10)
C(9)-C(8)-Fe(1)-C(1)	40.8(3)
C(7)-C(8)-Fe(1)-C(1)	160.3(3)
C(9)-C(8)-Fe(1)-C(6)	-82.03(10)
C(7)-C(8)-Fe(1)-C(6)	37.45(9)
C(9)-C(8)-Fe(1)-C(7)	-119.48(13)
C(9)-C(8)-Fe(1)-C(4)	157.38(10)
C(7)-C(8)-Fe(1)-C(4)	-83.14(11)
C(9)-C(8)-Fe(1)-C(5)	-167.85(14)
C(7)-C(8)-Fe(1)-C(5)	-48.37(18)
C(7)-C(8)-Fe(1)-C(9)	119.48(13)
C(9)-C(8)-Fe(1)-C(2)	73.64(12)
C(7)-C(8)-Fe(1)-C(2)	-166.88(10)
C(9)-C(8)-Fe(1)-C(3)	114.18(10)
C(7)-C(8)-Fe(1)-C(3)	-126.34(10)
C(9)-C(8)-Fe(1)-C(10)	-37.58(9)

C(7)-C(8)-Fe(1)-C(10)	81.90(10)
C(8)-C(9)-Fe(1)-C(1)	-168.57(10)
C(10)-C(9)-Fe(1)-C(1)	71.73(12)
C(8)-C(9)-Fe(1)-C(6)	81.74(10)
C(10)-C(9)-Fe(1)-C(6)	-37.97(9)
C(8)-C(9)-Fe(1)-C(7)	37.67(9)
C(10)-C(9)-Fe(1)-C(7)	-82.03(10)
C(8)-C(9)-Fe(1)-C(4)	-47.92(19)
C(10)-C(9)-Fe(1)-C(4)	-167.62(14)
C(8)-C(9)-Fe(1)-C(5)	156.4(3)
C(10)-C(9)-Fe(1)-C(5)	36.7(3)
C(10)-C(9)-Fe(1)-C(8)	-119.71(13)
C(8)-C(9)-Fe(1)-C(2)	-127.07(10)
C(10)-C(9)-Fe(1)-C(2)	113.23(10)
C(8)-C(9)-Fe(1)-C(3)	-83.96(11)
C(10)-C(9)-Fe(1)-C(3)	156.33(9)
C(8)-C(9)-Fe(1)-C(10)	119.71(13)
C(3)-C(2)-Fe(1)-C(1)	-119.32(16)
C(3)-C(2)-Fe(1)-C(6)	-165.49(14)
C(1)-C(2)-Fe(1)-C(6)	-46.2(2)
C(3)-C(2)-Fe(1)-C(7)	35.8(3)
C(1)-C(2)-Fe(1)-C(7)	155.1(3)
C(3)-C(2)-Fe(1)-C(4)	-37.81(12)
C(1)-C(2)-Fe(1)-C(4)	81.51(12)
C(3)-C(2)-Fe(1)-C(5)	-81.58(12)
C(1)-C(2)-Fe(1)-C(5)	37.74(12)
C(3)-C(2)-Fe(1)-C(8)	72.07(13)
C(1)-C(2)-Fe(1)-C(8)	-168.61(10)
C(3)-C(2)-Fe(1)-C(9)	113.40(11)
C(1)-C(2)-Fe(1)-C(9)	-127.28(11)
C(1)-C(2)-Fe(1)-C(3)	119.32(16)
C(3)-C(2)-Fe(1)-C(10)	156.99(11)
C(1)-C(2)-Fe(1)-C(10)	-83.69(12)
C(2)-C(3)-Fe(1)-C(1)	37.79(11)
C(4)-C(3)-Fe(1)-C(1)	-81.42(12)
C(2)-C(3)-Fe(1)-C(6)	154.7(2)

C(4)-C(3)-Fe(1)-C(6)	35.5(3)
C(2)-C(3)-Fe(1)-C(7)	-169.38(10)
C(4)-C(3)-Fe(1)-C(7)	71.40(13)
C(2)-C(3)-Fe(1)-C(4)	119.21(16)
C(2)-C(3)-Fe(1)-C(5)	81.60(12)
C(4)-C(3)-Fe(1)-C(5)	-37.61(11)
C(2)-C(3)-Fe(1)-C(8)	-128.01(11)
C(4)-C(3)-Fe(1)-C(8)	112.78(11)
C(2)-C(3)-Fe(1)-C(9)	-85.04(12)
C(4)-C(3)-Fe(1)-C(9)	155.75(11)
C(4)-C(3)-Fe(1)-C(2)	-119.21(16)
C(2)-C(3)-Fe(1)-C(10)	-49.3(2)
C(4)-C(3)-Fe(1)-C(10)	-168.51(14)
C(9)-C(10)-Fe(1)-C(1)	-128.45(10)
C(6)-C(10)-Fe(1)-C(1)	112.09(10)
P(1)-C(10)-Fe(1)-C(1)	-5.39(13)
C(9)-C(10)-Fe(1)-C(6)	119.45(13)
P(1)-C(10)-Fe(1)-C(6)	-117.49(15)
C(9)-C(10)-Fe(1)-C(7)	81.29(10)
C(6)-C(10)-Fe(1)-C(7)	-38.16(9)
P(1)-C(10)-Fe(1)-C(7)	-155.65(13)
C(9)-C(10)-Fe(1)-C(4)	158.3(3)
C(6)-C(10)-Fe(1)-C(4)	38.9(3)
P(1)-C(10)-Fe(1)-C(4)	-78.6(3)
C(9)-C(10)-Fe(1)-C(5)	-169.33(10)
C(6)-C(10)-Fe(1)-C(5)	71.22(12)
P(1)-C(10)-Fe(1)-C(5)	-46.27(14)
C(9)-C(10)-Fe(1)-C(8)	37.36(9)
C(6)-C(10)-Fe(1)-C(8)	-82.09(10)
P(1)-C(10)-Fe(1)-C(8)	160.42(13)
C(6)-C(10)-Fe(1)-C(9)	-119.45(13)
P(1)-C(10)-Fe(1)-C(9)	123.06(15)
C(9)-C(10)-Fe(1)-C(2)	-85.41(11)
C(6)-C(10)-Fe(1)-C(2)	155.14(10)
P(1)-C(10)-Fe(1)-C(2)	37.65(13)
C(9)-C(10)-Fe(1)-C(3)	-51.07(19)

C(6)-C(10)-Fe(1)-C(3)	-170.53(14)
P(1)-C(10)-Fe(1)-C(3)	71.99(19)
C(6)-C(11)-N(1)-C(13)	157.33(16)
C(12)-C(11)-N(1)-C(13)	-75.8(2)
C(6)-C(11)-N(1)-C(14)	-73.91(18)
C(12)-C(11)-N(1)-C(14)	53.0(2)
C(9)-C(10)-P(1)-C(15)	-88.96(16)
C(6)-C(10)-P(1)-C(15)	90.06(15)
Fe(1)-C(10)-P(1)-C(15)	178.49(10)
C(9)-C(10)-P(1)-C(25)	12.66(17)
C(6)-C(10)-P(1)-C(25)	-168.32(14)
Fe(1)-C(10)-P(1)-C(25)	-79.89(11)
C(16)-C(15)-P(1)-C(10)	5.72(16)
C(24)-C(15)-P(1)-C(10)	-174.15(13)
C(16)-C(15)-P(1)-C(25)	-96.23(15)
C(24)-C(15)-P(1)-C(25)	83.90(13)
C(26)-C(25)-P(1)-C(10)	-93.39(15)
C(30)-C(25)-P(1)-C(10)	87.22(14)
C(26)-C(25)-P(1)-C(15)	9.41(15)
C(30)-C(25)-P(1)-C(15)	-169.98(13)

Symmetry transformations used to generate equivalent atoms:

X-Ray crystal structure data for compound (R_C,S_{Fe},S_P)-6b

Table 1. Crystal data and structure refinement for (R_C,S_{Fe},S_P)-6b.

Identification code	(R _C ,S _{Fe} ,S _P)-6b	
Empirical formula	C ₄₀ H ₄₆ Fe P ₂	
Formula weight	644.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21	
Unit cell dimensions	a = 10.4857(17) Å	α = 90°.
	b = 11.0663(18) Å	β = 92.984(2)°.
	c = 28.974(5) Å	γ = 90°.
Volume	3357.5(9) Å ³	
Z	4	
Density (calculated)	1.275 Mg/m ³	
Absorption coefficient	0.572 mm ⁻¹	
F(000)	1368	
Theta range for data collection	3.81 to 25.10°.	
Index ranges	-12 ≤ h ≤ 11, -13 ≤ k ≤ 13, -34 ≤ l ≤ 24	
Reflections collected	12942	
Independent reflections	9533 [R(int) = 0.0372]	
Completeness to theta = 25.10°	89.3 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9533 / 1 / 720	
Goodness-of-fit on F ²	1.027	
Final R indices [I > 2σ(I)]	R1 = 0.0514, wR2 = 0.1079	
R indices (all data)	R1 = 0.0695, wR2 = 0.1161	
Absolute structure parameter	0.006(18)	
Largest diff. peak and hole	0.663 and -0.549 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (R_C, S_{Fe}, S_P)-**6b**. $U(eq)$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4470(2)	3612(2)	164(1)	24(1)
C(2)	5550(3)	2936(3)	291(1)	22(1)
C(3)	6352(2)	2537(3)	-45(1)	27(1)
C(4)	6074(2)	2814(3)	-507(1)	30(1)
C(5)	4995(2)	3489(2)	-634(1)	24(1)
C(6)	4193(2)	3888(2)	-299(1)	25(1)
C(7)	3113(2)	4563(2)	-426(1)	28(1)
C(8)	2835(2)	4840(3)	-888(1)	34(2)
C(9)	3638(3)	4441(3)	-1223(1)	37(2)
C(10)	4717(3)	3765(3)	-1096(1)	32(1)
C(11)	4468(5)	4270(5)	1116(2)	21(1)
C(12)	5222(5)	5304(5)	1102(2)	29(1)
C(13)	6030(5)	5621(5)	1467(2)	32(1)
C(14)	6131(5)	4909(5)	1856(2)	29(1)
C(15)	5416(5)	3867(5)	1878(2)	29(1)
C(16)	4577(5)	3555(5)	1513(2)	25(1)
C(17)	2663(5)	2531(5)	774(2)	22(1)
C(18)	3234(5)	1339(5)	747(2)	25(1)
C(19)	2332(5)	473(5)	887(2)	27(1)
C(20)	1217(5)	1101(5)	1011(2)	25(1)
C(21)	1403(5)	2371(5)	950(2)	21(1)
C(22)	1820(7)	416(7)	-241(2)	46(2)
C(23)	509(9)	350(8)	-91(2)	69(3)
C(24)	67(7)	1583(10)	-138(2)	67(3)
C(25)	1016(9)	2263(7)	-281(3)	62(2)
C(26)	2027(7)	1581(7)	-354(2)	47(2)
C(27)	527(4)	3355(4)	1095(2)	18(1)
C(28)	-896(4)	3089(5)	954(2)	22(1)
C(29)	723(5)	5354(5)	1760(2)	23(1)
C(30)	1895(5)	5993(5)	1588(2)	26(1)
C(31)	1845(6)	7354(5)	1684(2)	32(1)

C(32)	616(6)	7923(5)	1470(2)	34(2)
C(33)	-570(5)	7269(5)	1626(2)	32(1)
C(34)	-485(5)	5901(5)	1533(2)	27(1)
C(35)	-550(5)	3133(5)	2019(2)	23(1)
C(36)	-517(5)	1758(5)	2055(2)	31(1)
C(37)	-1657(5)	1240(5)	2299(2)	33(1)
C(38)	-1695(6)	1755(6)	2785(2)	40(2)
C(39)	-1729(6)	3128(6)	2768(2)	38(2)
C(40)	-603(5)	3650(5)	2511(2)	31(1)
C(41)	9445(3)	8848(3)	4780(1)	35(2)
C(42)	10490(3)	9525(3)	4655(1)	42(2)
C(43)	11378(3)	9931(3)	4993(2)	59(2)
C(44)	11221(3)	9661(3)	5455(1)	74(3)
C(45)	10176(3)	8984(3)	5580(1)	62(2)
C(46)	9288(3)	8578(2)	5242(1)	44(2)
C(47)	8243(3)	7901(3)	5366(1)	52(2)
C(48)	8086(4)	7631(4)	5828(1)	70(3)
C(49)	8974(5)	8037(4)	6166(1)	108(5)
C(50)	10019(5)	8714(4)	6042(1)	92(4)
C(51)	9218(5)	8041(5)	3831(2)	25(1)
C(52)	10069(5)	7083(5)	3892(2)	30(1)
C(53)	10751(5)	6663(6)	3523(2)	38(2)
C(54)	10601(6)	7196(6)	3099(2)	37(2)
C(55)	9768(6)	8162(5)	3036(2)	34(1)
C(56)	9090(5)	8590(5)	3406(2)	31(1)
C(57)	7488(5)	9831(5)	4136(2)	24(1)
C(58)	6160(5)	9922(4)	3980(2)	18(1)
C(59)	5930(5)	11161(5)	3853(2)	26(1)
C(60)	7088(5)	11814(5)	3940(2)	27(1)
C(61)	8037(5)	11021(5)	4109(2)	29(1)
C(62)	7133(5)	12037(5)	5117(2)	53(2)
C(63)	6987(7)	10800(5)	5233(2)	63(3)
C(64)	5708(9)	10459(7)	5110(2)	132(6)
C(65)	5064(4)	11485(11)	4918(2)	159(8)
C(66)	5945(8)	12460(6)	4922(2)	111(5)
C(67)	5244(5)	8868(5)	3915(2)	22(1)

C(68)	3880(5)	9195(5)	4032(2)	31(1)
C(69)	4489(5)	6815(5)	3329(2)	26(1)
C(70)	5075(5)	5925(5)	3684(2)	32(1)
C(71)	4379(6)	4701(5)	3681(2)	38(2)
C(72)	4303(6)	4146(6)	3198(2)	39(2)
C(73)	3693(6)	5029(5)	2847(2)	38(2)
C(74)	4427(5)	6219(5)	2849(2)	33(1)
C(75)	4547(5)	9349(5)	2953(2)	26(1)
C(76)	3094(5)	9182(5)	2883(2)	30(1)
C(77)	2507(6)	10283(6)	2638(2)	42(2)
C(78)	3092(5)	10523(6)	2176(2)	37(2)
C(79)	4546(6)	10633(5)	2243(2)	35(2)
C(80)	5137(5)	9527(5)	2485(2)	30(1)
Fe(1)	1594(1)	1434(1)	332(1)	23(1)
Fe(2)	6552(1)	11044(1)	4537(1)	24(1)
P(1)	3331(1)	3990(1)	629(1)	21(1)
P(2)	900(1)	3678(1)	1732(1)	21(1)
P(3)	8222(1)	8404(1)	4316(1)	25(1)
P(4)	5475(1)	8220(1)	3324(1)	23(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $(\text{R}_\text{C}, \text{S}_\text{Fe}, \text{S}_\text{P})$ -**6b**.

C(1)-C(2)	1.3900
C(1)-C(6)	1.3900
C(1)-P(1)	1.894(3)
C(2)-C(3)	1.3900
C(3)-C(4)	1.3900
C(4)-C(5)	1.3900
C(5)-C(6)	1.3900
C(5)-C(10)	1.3900
C(6)-C(7)	1.3900
C(7)-C(8)	1.3900
C(8)-C(9)	1.3900
C(9)-C(10)	1.3900
C(11)-C(12)	1.393(7)

C(11)-C(16)	1.396(7)
C(11)-P(1)	1.826(5)
C(12)-C(13)	1.366(7)
C(13)-C(14)	1.375(8)
C(14)-C(15)	1.378(7)
C(15)-C(16)	1.384(7)
C(17)-C(21)	1.451(7)
C(17)-C(18)	1.453(7)
C(17)-P(1)	1.817(5)
C(17)-Fe(1)	2.054(5)
C(18)-C(19)	1.421(7)
C(18)-Fe(1)	2.050(5)
C(19)-C(20)	1.423(7)
C(19)-Fe(1)	2.046(6)
C(20)-C(21)	1.431(7)
C(20)-Fe(1)	2.061(5)
C(21)-C(27)	1.500(7)
C(21)-Fe(1)	2.087(5)
C(22)-C(26)	1.350(9)
C(22)-C(23)	1.465(10)
C(22)-Fe(1)	2.030(6)
C(23)-C(24)	1.446(12)
C(23)-Fe(1)	2.022(6)
C(24)-C(25)	1.332(11)
C(24)-Fe(1)	2.054(7)
C(25)-C(26)	1.327(10)
C(25)-Fe(1)	2.063(8)
C(26)-Fe(1)	2.069(6)
C(27)-C(28)	1.555(6)
C(27)-P(2)	1.901(5)
C(29)-C(34)	1.523(7)
C(29)-C(30)	1.524(7)
C(29)-P(2)	1.866(5)
C(30)-C(31)	1.533(8)
C(31)-C(32)	1.535(8)
C(32)-C(33)	1.526(8)

C(33)-C(34)	1.541(7)
C(35)-C(36)	1.525(7)
C(35)-C(40)	1.540(7)
C(35)-P(2)	1.870(5)
C(36)-C(37)	1.532(7)
C(37)-C(38)	1.523(8)
C(38)-C(39)	1.521(8)
C(39)-C(40)	1.540(7)
C(41)-C(42)	1.3900
C(41)-C(46)	1.3900
C(41)-P(3)	1.874(3)
C(42)-C(43)	1.3900
C(43)-C(44)	1.3900
C(44)-C(45)	1.3900
C(45)-C(46)	1.3900
C(45)-C(50)	1.3900
C(46)-C(47)	1.3900
C(47)-C(48)	1.3900
C(48)-C(49)	1.3900
C(49)-C(50)	1.3900
C(51)-C(56)	1.373(7)
C(51)-C(52)	1.391(7)
C(51)-P(3)	1.838(5)
C(52)-C(53)	1.397(8)
C(53)-C(54)	1.364(8)
C(54)-C(55)	1.386(8)
C(55)-C(56)	1.400(7)
C(57)-C(61)	1.441(7)
C(57)-C(58)	1.444(7)
C(57)-P(3)	1.821(6)
C(57)-Fe(2)	2.057(5)
C(58)-C(59)	1.437(7)
C(58)-C(67)	1.518(7)
C(58)-Fe(2)	2.058(5)
C(59)-C(60)	1.424(7)
C(59)-Fe(2)	2.058(5)

C(60)-C(61)	1.396(7)
C(60)-Fe(2)	2.033(5)
C(61)-Fe(2)	2.041(5)
C(62)-C(63)	1.4200
C(62)-C(66)	1.4200
C(62)-Fe(2)	2.073(4)
C(63)-C(64)	1.4200
C(63)-Fe(2)	2.063(5)
C(64)-C(65)	1.4200
C(64)-Fe(2)	2.029(5)
C(65)-C(66)	1.4200
C(65)-Fe(2)	2.018(5)
C(66)-Fe(2)	2.045(5)
C(67)-C(68)	1.531(7)
C(67)-P(4)	1.883(5)
C(69)-C(70)	1.528(7)
C(69)-C(74)	1.539(7)
C(69)-P(4)	1.867(5)
C(70)-C(71)	1.538(8)
C(71)-C(72)	1.525(8)
C(72)-C(73)	1.528(8)
C(73)-C(74)	1.526(8)
C(75)-C(80)	1.531(7)
C(75)-C(76)	1.538(7)
C(75)-P(4)	1.886(5)
C(76)-C(77)	1.524(8)
C(77)-C(78)	1.525(8)
C(78)-C(79)	1.531(8)
C(79)-C(80)	1.526(8)
C(2)-C(1)-C(6)	120.0
C(2)-C(1)-P(1)	117.75(12)
C(6)-C(1)-P(1)	121.96(12)
C(1)-C(2)-C(3)	120.0
C(2)-C(3)-C(4)	120.0
C(3)-C(4)-C(5)	120.0

C(6)-C(5)-C(4)	120.0
C(6)-C(5)-C(10)	120.0
C(4)-C(5)-C(10)	120.0
C(7)-C(6)-C(5)	120.0
C(7)-C(6)-C(1)	120.0
C(5)-C(6)-C(1)	120.0
C(6)-C(7)-C(8)	120.0
C(9)-C(8)-C(7)	120.0
C(10)-C(9)-C(8)	120.0
C(9)-C(10)-C(5)	120.0
C(12)-C(11)-C(16)	117.9(5)
C(12)-C(11)-P(1)	117.8(4)
C(16)-C(11)-P(1)	124.2(4)
C(13)-C(12)-C(11)	121.2(5)
C(12)-C(13)-C(14)	120.4(5)
C(13)-C(14)-C(15)	119.9(5)
C(14)-C(15)-C(16)	120.0(5)
C(15)-C(16)-C(11)	120.6(5)
C(21)-C(17)-C(18)	107.1(4)
C(21)-C(17)-P(1)	123.9(4)
C(18)-C(17)-P(1)	129.0(4)
C(21)-C(17)-Fe(1)	70.7(3)
C(18)-C(17)-Fe(1)	69.1(3)
P(1)-C(17)-Fe(1)	125.8(3)
C(19)-C(18)-C(17)	108.3(4)
C(19)-C(18)-Fe(1)	69.6(3)
C(17)-C(18)-Fe(1)	69.4(3)
C(18)-C(19)-C(20)	108.1(5)
C(18)-C(19)-Fe(1)	69.9(3)
C(20)-C(19)-Fe(1)	70.3(3)
C(19)-C(20)-C(21)	109.2(5)
C(19)-C(20)-Fe(1)	69.2(3)
C(21)-C(20)-Fe(1)	70.8(3)
C(20)-C(21)-C(17)	107.3(5)
C(20)-C(21)-C(27)	126.0(5)
C(17)-C(21)-C(27)	126.3(5)

C(20)-C(21)-Fe(1)	68.8(3)
C(17)-C(21)-Fe(1)	68.3(3)
C(27)-C(21)-Fe(1)	133.6(4)
C(26)-C(22)-C(23)	106.6(6)
C(26)-C(22)-Fe(1)	72.3(4)
C(23)-C(22)-Fe(1)	68.5(4)
C(24)-C(23)-C(22)	103.1(6)
C(24)-C(23)-Fe(1)	70.4(4)
C(22)-C(23)-Fe(1)	69.1(4)
C(25)-C(24)-C(23)	108.7(7)
C(25)-C(24)-Fe(1)	71.5(4)
C(23)-C(24)-Fe(1)	68.0(4)
C(26)-C(25)-C(24)	110.1(8)
C(26)-C(25)-Fe(1)	71.5(4)
C(24)-C(25)-Fe(1)	70.7(5)
C(25)-C(26)-C(22)	111.4(7)
C(25)-C(26)-Fe(1)	71.0(5)
C(22)-C(26)-Fe(1)	69.3(4)
C(21)-C(27)-C(28)	112.4(4)
C(21)-C(27)-P(2)	108.1(3)
C(28)-C(27)-P(2)	116.0(3)
C(34)-C(29)-C(30)	109.9(4)
C(34)-C(29)-P(2)	117.3(4)
C(30)-C(29)-P(2)	111.3(4)
C(29)-C(30)-C(31)	111.2(4)
C(30)-C(31)-C(32)	111.4(4)
C(33)-C(32)-C(31)	111.5(5)
C(32)-C(33)-C(34)	111.0(5)
C(29)-C(34)-C(33)	111.7(4)
C(36)-C(35)-C(40)	108.0(4)
C(36)-C(35)-P(2)	109.6(4)
C(40)-C(35)-P(2)	111.1(4)
C(35)-C(36)-C(37)	112.9(4)
C(38)-C(37)-C(36)	110.2(5)
C(39)-C(38)-C(37)	110.2(5)
C(38)-C(39)-C(40)	111.9(5)

C(39)-C(40)-C(35)	111.9(5)
C(42)-C(41)-C(46)	120.0
C(42)-C(41)-P(3)	118.32(15)
C(46)-C(41)-P(3)	121.57(15)
C(41)-C(42)-C(43)	120.0
C(42)-C(43)-C(44)	120.0
C(45)-C(44)-C(43)	120.0
C(44)-C(45)-C(46)	120.0
C(44)-C(45)-C(50)	120.0
C(46)-C(45)-C(50)	120.0
C(47)-C(46)-C(45)	120.0
C(47)-C(46)-C(41)	120.0
C(45)-C(46)-C(41)	120.0
C(46)-C(47)-C(48)	120.0
C(49)-C(48)-C(47)	120.0
C(48)-C(49)-C(50)	120.0
C(49)-C(50)-C(45)	120.0
C(56)-C(51)-C(52)	118.9(5)
C(56)-C(51)-P(3)	123.8(4)
C(52)-C(51)-P(3)	117.1(4)
C(51)-C(52)-C(53)	120.4(5)
C(54)-C(53)-C(52)	120.4(6)
C(53)-C(54)-C(55)	119.6(6)
C(54)-C(55)-C(56)	120.1(6)
C(51)-C(56)-C(55)	120.5(5)
C(61)-C(57)-C(58)	107.5(5)
C(61)-C(57)-P(3)	130.1(4)
C(58)-C(57)-P(3)	122.4(4)
C(61)-C(57)-Fe(2)	68.8(3)
C(58)-C(57)-Fe(2)	69.5(3)
P(3)-C(57)-Fe(2)	127.7(3)
C(59)-C(58)-C(57)	107.1(4)
C(59)-C(58)-C(67)	127.2(4)
C(57)-C(58)-C(67)	125.4(4)
C(59)-C(58)-Fe(2)	69.5(3)
C(57)-C(58)-Fe(2)	69.4(3)

C(67)-C(58)-Fe(2)	131.4(4)
C(60)-C(59)-C(58)	107.9(5)
C(60)-C(59)-Fe(2)	68.7(3)
C(58)-C(59)-Fe(2)	69.6(3)
C(61)-C(60)-C(59)	109.2(5)
C(61)-C(60)-Fe(2)	70.3(3)
C(59)-C(60)-Fe(2)	70.6(3)
C(60)-C(61)-C(57)	108.3(5)
C(60)-C(61)-Fe(2)	69.6(3)
C(57)-C(61)-Fe(2)	70.0(3)
C(63)-C(62)-C(66)	108.0
C(63)-C(62)-Fe(2)	69.5(2)
C(66)-C(62)-Fe(2)	68.8(2)
C(62)-C(63)-C(64)	108.0
C(62)-C(63)-Fe(2)	70.3(2)
C(64)-C(63)-Fe(2)	68.43(19)
C(65)-C(64)-C(63)	108.0
C(65)-C(64)-Fe(2)	69.0(2)
C(63)-C(64)-Fe(2)	70.97(18)
C(64)-C(65)-C(66)	108.0
C(64)-C(65)-Fe(2)	69.9(2)
C(66)-C(65)-Fe(2)	70.6(2)
C(62)-C(66)-C(65)	108.0
C(62)-C(66)-Fe(2)	70.86(19)
C(65)-C(66)-Fe(2)	68.52(19)
C(58)-C(67)-C(68)	112.5(4)
C(58)-C(67)-P(4)	107.2(3)
C(68)-C(67)-P(4)	117.3(4)
C(70)-C(69)-C(74)	109.2(4)
C(70)-C(69)-P(4)	109.8(4)
C(74)-C(69)-P(4)	110.3(4)
C(69)-C(70)-C(71)	113.0(5)
C(72)-C(71)-C(70)	111.2(5)
C(71)-C(72)-C(73)	110.7(5)
C(74)-C(73)-C(72)	110.9(5)
C(73)-C(74)-C(69)	111.7(4)

C(80)-C(75)-C(76)	110.1(4)
C(80)-C(75)-P(4)	111.8(4)
C(76)-C(75)-P(4)	118.2(4)
C(77)-C(76)-C(75)	109.8(4)
C(76)-C(77)-C(78)	112.1(5)
C(77)-C(78)-C(79)	110.3(5)
C(80)-C(79)-C(78)	111.8(5)
C(79)-C(80)-C(75)	109.7(5)
C(23)-Fe(1)-C(22)	42.4(3)
C(23)-Fe(1)-C(19)	110.2(3)
C(22)-Fe(1)-C(19)	107.4(3)
C(23)-Fe(1)-C(18)	138.9(3)
C(22)-Fe(1)-C(18)	108.7(2)
C(19)-Fe(1)-C(18)	40.6(2)
C(23)-Fe(1)-C(24)	41.5(3)
C(22)-Fe(1)-C(24)	67.8(3)
C(19)-Fe(1)-C(24)	144.4(4)
C(18)-Fe(1)-C(24)	174.1(3)
C(23)-Fe(1)-C(17)	178.6(3)
C(22)-Fe(1)-C(17)	139.0(3)
C(19)-Fe(1)-C(17)	69.2(2)
C(18)-Fe(1)-C(17)	41.5(2)
C(24)-Fe(1)-C(17)	138.3(3)
C(23)-Fe(1)-C(20)	110.0(2)
C(22)-Fe(1)-C(20)	135.9(3)
C(19)-Fe(1)-C(20)	40.5(2)
C(18)-Fe(1)-C(20)	68.1(2)
C(24)-Fe(1)-C(20)	117.7(3)
C(17)-Fe(1)-C(20)	68.7(2)
C(23)-Fe(1)-C(25)	67.1(3)
C(22)-Fe(1)-C(25)	65.4(3)
C(19)-Fe(1)-C(25)	172.1(3)
C(18)-Fe(1)-C(25)	136.7(3)
C(24)-Fe(1)-C(25)	37.8(3)
C(17)-Fe(1)-C(25)	113.6(3)
C(20)-Fe(1)-C(25)	147.1(3)

C(23)-Fe(1)-C(26)	67.0(3)
C(22)-Fe(1)-C(26)	38.4(3)
C(19)-Fe(1)-C(26)	134.7(3)
C(18)-Fe(1)-C(26)	110.4(3)
C(24)-Fe(1)-C(26)	63.9(3)
C(17)-Fe(1)-C(26)	114.4(2)
C(20)-Fe(1)-C(26)	174.0(3)
C(25)-Fe(1)-C(26)	37.5(3)
C(23)-Fe(1)-C(21)	137.6(3)
C(22)-Fe(1)-C(21)	175.8(3)
C(19)-Fe(1)-C(21)	68.5(2)
C(18)-Fe(1)-C(21)	68.7(2)
C(24)-Fe(1)-C(21)	115.0(3)
C(17)-Fe(1)-C(21)	41.01(19)
C(20)-Fe(1)-C(21)	40.4(2)
C(25)-Fe(1)-C(21)	118.7(3)
C(26)-Fe(1)-C(21)	145.2(3)
C(65)-Fe(2)-C(64)	41.08(9)
C(65)-Fe(2)-C(60)	128.3(3)
C(64)-Fe(2)-C(60)	169.1(4)
C(65)-Fe(2)-C(61)	166.4(4)
C(64)-Fe(2)-C(61)	150.8(4)
C(60)-Fe(2)-C(61)	40.1(2)
C(65)-Fe(2)-C(66)	40.90(9)
C(64)-Fe(2)-C(66)	68.65(11)
C(60)-Fe(2)-C(66)	104.5(2)
C(61)-Fe(2)-C(66)	127.6(3)
C(65)-Fe(2)-C(59)	107.3(2)
C(64)-Fe(2)-C(59)	132.8(3)
C(60)-Fe(2)-C(59)	40.7(2)
C(61)-Fe(2)-C(59)	68.2(2)
C(66)-Fe(2)-C(59)	112.7(2)
C(65)-Fe(2)-C(57)	150.7(3)
C(64)-Fe(2)-C(57)	119.7(3)
C(60)-Fe(2)-C(57)	68.4(2)
C(61)-Fe(2)-C(57)	41.2(2)

C(66)-Fe(2)-C(57)	168.3(3)
C(59)-Fe(2)-C(57)	68.5(2)
C(65)-Fe(2)-C(58)	116.5(2)
C(64)-Fe(2)-C(58)	111.8(2)
C(60)-Fe(2)-C(58)	68.9(2)
C(61)-Fe(2)-C(58)	69.1(2)
C(66)-Fe(2)-C(58)	146.6(2)
C(59)-Fe(2)-C(58)	40.9(2)
C(57)-Fe(2)-C(58)	41.1(2)
C(65)-Fe(2)-C(63)	68.52(11)
C(64)-Fe(2)-C(63)	40.60(9)
C(60)-Fe(2)-C(63)	146.1(3)
C(61)-Fe(2)-C(63)	117.1(2)
C(66)-Fe(2)-C(63)	68.01(10)
C(59)-Fe(2)-C(63)	173.2(3)
C(57)-Fe(2)-C(63)	112.3(2)
C(58)-Fe(2)-C(63)	135.4(2)
C(65)-Fe(2)-C(62)	68.33(10)
C(64)-Fe(2)-C(62)	68.13(10)
C(60)-Fe(2)-C(62)	112.6(2)
C(61)-Fe(2)-C(62)	107.3(2)
C(66)-Fe(2)-C(62)	40.34(8)
C(59)-Fe(2)-C(62)	144.3(2)
C(57)-Fe(2)-C(62)	132.4(2)
C(58)-Fe(2)-C(62)	173.0(2)
C(63)-Fe(2)-C(62)	40.17(8)
C(17)-P(1)-C(11)	102.5(2)
C(17)-P(1)-C(1)	103.49(19)
C(11)-P(1)-C(1)	100.19(18)
C(29)-P(2)-C(35)	102.5(2)
C(29)-P(2)-C(27)	102.3(2)
C(35)-P(2)-C(27)	103.9(2)
C(57)-P(3)-C(51)	102.6(3)
C(57)-P(3)-C(41)	103.9(2)
C(51)-P(3)-C(41)	102.2(2)
C(69)-P(4)-C(67)	102.2(2)

C(69)-P(4)-C(75)	106.7(2)
C(67)-P(4)-C(75)	100.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (R_C, S_{Fc}, S_P) -**6b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(3)	19(3)	29(3)	-5(2)	5(2)	-6(2)
C(2)	23(3)	17(3)	26(3)	0(2)	3(2)	-8(2)
C(3)	19(3)	24(3)	39(4)	-1(3)	4(3)	-5(2)
C(4)	32(3)	25(3)	34(3)	-6(3)	15(3)	-9(3)
C(5)	24(3)	23(3)	27(3)	0(3)	8(2)	-8(2)
C(6)	28(3)	19(3)	26(3)	-4(3)	-4(3)	-11(2)
C(7)	36(3)	23(3)	26(3)	2(3)	6(3)	-5(3)
C(8)	39(4)	26(3)	38(4)	6(3)	1(3)	2(3)
C(9)	52(4)	37(4)	22(3)	5(3)	3(3)	-13(3)
C(10)	36(3)	30(3)	31(3)	5(3)	10(3)	-6(3)
C(11)	16(3)	23(3)	25(3)	2(2)	4(2)	1(2)
C(12)	26(3)	25(3)	34(4)	5(3)	2(3)	0(3)
C(13)	26(3)	21(3)	47(4)	0(3)	-3(3)	-5(2)
C(14)	28(3)	27(3)	33(4)	0(3)	-4(3)	4(3)
C(15)	29(3)	36(4)	21(3)	7(3)	-2(2)	-1(3)
C(16)	16(3)	22(3)	37(3)	0(3)	-1(2)	-8(2)
C(17)	18(3)	26(3)	21(3)	-1(2)	5(2)	-1(2)
C(18)	20(3)	28(3)	26(3)	3(3)	0(2)	6(2)
C(19)	33(3)	15(3)	33(3)	3(3)	5(3)	0(2)
C(20)	28(3)	17(3)	31(3)	5(3)	3(2)	-3(3)
C(21)	21(3)	21(3)	21(3)	5(2)	1(2)	-2(2)
C(22)	55(5)	46(4)	37(4)	-15(4)	-6(4)	19(4)
C(23)	110(7)	66(6)	31(4)	-1(4)	-6(4)	-78(6)
C(24)	26(4)	132(9)	44(5)	-39(5)	-8(3)	19(5)
C(25)	82(6)	46(5)	55(5)	-19(4)	-29(5)	8(5)
C(26)	56(4)	54(5)	31(4)	-3(4)	0(3)	-20(4)

C(27)	16(3)	10(3)	27(3)	1(2)	4(2)	-1(2)
C(28)	22(3)	18(3)	25(3)	-2(2)	-4(2)	1(2)
C(29)	25(3)	22(3)	21(3)	-3(2)	2(2)	-3(2)
C(30)	27(3)	23(3)	28(3)	1(3)	4(2)	-1(3)
C(31)	46(4)	30(3)	21(3)	-2(3)	7(3)	-15(3)
C(32)	47(4)	25(3)	30(3)	-1(3)	-2(3)	-4(3)
C(33)	31(3)	20(3)	45(4)	-2(3)	4(3)	8(3)
C(34)	21(3)	23(3)	35(3)	1(3)	0(2)	-2(2)
C(35)	24(3)	26(3)	19(3)	4(2)	4(2)	1(2)
C(36)	33(3)	24(3)	37(4)	13(3)	10(3)	3(3)
C(37)	42(3)	22(3)	37(3)	8(3)	6(3)	-4(3)
C(38)	35(4)	55(5)	29(3)	21(3)	2(3)	-6(3)
C(39)	43(4)	51(4)	20(3)	1(3)	-2(3)	-9(3)
C(40)	29(3)	40(4)	23(3)	5(3)	1(2)	-7(3)
C(41)	35(4)	32(3)	37(4)	-6(3)	-3(3)	16(3)
C(42)	45(4)	29(4)	50(4)	-10(3)	-14(3)	15(3)
C(43)	39(4)	45(4)	91(7)	-37(4)	-20(4)	23(3)
C(44)	80(6)	77(6)	59(6)	-44(5)	-47(5)	58(5)
C(45)	70(5)	71(6)	43(5)	-18(4)	-18(4)	49(5)
C(46)	53(4)	46(4)	31(4)	-2(3)	-8(3)	32(4)
C(47)	78(5)	49(5)	30(4)	6(3)	3(4)	34(4)
C(48)	118(7)	60(5)	32(4)	7(4)	13(5)	47(5)
C(49)	183(11)	116(9)	25(4)	9(5)	9(6)	124(9)
C(50)	127(8)	110(8)	34(5)	-18(5)	-31(5)	87(7)
C(51)	20(3)	25(3)	29(3)	-2(3)	4(2)	-4(2)
C(52)	33(3)	28(3)	28(3)	5(3)	5(3)	4(3)
C(53)	31(3)	32(4)	52(4)	1(3)	19(3)	2(3)
C(54)	32(3)	39(4)	42(4)	-10(3)	17(3)	-10(3)
C(55)	39(4)	39(4)	25(3)	-2(3)	8(3)	-8(3)
C(56)	29(3)	31(3)	33(3)	-4(3)	3(3)	4(3)
C(57)	35(3)	25(3)	13(3)	-1(2)	5(2)	-4(3)
C(58)	21(3)	19(3)	14(3)	2(2)	0(2)	4(2)
C(59)	33(3)	24(3)	21(3)	3(3)	-2(2)	2(3)
C(60)	30(3)	23(3)	28(3)	0(3)	5(3)	1(3)
C(61)	28(3)	32(3)	27(3)	1(3)	1(2)	-7(3)
C(62)	79(5)	62(5)	17(3)	-19(3)	7(3)	-30(4)

C(63)	116(7)	56(5)	19(3)	1(3)	25(4)	61(5)
C(64)	221(15)	139(10)	43(6)	-61(7)	88(8)	-145(11)
C(65)	48(5)	360(20)	71(8)	-141(12)	28(5)	-21(10)
C(66)	210(12)	102(8)	20(4)	-24(5)	-21(6)	128(9)
C(67)	27(3)	20(3)	20(3)	2(2)	1(2)	0(2)
C(68)	36(3)	32(3)	26(3)	0(3)	10(3)	2(3)
C(69)	32(3)	25(3)	20(3)	-1(2)	0(2)	0(2)
C(70)	44(4)	28(3)	26(3)	-1(3)	3(3)	1(3)
C(71)	57(4)	23(3)	35(4)	0(3)	4(3)	-5(3)
C(72)	47(4)	34(4)	35(4)	-6(3)	6(3)	1(3)
C(73)	45(4)	35(4)	34(4)	-10(3)	3(3)	-1(3)
C(74)	39(3)	32(4)	27(3)	-5(3)	3(3)	3(3)
C(75)	29(3)	26(3)	22(3)	3(3)	2(2)	-6(3)
C(76)	27(3)	28(3)	33(3)	6(3)	-3(3)	-8(3)
C(77)	33(4)	40(4)	52(4)	13(3)	-1(3)	-1(3)
C(78)	36(4)	35(4)	39(4)	13(3)	-6(3)	-1(3)
C(79)	50(4)	27(3)	28(3)	2(3)	9(3)	-4(3)
C(80)	40(4)	28(3)	22(3)	10(3)	6(3)	-2(3)
Fe(1)	23(1)	18(1)	28(1)	-4(1)	2(1)	-3(1)
Fe(2)	26(1)	22(1)	25(1)	-4(1)	1(1)	1(1)
P(1)	22(1)	17(1)	23(1)	1(1)	1(1)	-2(1)
P(2)	21(1)	19(1)	22(1)	2(1)	1(1)	0(1)
P(3)	29(1)	25(1)	22(1)	1(1)	2(1)	7(1)
P(4)	25(1)	24(1)	21(1)	0(1)	1(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for (R_C, S_{Fe}, S_P)-**6b**.

	x	y	z	U(eq)
H(2)	5739	2748	607	26
H(3)	7090	2076	42	33
H(4)	6623	2541	-736	36
H(7)	2564	4836	-196	34

H(8)	2097	5301	-975	41
H(9)	3448	4630	-1539	44
H(10)	5266	3493	-1326	39
H(12)	5174	5798	834	34
H(13)	6525	6337	1452	38
H(14)	6692	5134	2110	35
H(15)	5498	3364	2144	35
H(16)	4071	2846	1533	30
H(18)	4107	1158	642	29
H(19)	2461	-422	899	32
H(20)	423	715	1119	31
H(22)	2425	-274	-271	55
H(23)	13	-383	-8	83
H(24)	-804	1879	-69	81
H(25)	971	3157	-331	75
H(26)	2855	1897	-461	57
H(27)	764	4099	923	22
H(28A)	-982	2919	621	33
H(28B)	-1418	3793	1024	33
H(28C)	-1185	2387	1126	33
H(29)	703	5557	2096	27
H(30A)	1940	5857	1251	31
H(30B)	2675	5648	1743	31
H(31A)	2593	7750	1554	38
H(31B)	1891	7492	2022	38
H(32A)	577	8783	1563	41
H(32B)	629	7889	1129	41
H(33A)	-1338	7603	1458	38
H(33B)	-657	7408	1960	38
H(34A)	-1241	5494	1653	32
H(34B)	-495	5760	1195	32
H(35)	-1332	3385	1831	27
H(36A)	282	1511	2227	37
H(36B)	-506	1411	1740	37
H(37A)	-2459	1444	2120	40
H(37B)	-1586	348	2315	40

H(38A)	-2461	1452	2934	48
H(38B)	-931	1486	2973	48
H(39A)	-1700	3451	3087	46
H(39B)	-2542	3393	2610	46
H(40A)	206	3462	2688	37
H(40B)	-687	4540	2493	37
H(42)	10597	9709	4340	50
H(43)	12092	10393	4908	71
H(44)	11828	9938	5686	88
H(47)	7636	7623	5135	63
H(48)	7372	7168	5913	84
H(49)	8867	7852	6482	129
H(50)	10626	8991	6272	110
H(52)	10188	6713	4187	35
H(53)	11322	6003	3567	45
H(54)	11065	6907	2849	44
H(55)	9656	8533	2741	41
H(56)	8538	9266	3363	37
H(59)	5097	11507	3732	31
H(60)	7203	12700	3888	33
H(61)	8942	11242	4197	35
H(62)	7938	12519	5156	63
H(63)	7669	10259	5371	75
H(64)	5326	9642	5154	158
H(65)	4147	11519	4806	191
H(66)	5762	13297	4807	134
H(67)	5541	8235	4142	27
H(68A)	3871	9433	4358	46
H(68B)	3321	8494	3977	46
H(68C)	3573	9869	3837	46
H(69)	3605	7026	3415	31
H(70A)	5051	6286	3996	39
H(70B)	5981	5790	3618	39
H(71A)	4839	4143	3898	46
H(71B)	3505	4816	3787	46
H(72A)	3791	3395	3201	47

H(72B)	5172	3934	3108	47
H(73A)	3685	4666	2534	46
H(73B)	2797	5185	2922	46
H(74A)	4006	6778	2621	39
H(74B)	5305	6068	2753	39
H(75)	4663	10139	3116	31
H(76A)	2906	8448	2696	35
H(76B)	2716	9077	3187	35
H(77A)	2635	11001	2839	50
H(77B)	1576	10155	2585	50
H(78A)	2736	11279	2040	44
H(78B)	2874	9853	1960	44
H(79A)	4916	10731	1937	42
H(79B)	4760	11364	2428	42
H(80A)	6071	9640	2531	36
H(80B)	4981	8802	2290	36

Table 6. Torsion angles [°] for (R_C,S_{Fe},S_P)-**6b**.

C(6)-C(1)-C(2)-C(3)	0.0
P(1)-C(1)-C(2)-C(3)	173.90(19)
C(1)-C(2)-C(3)-C(4)	0.0
C(2)-C(3)-C(4)-C(5)	0.0
C(3)-C(4)-C(5)-C(6)	0.0
C(3)-C(4)-C(5)-C(10)	180.0
C(4)-C(5)-C(6)-C(7)	180.0
C(10)-C(5)-C(6)-C(7)	0.0
C(4)-C(5)-C(6)-C(1)	0.0
C(10)-C(5)-C(6)-C(1)	180.0
C(2)-C(1)-C(6)-C(7)	180.0
P(1)-C(1)-C(6)-C(7)	6.4(2)
C(2)-C(1)-C(6)-C(5)	0.0
P(1)-C(1)-C(6)-C(5)	-173.6(2)
C(5)-C(6)-C(7)-C(8)	0.0
C(1)-C(6)-C(7)-C(8)	180.0

C(6)-C(7)-C(8)-C(9)	0.0
C(7)-C(8)-C(9)-C(10)	0.0
C(8)-C(9)-C(10)-C(5)	0.0
C(6)-C(5)-C(10)-C(9)	0.0
C(4)-C(5)-C(10)-C(9)	180.0
C(16)-C(11)-C(12)-C(13)	-1.0(8)
P(1)-C(11)-C(12)-C(13)	175.4(4)
C(11)-C(12)-C(13)-C(14)	1.1(9)
C(12)-C(13)-C(14)-C(15)	0.2(8)
C(13)-C(14)-C(15)-C(16)	-1.5(8)
C(14)-C(15)-C(16)-C(11)	1.5(8)
C(12)-C(11)-C(16)-C(15)	-0.3(8)
P(1)-C(11)-C(16)-C(15)	-176.4(4)
C(21)-C(17)-C(18)-C(19)	2.0(6)
P(1)-C(17)-C(18)-C(19)	-178.6(4)
Fe(1)-C(17)-C(18)-C(19)	-58.8(4)
C(21)-C(17)-C(18)-Fe(1)	60.8(3)
P(1)-C(17)-C(18)-Fe(1)	-119.8(4)
C(17)-C(18)-C(19)-C(20)	-1.4(6)
Fe(1)-C(18)-C(19)-C(20)	-60.1(4)
C(17)-C(18)-C(19)-Fe(1)	58.8(3)
C(18)-C(19)-C(20)-C(21)	0.2(6)
Fe(1)-C(19)-C(20)-C(21)	-59.7(4)
C(18)-C(19)-C(20)-Fe(1)	59.9(4)
C(19)-C(20)-C(21)-C(17)	1.0(6)
Fe(1)-C(20)-C(21)-C(17)	-57.6(3)
C(19)-C(20)-C(21)-C(27)	-172.1(5)
Fe(1)-C(20)-C(21)-C(27)	129.2(5)
C(19)-C(20)-C(21)-Fe(1)	58.7(4)
C(18)-C(17)-C(21)-C(20)	-1.8(6)
P(1)-C(17)-C(21)-C(20)	178.7(4)
Fe(1)-C(17)-C(21)-C(20)	58.0(4)
C(18)-C(17)-C(21)-C(27)	171.3(5)
P(1)-C(17)-C(21)-C(27)	-8.2(7)
Fe(1)-C(17)-C(21)-C(27)	-128.9(5)
C(18)-C(17)-C(21)-Fe(1)	-59.8(3)

P(1)-C(17)-C(21)-Fe(1)	120.8(4)
C(26)-C(22)-C(23)-C(24)	0.1(7)
Fe(1)-C(22)-C(23)-C(24)	62.8(4)
C(26)-C(22)-C(23)-Fe(1)	-62.7(5)
C(22)-C(23)-C(24)-C(25)	-1.8(8)
Fe(1)-C(23)-C(24)-C(25)	60.1(5)
C(22)-C(23)-C(24)-Fe(1)	-61.9(4)
C(23)-C(24)-C(25)-C(26)	2.9(9)
Fe(1)-C(24)-C(25)-C(26)	60.9(5)
C(23)-C(24)-C(25)-Fe(1)	-58.0(5)
C(24)-C(25)-C(26)-C(22)	-3.0(9)
Fe(1)-C(25)-C(26)-C(22)	57.5(5)
C(24)-C(25)-C(26)-Fe(1)	-60.5(6)
C(23)-C(22)-C(26)-C(25)	1.7(8)
Fe(1)-C(22)-C(26)-C(25)	-58.5(5)
C(23)-C(22)-C(26)-Fe(1)	60.2(5)
C(20)-C(21)-C(27)-C(28)	-46.6(7)
C(17)-C(21)-C(27)-C(28)	141.5(5)
Fe(1)-C(21)-C(27)-C(28)	47.7(6)
C(20)-C(21)-C(27)-P(2)	82.7(6)
C(17)-C(21)-C(27)-P(2)	-89.1(5)
Fe(1)-C(21)-C(27)-P(2)	177.1(3)
C(34)-C(29)-C(30)-C(31)	57.6(6)
P(2)-C(29)-C(30)-C(31)	-170.7(4)
C(29)-C(30)-C(31)-C(32)	-56.1(6)
C(30)-C(31)-C(32)-C(33)	53.9(6)
C(31)-C(32)-C(33)-C(34)	-53.3(6)
C(30)-C(29)-C(34)-C(33)	-57.5(6)
P(2)-C(29)-C(34)-C(33)	174.0(4)
C(32)-C(33)-C(34)-C(29)	55.7(6)
C(40)-C(35)-C(36)-C(37)	57.2(6)
P(2)-C(35)-C(36)-C(37)	178.4(4)
C(35)-C(36)-C(37)-C(38)	-58.9(6)
C(36)-C(37)-C(38)-C(39)	56.1(6)
C(37)-C(38)-C(39)-C(40)	-55.5(6)
C(38)-C(39)-C(40)-C(35)	55.9(6)

C(36)-C(35)-C(40)-C(39)	-54.9(6)
P(2)-C(35)-C(40)-C(39)	-175.2(4)
C(46)-C(41)-C(42)-C(43)	0.0
P(3)-C(41)-C(42)-C(43)	176.3(2)
C(41)-C(42)-C(43)-C(44)	0.0
C(42)-C(43)-C(44)-C(45)	0.0
C(43)-C(44)-C(45)-C(46)	0.0
C(43)-C(44)-C(45)-C(50)	180.0
C(44)-C(45)-C(46)-C(47)	180.0
C(50)-C(45)-C(46)-C(47)	0.0
C(44)-C(45)-C(46)-C(41)	0.0
C(50)-C(45)-C(46)-C(41)	180.0
C(42)-C(41)-C(46)-C(47)	180.0
P(3)-C(41)-C(46)-C(47)	3.9(2)
C(42)-C(41)-C(46)-C(45)	0.0
P(3)-C(41)-C(46)-C(45)	-176.1(2)
C(45)-C(46)-C(47)-C(48)	0.0
C(41)-C(46)-C(47)-C(48)	180.0
C(46)-C(47)-C(48)-C(49)	0.0
C(47)-C(48)-C(49)-C(50)	0.0
C(48)-C(49)-C(50)-C(45)	0.0
C(44)-C(45)-C(50)-C(49)	180.0
C(46)-C(45)-C(50)-C(49)	0.0
C(56)-C(51)-C(52)-C(53)	-2.1(8)
P(3)-C(51)-C(52)-C(53)	172.6(4)
C(51)-C(52)-C(53)-C(54)	0.8(9)
C(52)-C(53)-C(54)-C(55)	0.1(9)
C(53)-C(54)-C(55)-C(56)	0.4(9)
C(52)-C(51)-C(56)-C(55)	2.5(8)
P(3)-C(51)-C(56)-C(55)	-171.7(4)
C(54)-C(55)-C(56)-C(51)	-1.7(8)
C(61)-C(57)-C(58)-C(59)	1.1(6)
P(3)-C(57)-C(58)-C(59)	-178.0(4)
Fe(2)-C(57)-C(58)-C(59)	59.6(3)
C(61)-C(57)-C(58)-C(67)	174.7(5)
P(3)-C(57)-C(58)-C(67)	-4.4(7)

Fe(2)-C(57)-C(58)-C(67)	-126.8(5)
C(61)-C(57)-C(58)-Fe(2)	-58.5(4)
P(3)-C(57)-C(58)-Fe(2)	122.4(4)
C(57)-C(58)-C(59)-C(60)	-1.4(6)
C(67)-C(58)-C(59)-C(60)	-174.8(5)
Fe(2)-C(58)-C(59)-C(60)	58.1(4)
C(57)-C(58)-C(59)-Fe(2)	-59.5(3)
C(67)-C(58)-C(59)-Fe(2)	127.0(5)
C(58)-C(59)-C(60)-C(61)	1.2(6)
Fe(2)-C(59)-C(60)-C(61)	59.9(4)
C(58)-C(59)-C(60)-Fe(2)	-58.7(4)
C(59)-C(60)-C(61)-C(57)	-0.5(6)
Fe(2)-C(60)-C(61)-C(57)	59.6(4)
C(59)-C(60)-C(61)-Fe(2)	-60.1(4)
C(58)-C(57)-C(61)-C(60)	-0.4(6)
P(3)-C(57)-C(61)-C(60)	178.7(4)
Fe(2)-C(57)-C(61)-C(60)	-59.3(4)
C(58)-C(57)-C(61)-Fe(2)	59.0(4)
P(3)-C(57)-C(61)-Fe(2)	-122.0(5)
C(66)-C(62)-C(63)-C(64)	0.0
Fe(2)-C(62)-C(63)-C(64)	-58.19(19)
C(66)-C(62)-C(63)-Fe(2)	58.19(19)
C(62)-C(63)-C(64)-C(65)	0.0
Fe(2)-C(63)-C(64)-C(65)	-59.4(2)
C(62)-C(63)-C(64)-Fe(2)	59.4(2)
C(63)-C(64)-C(65)-C(66)	0.0
Fe(2)-C(64)-C(65)-C(66)	-60.56(18)
C(63)-C(64)-C(65)-Fe(2)	60.56(18)
C(63)-C(62)-C(66)-C(65)	0.0
Fe(2)-C(62)-C(66)-C(65)	58.65(19)
C(63)-C(62)-C(66)-Fe(2)	-58.7(2)
C(64)-C(65)-C(66)-C(62)	0.0
Fe(2)-C(65)-C(66)-C(62)	-60.12(19)
C(64)-C(65)-C(66)-Fe(2)	60.12(19)
C(59)-C(58)-C(67)-C(68)	-42.0(7)
C(57)-C(58)-C(67)-C(68)	145.7(5)

Fe(2)-C(58)-C(67)-C(68)	52.7(6)
C(59)-C(58)-C(67)-P(4)	88.4(6)
C(57)-C(58)-C(67)-P(4)	-83.9(5)
Fe(2)-C(58)-C(67)-P(4)	-176.9(3)
C(74)-C(69)-C(70)-C(71)	-54.3(6)
P(4)-C(69)-C(70)-C(71)	-175.3(4)
C(69)-C(70)-C(71)-C(72)	54.6(7)
C(70)-C(71)-C(72)-C(73)	-54.6(7)
C(71)-C(72)-C(73)-C(74)	56.8(7)
C(72)-C(73)-C(74)-C(69)	-58.2(6)
C(70)-C(69)-C(74)-C(73)	56.0(6)
P(4)-C(69)-C(74)-C(73)	176.7(4)
C(80)-C(75)-C(76)-C(77)	-58.7(6)
P(4)-C(75)-C(76)-C(77)	171.3(4)
C(75)-C(76)-C(77)-C(78)	57.0(6)
C(76)-C(77)-C(78)-C(79)	-54.8(7)
C(77)-C(78)-C(79)-C(80)	55.0(7)
C(78)-C(79)-C(80)-C(75)	-57.5(6)
C(76)-C(75)-C(80)-C(79)	59.0(6)
P(4)-C(75)-C(80)-C(79)	-167.5(4)
C(24)-C(23)-Fe(1)-C(22)	-113.1(6)
C(24)-C(23)-Fe(1)-C(19)	152.9(5)
C(22)-C(23)-Fe(1)-C(19)	-94.0(4)
C(24)-C(23)-Fe(1)-C(18)	-171.1(4)
C(22)-C(23)-Fe(1)-C(18)	-57.9(5)
C(22)-C(23)-Fe(1)-C(24)	113.1(6)
C(24)-C(23)-Fe(1)-C(17)	85(13)
C(22)-C(23)-Fe(1)-C(17)	-161(13)
C(24)-C(23)-Fe(1)-C(20)	109.6(5)
C(22)-C(23)-Fe(1)-C(20)	-137.3(4)
C(24)-C(23)-Fe(1)-C(25)	-35.1(5)
C(22)-C(23)-Fe(1)-C(25)	78.0(4)
C(24)-C(23)-Fe(1)-C(26)	-76.0(5)
C(22)-C(23)-Fe(1)-C(26)	37.2(4)
C(24)-C(23)-Fe(1)-C(21)	73.0(6)
C(22)-C(23)-Fe(1)-C(21)	-173.8(4)

C(26)-C(22)-Fe(1)-C(23)	116.6(6)
C(26)-C(22)-Fe(1)-C(19)	-142.2(4)
C(23)-C(22)-Fe(1)-C(19)	101.2(5)
C(26)-C(22)-Fe(1)-C(18)	-99.5(5)
C(23)-C(22)-Fe(1)-C(18)	144.0(4)
C(26)-C(22)-Fe(1)-C(24)	75.4(5)
C(23)-C(22)-Fe(1)-C(24)	-41.2(5)
C(26)-C(22)-Fe(1)-C(17)	-64.1(6)
C(23)-C(22)-Fe(1)-C(17)	179.3(4)
C(26)-C(22)-Fe(1)-C(20)	-177.0(4)
C(23)-C(22)-Fe(1)-C(20)	66.4(5)
C(26)-C(22)-Fe(1)-C(25)	34.2(5)
C(23)-C(22)-Fe(1)-C(25)	-82.4(5)
C(23)-C(22)-Fe(1)-C(26)	-116.6(6)
C(26)-C(22)-Fe(1)-C(21)	-151(3)
C(23)-C(22)-Fe(1)-C(21)	92(4)
C(18)-C(19)-Fe(1)-C(23)	143.5(4)
C(20)-C(19)-Fe(1)-C(23)	-97.5(4)
C(18)-C(19)-Fe(1)-C(22)	98.7(4)
C(20)-C(19)-Fe(1)-C(22)	-142.3(3)
C(20)-C(19)-Fe(1)-C(18)	118.9(4)
C(18)-C(19)-Fe(1)-C(24)	174.8(4)
C(20)-C(19)-Fe(1)-C(24)	-66.3(6)
C(18)-C(19)-Fe(1)-C(17)	-37.9(3)
C(20)-C(19)-Fe(1)-C(17)	81.0(3)
C(18)-C(19)-Fe(1)-C(20)	-118.9(4)
C(18)-C(19)-Fe(1)-C(25)	74(2)
C(20)-C(19)-Fe(1)-C(25)	-167(2)
C(18)-C(19)-Fe(1)-C(26)	66.4(5)
C(20)-C(19)-Fe(1)-C(26)	-174.7(4)
C(18)-C(19)-Fe(1)-C(21)	-82.0(3)
C(20)-C(19)-Fe(1)-C(21)	36.9(3)
C(19)-C(18)-Fe(1)-C(23)	-58.0(5)
C(17)-C(18)-Fe(1)-C(23)	-177.9(4)
C(19)-C(18)-Fe(1)-C(22)	-95.1(4)
C(17)-C(18)-Fe(1)-C(22)	145.0(3)

C(17)-C(18)-Fe(1)-C(19)	-119.9(4)
C(19)-C(18)-Fe(1)-C(24)	-149(3)
C(17)-C(18)-Fe(1)-C(24)	91(3)
C(19)-C(18)-Fe(1)-C(17)	119.9(4)
C(19)-C(18)-Fe(1)-C(20)	37.8(3)
C(17)-C(18)-Fe(1)-C(20)	-82.1(3)
C(19)-C(18)-Fe(1)-C(25)	-168.8(4)
C(17)-C(18)-Fe(1)-C(25)	71.3(5)
C(19)-C(18)-Fe(1)-C(26)	-136.0(4)
C(17)-C(18)-Fe(1)-C(26)	104.1(4)
C(19)-C(18)-Fe(1)-C(21)	81.4(3)
C(17)-C(18)-Fe(1)-C(21)	-38.5(3)
C(25)-C(24)-Fe(1)-C(23)	-120.0(7)
C(25)-C(24)-Fe(1)-C(22)	-78.0(5)
C(23)-C(24)-Fe(1)-C(22)	42.0(4)
C(25)-C(24)-Fe(1)-C(19)	-167.2(5)
C(23)-C(24)-Fe(1)-C(19)	-47.2(7)
C(25)-C(24)-Fe(1)-C(18)	-22(4)
C(23)-C(24)-Fe(1)-C(18)	98(3)
C(25)-C(24)-Fe(1)-C(17)	62.1(6)
C(23)-C(24)-Fe(1)-C(17)	-177.9(4)
C(25)-C(24)-Fe(1)-C(20)	150.6(4)
C(23)-C(24)-Fe(1)-C(20)	-89.4(5)
C(23)-C(24)-Fe(1)-C(25)	120.0(7)
C(25)-C(24)-Fe(1)-C(26)	-35.9(4)
C(23)-C(24)-Fe(1)-C(26)	84.1(5)
C(25)-C(24)-Fe(1)-C(21)	105.4(5)
C(23)-C(24)-Fe(1)-C(21)	-134.6(4)
C(21)-C(17)-Fe(1)-C(23)	-13(14)
C(18)-C(17)-Fe(1)-C(23)	105(13)
P(1)-C(17)-Fe(1)-C(23)	-131(13)
C(21)-C(17)-Fe(1)-C(22)	-173.7(4)
C(18)-C(17)-Fe(1)-C(22)	-55.8(5)
P(1)-C(17)-Fe(1)-C(22)	67.9(5)
C(21)-C(17)-Fe(1)-C(19)	-80.7(3)
C(18)-C(17)-Fe(1)-C(19)	37.1(3)

P(1)-C(17)-Fe(1)-C(19)	160.8(4)
C(21)-C(17)-Fe(1)-C(18)	-117.8(4)
P(1)-C(17)-Fe(1)-C(18)	123.7(5)
C(21)-C(17)-Fe(1)-C(24)	71.1(5)
C(18)-C(17)-Fe(1)-C(24)	-171.1(4)
P(1)-C(17)-Fe(1)-C(24)	-47.4(6)
C(21)-C(17)-Fe(1)-C(20)	-37.1(3)
C(18)-C(17)-Fe(1)-C(20)	80.7(3)
P(1)-C(17)-Fe(1)-C(20)	-155.6(4)
C(21)-C(17)-Fe(1)-C(25)	107.3(4)
C(18)-C(17)-Fe(1)-C(25)	-134.9(4)
P(1)-C(17)-Fe(1)-C(25)	-11.2(5)
C(21)-C(17)-Fe(1)-C(26)	148.5(3)
C(18)-C(17)-Fe(1)-C(26)	-93.7(4)
P(1)-C(17)-Fe(1)-C(26)	30.0(4)
C(18)-C(17)-Fe(1)-C(21)	117.8(4)
P(1)-C(17)-Fe(1)-C(21)	-118.5(5)
C(19)-C(20)-Fe(1)-C(23)	98.0(5)
C(21)-C(20)-Fe(1)-C(23)	-141.7(4)
C(19)-C(20)-Fe(1)-C(22)	56.9(5)
C(21)-C(20)-Fe(1)-C(22)	177.2(4)
C(21)-C(20)-Fe(1)-C(19)	120.3(4)
C(19)-C(20)-Fe(1)-C(18)	-37.9(3)
C(21)-C(20)-Fe(1)-C(18)	82.5(3)
C(19)-C(20)-Fe(1)-C(24)	142.9(4)
C(21)-C(20)-Fe(1)-C(24)	-96.8(4)
C(19)-C(20)-Fe(1)-C(17)	-82.6(3)
C(21)-C(20)-Fe(1)-C(17)	37.7(3)
C(19)-C(20)-Fe(1)-C(25)	176.6(5)
C(21)-C(20)-Fe(1)-C(25)	-63.1(6)
C(19)-C(20)-Fe(1)-C(26)	39(2)
C(21)-C(20)-Fe(1)-C(26)	159(2)
C(19)-C(20)-Fe(1)-C(21)	-120.3(4)
C(26)-C(25)-Fe(1)-C(23)	-81.5(5)
C(24)-C(25)-Fe(1)-C(23)	38.6(5)
C(26)-C(25)-Fe(1)-C(22)	-35.0(4)

C(24)-C(25)-Fe(1)-C(22)	85.0(5)
C(26)-C(25)-Fe(1)-C(19)	-9(2)
C(24)-C(25)-Fe(1)-C(19)	111(2)
C(26)-C(25)-Fe(1)-C(18)	56.7(6)
C(24)-C(25)-Fe(1)-C(18)	176.7(5)
C(26)-C(25)-Fe(1)-C(24)	-120.1(7)
C(26)-C(25)-Fe(1)-C(17)	99.8(4)
C(24)-C(25)-Fe(1)-C(17)	-140.1(5)
C(26)-C(25)-Fe(1)-C(20)	-173.4(4)
C(24)-C(25)-Fe(1)-C(20)	-53.3(7)
C(24)-C(25)-Fe(1)-C(26)	120.1(7)
C(26)-C(25)-Fe(1)-C(21)	145.4(4)
C(24)-C(25)-Fe(1)-C(21)	-94.5(5)
C(25)-C(26)-Fe(1)-C(23)	82.0(5)
C(22)-C(26)-Fe(1)-C(23)	-40.9(5)
C(25)-C(26)-Fe(1)-C(22)	122.9(7)
C(25)-C(26)-Fe(1)-C(19)	178.2(4)
C(22)-C(26)-Fe(1)-C(19)	55.3(6)
C(25)-C(26)-Fe(1)-C(18)	-142.3(4)
C(22)-C(26)-Fe(1)-C(18)	94.8(5)
C(25)-C(26)-Fe(1)-C(24)	36.2(5)
C(22)-C(26)-Fe(1)-C(24)	-86.7(5)
C(25)-C(26)-Fe(1)-C(17)	-97.5(5)
C(22)-C(26)-Fe(1)-C(17)	139.6(4)
C(25)-C(26)-Fe(1)-C(20)	143(2)
C(22)-C(26)-Fe(1)-C(20)	20(3)
C(22)-C(26)-Fe(1)-C(25)	-122.9(7)
C(25)-C(26)-Fe(1)-C(21)	-60.6(6)
C(22)-C(26)-Fe(1)-C(21)	176.5(4)
C(20)-C(21)-Fe(1)-C(23)	59.8(5)
C(17)-C(21)-Fe(1)-C(23)	179.5(5)
C(27)-C(21)-Fe(1)-C(23)	-60.4(7)
C(20)-C(21)-Fe(1)-C(22)	-28(4)
C(17)-C(21)-Fe(1)-C(22)	92(4)
C(27)-C(21)-Fe(1)-C(22)	-148(3)
C(20)-C(21)-Fe(1)-C(19)	-37.1(3)

C(17)-C(21)-Fe(1)-C(19)	82.7(3)
C(27)-C(21)-Fe(1)-C(19)	-157.2(5)
C(20)-C(21)-Fe(1)-C(18)	-80.8(3)
C(17)-C(21)-Fe(1)-C(18)	38.9(3)
C(27)-C(21)-Fe(1)-C(18)	159.0(5)
C(20)-C(21)-Fe(1)-C(24)	104.2(5)
C(17)-C(21)-Fe(1)-C(24)	-136.1(4)
C(27)-C(21)-Fe(1)-C(24)	-16.0(6)
C(20)-C(21)-Fe(1)-C(17)	-119.8(4)
C(27)-C(21)-Fe(1)-C(17)	120.1(6)
C(17)-C(21)-Fe(1)-C(20)	119.8(4)
C(27)-C(21)-Fe(1)-C(20)	-120.1(6)
C(20)-C(21)-Fe(1)-C(25)	146.5(4)
C(17)-C(21)-Fe(1)-C(25)	-93.7(4)
C(27)-C(21)-Fe(1)-C(25)	26.4(6)
C(20)-C(21)-Fe(1)-C(26)	-176.3(4)
C(17)-C(21)-Fe(1)-C(26)	-56.5(5)
C(27)-C(21)-Fe(1)-C(26)	63.6(7)
C(66)-C(65)-Fe(2)-C(64)	118.57(10)
C(64)-C(65)-Fe(2)-C(60)	176.6(3)
C(66)-C(65)-Fe(2)-C(60)	-64.9(3)
C(64)-C(65)-Fe(2)-C(61)	-154.9(9)
C(66)-C(65)-Fe(2)-C(61)	-36.3(9)
C(64)-C(65)-Fe(2)-C(66)	-118.57(10)
C(64)-C(65)-Fe(2)-C(59)	136.5(3)
C(66)-C(65)-Fe(2)-C(59)	-104.9(3)
C(64)-C(65)-Fe(2)-C(57)	59.7(4)
C(66)-C(65)-Fe(2)-C(57)	178.3(4)
C(64)-C(65)-Fe(2)-C(58)	93.4(3)
C(66)-C(65)-Fe(2)-C(58)	-148.0(2)
C(64)-C(65)-Fe(2)-C(63)	-37.79(9)
C(66)-C(65)-Fe(2)-C(63)	80.78(12)
C(64)-C(65)-Fe(2)-C(62)	-81.13(13)
C(66)-C(65)-Fe(2)-C(62)	37.44(9)
C(63)-C(64)-Fe(2)-C(65)	-118.82(11)
C(65)-C(64)-Fe(2)-C(60)	-14.4(12)

C(63)-C(64)-Fe(2)-C(60)	-133.2(12)
C(65)-C(64)-Fe(2)-C(61)	168.2(5)
C(63)-C(64)-Fe(2)-C(61)	49.3(5)
C(65)-C(64)-Fe(2)-C(66)	38.13(9)
C(63)-C(64)-Fe(2)-C(66)	-80.70(12)
C(65)-C(64)-Fe(2)-C(59)	-63.6(3)
C(63)-C(64)-Fe(2)-C(59)	177.6(3)
C(65)-C(64)-Fe(2)-C(57)	-150.9(3)
C(63)-C(64)-Fe(2)-C(57)	90.3(3)
C(65)-C(64)-Fe(2)-C(58)	-105.9(3)
C(63)-C(64)-Fe(2)-C(58)	135.3(3)
C(65)-C(64)-Fe(2)-C(63)	118.82(11)
C(65)-C(64)-Fe(2)-C(62)	81.66(14)
C(63)-C(64)-Fe(2)-C(62)	-37.16(9)
C(61)-C(60)-Fe(2)-C(65)	169.9(4)
C(59)-C(60)-Fe(2)-C(65)	-70.3(4)
C(61)-C(60)-Fe(2)-C(64)	-178.1(11)
C(59)-C(60)-Fe(2)-C(64)	-58.3(12)
C(59)-C(60)-Fe(2)-C(61)	119.8(4)
C(61)-C(60)-Fe(2)-C(66)	132.2(4)
C(59)-C(60)-Fe(2)-C(66)	-108.1(4)
C(61)-C(60)-Fe(2)-C(59)	-119.8(4)
C(61)-C(60)-Fe(2)-C(57)	-38.1(3)
C(59)-C(60)-Fe(2)-C(57)	81.7(3)
C(61)-C(60)-Fe(2)-C(58)	-82.3(3)
C(59)-C(60)-Fe(2)-C(58)	37.5(3)
C(61)-C(60)-Fe(2)-C(63)	60.1(5)
C(59)-C(60)-Fe(2)-C(63)	179.9(3)
C(61)-C(60)-Fe(2)-C(62)	90.3(4)
C(59)-C(60)-Fe(2)-C(62)	-149.9(3)
C(60)-C(61)-Fe(2)-C(65)	-35.6(10)
C(57)-C(61)-Fe(2)-C(65)	-155.1(8)
C(60)-C(61)-Fe(2)-C(64)	179.3(4)
C(57)-C(61)-Fe(2)-C(64)	59.8(5)
C(57)-C(61)-Fe(2)-C(60)	-119.4(5)
C(60)-C(61)-Fe(2)-C(66)	-64.9(4)

C(57)-C(61)-Fe(2)-C(66)	175.6(3)
C(60)-C(61)-Fe(2)-C(59)	37.6(3)
C(57)-C(61)-Fe(2)-C(59)	-81.8(3)
C(60)-C(61)-Fe(2)-C(57)	119.4(5)
C(60)-C(61)-Fe(2)-C(58)	81.6(3)
C(57)-C(61)-Fe(2)-C(58)	-37.9(3)
C(60)-C(61)-Fe(2)-C(63)	-147.1(3)
C(57)-C(61)-Fe(2)-C(63)	93.5(3)
C(60)-C(61)-Fe(2)-C(62)	-104.8(4)
C(57)-C(61)-Fe(2)-C(62)	135.8(3)
C(62)-C(66)-Fe(2)-C(65)	119.21(11)
C(62)-C(66)-Fe(2)-C(64)	80.92(13)
C(65)-C(66)-Fe(2)-C(64)	-38.29(9)
C(62)-C(66)-Fe(2)-C(60)	-108.0(3)
C(65)-C(66)-Fe(2)-C(60)	132.8(3)
C(62)-C(66)-Fe(2)-C(61)	-70.9(3)
C(65)-C(66)-Fe(2)-C(61)	169.9(4)
C(62)-C(66)-Fe(2)-C(59)	-150.2(3)
C(65)-C(66)-Fe(2)-C(59)	90.5(3)
C(62)-C(66)-Fe(2)-C(57)	-56.6(10)
C(65)-C(66)-Fe(2)-C(57)	-175.8(10)
C(62)-C(66)-Fe(2)-C(58)	178.5(4)
C(65)-C(66)-Fe(2)-C(58)	59.3(4)
C(62)-C(66)-Fe(2)-C(63)	37.09(9)
C(65)-C(66)-Fe(2)-C(63)	-82.12(13)
C(65)-C(66)-Fe(2)-C(62)	-119.21(11)
C(60)-C(59)-Fe(2)-C(65)	129.3(4)
C(58)-C(59)-Fe(2)-C(65)	-110.8(4)
C(60)-C(59)-Fe(2)-C(64)	167.4(4)
C(58)-C(59)-Fe(2)-C(64)	-72.8(5)
C(58)-C(59)-Fe(2)-C(60)	119.9(4)
C(60)-C(59)-Fe(2)-C(61)	-37.0(3)
C(58)-C(59)-Fe(2)-C(61)	82.9(3)
C(60)-C(59)-Fe(2)-C(66)	86.0(4)
C(58)-C(59)-Fe(2)-C(66)	-154.1(4)
C(60)-C(59)-Fe(2)-C(57)	-81.4(3)

C(58)-C(59)-Fe(2)-C(57)	38.4(3)
C(60)-C(59)-Fe(2)-C(58)	-119.9(4)
C(60)-C(59)-Fe(2)-C(63)	-180(95)
C(58)-C(59)-Fe(2)-C(63)	-59.6(18)
C(60)-C(59)-Fe(2)-C(62)	52.6(5)
C(58)-C(59)-Fe(2)-C(62)	172.5(4)
C(61)-C(57)-Fe(2)-C(65)	168.3(5)
C(58)-C(57)-Fe(2)-C(65)	49.0(6)
P(3)-C(57)-Fe(2)-C(65)	-66.7(7)
C(61)-C(57)-Fe(2)-C(64)	-150.9(4)
C(58)-C(57)-Fe(2)-C(64)	89.8(4)
P(3)-C(57)-Fe(2)-C(64)	-25.9(5)
C(61)-C(57)-Fe(2)-C(60)	37.1(3)
C(58)-C(57)-Fe(2)-C(60)	-82.2(3)
P(3)-C(57)-Fe(2)-C(60)	162.1(4)
C(58)-C(57)-Fe(2)-C(61)	-119.2(4)
P(3)-C(57)-Fe(2)-C(61)	125.0(5)
C(61)-C(57)-Fe(2)-C(66)	-17.3(11)
C(58)-C(57)-Fe(2)-C(66)	-136.5(9)
P(3)-C(57)-Fe(2)-C(66)	107.7(10)
C(61)-C(57)-Fe(2)-C(59)	81.0(3)
C(58)-C(57)-Fe(2)-C(59)	-38.2(3)
P(3)-C(57)-Fe(2)-C(59)	-154.0(4)
C(61)-C(57)-Fe(2)-C(58)	119.2(4)
P(3)-C(57)-Fe(2)-C(58)	-115.8(5)
C(61)-C(57)-Fe(2)-C(63)	-106.3(4)
C(58)-C(57)-Fe(2)-C(63)	134.5(4)
P(3)-C(57)-Fe(2)-C(63)	18.7(5)
C(61)-C(57)-Fe(2)-C(62)	-64.4(4)
C(58)-C(57)-Fe(2)-C(62)	176.4(3)
P(3)-C(57)-Fe(2)-C(62)	60.6(5)
C(59)-C(58)-Fe(2)-C(65)	86.0(5)
C(57)-C(58)-Fe(2)-C(65)	-155.6(4)
C(67)-C(58)-Fe(2)-C(65)	-36.0(6)
C(59)-C(58)-Fe(2)-C(64)	131.0(4)
C(57)-C(58)-Fe(2)-C(64)	-110.7(4)

C(67)-C(58)-Fe(2)-C(64)	8.9(6)
C(59)-C(58)-Fe(2)-C(60)	-37.4(3)
C(57)-C(58)-Fe(2)-C(60)	81.0(3)
C(67)-C(58)-Fe(2)-C(60)	-159.4(5)
C(59)-C(58)-Fe(2)-C(61)	-80.4(3)
C(57)-C(58)-Fe(2)-C(61)	37.9(3)
C(67)-C(58)-Fe(2)-C(61)	157.5(5)
C(59)-C(58)-Fe(2)-C(66)	47.0(6)
C(57)-C(58)-Fe(2)-C(66)	165.4(5)
C(67)-C(58)-Fe(2)-C(66)	-75.0(7)
C(57)-C(58)-Fe(2)-C(59)	118.4(4)
C(67)-C(58)-Fe(2)-C(59)	-122.0(6)
C(59)-C(58)-Fe(2)-C(57)	-118.4(4)
C(67)-C(58)-Fe(2)-C(57)	119.6(6)
C(59)-C(58)-Fe(2)-C(63)	171.6(4)
C(57)-C(58)-Fe(2)-C(63)	-70.0(4)
C(67)-C(58)-Fe(2)-C(63)	49.6(6)
C(59)-C(58)-Fe(2)-C(62)	-141.0(16)
C(57)-C(58)-Fe(2)-C(62)	-22.6(18)
C(67)-C(58)-Fe(2)-C(62)	97.0(17)
C(62)-C(63)-Fe(2)-C(65)	-81.42(14)
C(64)-C(63)-Fe(2)-C(65)	38.22(9)
C(62)-C(63)-Fe(2)-C(64)	-119.64(12)
C(62)-C(63)-Fe(2)-C(60)	46.1(5)
C(64)-C(63)-Fe(2)-C(60)	165.7(5)
C(62)-C(63)-Fe(2)-C(61)	84.9(4)
C(64)-C(63)-Fe(2)-C(61)	-155.4(4)
C(62)-C(63)-Fe(2)-C(66)	-37.24(9)
C(64)-C(63)-Fe(2)-C(66)	82.40(13)
C(62)-C(63)-Fe(2)-C(59)	-134.5(17)
C(64)-C(63)-Fe(2)-C(59)	-14.8(17)
C(62)-C(63)-Fe(2)-C(57)	130.2(3)
C(64)-C(63)-Fe(2)-C(57)	-110.2(3)
C(62)-C(63)-Fe(2)-C(58)	172.0(3)
C(64)-C(63)-Fe(2)-C(58)	-68.3(3)
C(64)-C(63)-Fe(2)-C(62)	119.64(12)

C(63)-C(62)-Fe(2)-C(65)	81.95(14)
C(66)-C(62)-Fe(2)-C(65)	-37.95(10)
C(63)-C(62)-Fe(2)-C(64)	37.55(10)
C(66)-C(62)-Fe(2)-C(64)	-82.34(14)
C(63)-C(62)-Fe(2)-C(60)	-154.2(3)
C(66)-C(62)-Fe(2)-C(60)	85.9(4)
C(63)-C(62)-Fe(2)-C(61)	-111.8(4)
C(66)-C(62)-Fe(2)-C(61)	128.3(4)
C(63)-C(62)-Fe(2)-C(66)	119.90(11)
C(63)-C(62)-Fe(2)-C(59)	171.6(4)
C(66)-C(62)-Fe(2)-C(59)	51.8(4)
C(63)-C(62)-Fe(2)-C(57)	-73.3(4)
C(66)-C(62)-Fe(2)-C(57)	166.8(4)
C(63)-C(62)-Fe(2)-C(58)	-53.3(17)
C(66)-C(62)-Fe(2)-C(58)	-173.2(17)
C(66)-C(62)-Fe(2)-C(63)	-119.90(11)
C(21)-C(17)-P(1)-C(11)	104.2(4)
C(18)-C(17)-P(1)-C(11)	-75.1(5)
Fe(1)-C(17)-P(1)-C(11)	-166.1(3)
C(21)-C(17)-P(1)-C(1)	-152.0(4)
C(18)-C(17)-P(1)-C(1)	28.8(5)
Fe(1)-C(17)-P(1)-C(1)	-62.3(3)
C(12)-C(11)-P(1)-C(17)	176.1(4)
C(16)-C(11)-P(1)-C(17)	-7.8(5)
C(12)-C(11)-P(1)-C(1)	69.7(4)
C(16)-C(11)-P(1)-C(1)	-114.2(4)
C(2)-C(1)-P(1)-C(17)	-67.5(2)
C(6)-C(1)-P(1)-C(17)	106.2(2)
C(2)-C(1)-P(1)-C(11)	38.1(2)
C(6)-C(1)-P(1)-C(11)	-148.1(2)
C(34)-C(29)-P(2)-C(35)	-58.2(4)
C(30)-C(29)-P(2)-C(35)	173.9(4)
C(34)-C(29)-P(2)-C(27)	49.2(4)
C(30)-C(29)-P(2)-C(27)	-78.6(4)
C(36)-C(35)-P(2)-C(29)	-176.3(4)
C(40)-C(35)-P(2)-C(29)	-57.0(4)

C(36)-C(35)-P(2)-C(27)	77.5(4)
C(40)-C(35)-P(2)-C(27)	-163.2(4)
C(21)-C(27)-P(2)-C(29)	142.0(3)
C(28)-C(27)-P(2)-C(29)	-90.7(4)
C(21)-C(27)-P(2)-C(35)	-111.6(3)
C(28)-C(27)-P(2)-C(35)	15.7(4)
C(61)-C(57)-P(3)-C(51)	-72.2(5)
C(58)-C(57)-P(3)-C(51)	106.7(4)
Fe(2)-C(57)-P(3)-C(51)	-165.3(3)
C(61)-C(57)-P(3)-C(41)	33.9(5)
C(58)-C(57)-P(3)-C(41)	-147.2(4)
Fe(2)-C(57)-P(3)-C(41)	-59.1(4)
C(56)-C(51)-P(3)-C(57)	-15.4(5)
C(52)-C(51)-P(3)-C(57)	170.3(4)
C(56)-C(51)-P(3)-C(41)	-122.9(5)
C(52)-C(51)-P(3)-C(41)	62.8(4)
C(42)-C(41)-P(3)-C(57)	-67.4(2)
C(46)-C(41)-P(3)-C(57)	108.8(2)
C(42)-C(41)-P(3)-C(51)	39.1(2)
C(46)-C(41)-P(3)-C(51)	-144.6(2)
C(70)-C(69)-P(4)-C(67)	-66.2(4)
C(74)-C(69)-P(4)-C(67)	173.4(4)
C(70)-C(69)-P(4)-C(75)	-171.1(4)
C(74)-C(69)-P(4)-C(75)	68.6(4)
C(58)-C(67)-P(4)-C(69)	171.7(3)
C(68)-C(67)-P(4)-C(69)	-60.6(4)
C(58)-C(67)-P(4)-C(75)	-78.6(4)
C(68)-C(67)-P(4)-C(75)	49.1(4)
C(80)-C(75)-P(4)-C(69)	-106.8(4)
C(76)-C(75)-P(4)-C(69)	22.5(5)
C(80)-C(75)-P(4)-C(67)	146.9(4)
C(76)-C(75)-P(4)-C(67)	-83.8(5)

Symmetry transformations used to generate equivalent atoms: