Supporting Information for
Chiral Copper Complexes of Phosphino Sulfenyl Ferrocenes as Efficient
Catalysts for Enantioselective Formal Aza Diels-Alder Reactions of *N*-
Sulfonyl Imines

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General: Aldehydes, arylsulfonamides, copper salts and Danishefsky's diene **2a** were purchased from commercial suppliers and were used without further purification. Methyl substituted Danishefsky's diene **2b** was prepared according to literature's procedures.¹ *N*-Sulfonyl aldimines derived from aromatic aldehydes,^{2a,b} cinnamaldehyde^{2a,b} and butyraldehyde^{2c} were synthesized from the corresponding aldehyde and the aromatic sulfonamide using well established protocols. The preparation of ligands (*R*)-**1a-f** have been previously reported by us.³ Racemic piperidones **5** were obtained using AgClO₄ (20 mol %) as catalyst.⁴ Toluene and CH₂Cl₂ were dried over microwave-activated MS 4Å. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm Merck silica gel plates (Merck-60 230-400 mesh). Merck-60 230-400 mesh silica gel was used for flash column chromatography. NMR spectra were recorded on Bruker AC-200 or AC-300 instruments in CDCl₃ (calibrated at 7.26 and 77.0 ppm for ¹H and ¹³C experiments respectively). Mass spectra were determined on a Hewlett-Packard HP-5985 mass spectrometer at 70 eV ionising voltage (EI) or under fast atom bombardment (FAB) conditions. Melting points were determined in open-end capillary tubes on a GallemKamp apparatus. Optical rotations were measured on a Perkin-Elmer 241C polarimeter. High-Performance Liquid Chromatography (HPLC) was conducted on an Agilent 1100 instrument, using Daicel Chiralpak AD, AS and Chiralcel OD columns.

General procedure for the synthesis of chiral Cu(I) complexes: A solution of ligand (*R*)-**1** (0.4 mmol) and CuCl or CuBr (0.41 mmol) in a 2:3 mixture of THF/MeOH (5 mL) were stirred at room temperature under argon for 5-10 min. The mixture was concentrated to dryness, a 4:1 mixture of *n*-

hexane/EtOAc was added and it was passed through a short pad of silica gel to obtain pure complexes **6-7** after evaporation of the solvent under reduced pressure.

(*R_P*,*R_S*)-2-(*tert*-Butylsulfenyl)-1-(diphenylphosphino)ferrocene copper (I) chloride dimer [6a]

According to the general procedure, the reaction of (*R*)-**1a** with CuCl gave complex **6a** as an orange solid (99%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -330$ (c 0.1, CHCl₃). ¹H NMR (300 MHz): δ 8.15 (m, 2H), 7.70 (t, 2H, *J* = 8.6 Hz), 7.42 (m, 3H), 7.25 (m, 3H), 4.42 (m, 1H), 4.63 (m, 1H), 4.50 (m, 1H), 4.00 (s, 5H), 1.12 (s, 9H). ¹³C NMR (75 MHz): δ 135.2 (d, *J*_{C-P} = 30.3 Hz), 134.8 (d, *J*_{C-P} = 16.7 Hz), 134.4 (d, *J*_{C-P} = 34.5 Hz), 132.5 (d, *J*_{C-P} = 15.7 Hz), 130.0, 128.9, 128.3, 128.2, 128.1, 84.6 (d, *J*_{C-P} = 35.6 Hz), 78.7 (d, *J*_{C-P} = 46.0 Hz), 77.6, 73.3 (d, *J*_{C-P} = 4.2 Hz), 72.0, 71.4, 50.0, 30.3. MS (FAB+) *m/z* 1079 [*M*⁺+H-Cl (32)], 458 (100), 402 (50).

(*R_P*,*R_S*)-2-(*tert*-Butylsulfenyl)-1-[bis(4-fluorophenyl)phosphino]ferrocene copper (I) chloride dimer [6b]

According to the general procedure, the reaction of (*R*)-**1b** with CuCl gave complex **6b** as an orange solid (99%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -244$ (c 0.1, CHCl₃). ¹H NMR (300 MHz): δ 8.11 (m, 2H), 7.68 (m, 2H), 7.15 (dt, 2H, *J* = 1.0, 8.9 Hz), 7.03 (dt, 2H, *J* = 1.0, 8.7 Hz), 4.82 (q, 1H, *J* = 1.2 Hz), 4.65 (t, 1H, *J* = 2.6 Hz), 4.46 (dd, 1H, *J* = 1.2, 2.6 Hz), 4.07 (s, 5H), 1.21 (s, 9H). ¹³C NMR (75 MHz): δ 165.4 (d, *J* = 46.0 Hz), 162.1 (d, *J* = 47.1 Hz), 137.0, 136.9, 136.8, 136.7, 134.7, 134.6, 134.5, 134.4, 130.9 (dd, *J* = 3.1, 30.3 Hz), 130.9 (dd, *J* = 3.1, 30.3 Hz), 130.0 (dd, *J* = 3.1, 34.5 Hz), 115.8, 115.7, 115.5, 115.4, 84.7 (d, *J* = 36.6 Hz), 78.7 (d, *J* = 47.1 Hz), 77.8 (d, *J* = 4.2 Hz), 73.5 (d, *J* = 3.1 Hz), 50.1, 30.3. MS (FAB+) *m/z* 1186 [*M*⁺ (6)], 1151 [*M*⁺-Cl (21)], 494 (100).

(*R_P*,*R_S*)-2-(*tert*-Butylsulfenyl)-1-(difurylphosphino)ferrocene copper (I) chloride dimer [6c]

According to the general procedure, the reaction of (*R*)-**1c** with CuCl gave complex **6c** as an orange solid (99%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -393$ (c

0.1, CHCl₃). ¹H NMR (300 MHz): δ 7.74 (d, 1H, *J* = 1.2 Hz), 7.62 (t, 1H, *J* = 3.6 Hz), 7.57 (d, 1H, *J* = 1.4 Hz), 7.21 (t, 1H, *J* = 3.1 Hz), 6.46 (m, 1H), 6.29 (m, 1H), 5.06 (dd, 1H, *J* = 1.2, 2.5 Hz), 4.72 (m, 1H), 4.60 (t, 1H, *J* = 2.5 Hz), 4.10 (s, 5H), 1.32 (s, 9H). ¹³C NMR (75 MHz): δ 148.7, 148.5, 148.2, 148.0, 147.1-147.0 (m), 123.1 (d, *J* = 34.5 Hz), 121.8 (d, *J* = 30.3 Hz), 111.0, 110.8, 110.5, 110.4, 84.3 (d, *J* = 40.8 Hz), 81.6 (d, *J* = 68.0 Hz), 77.7, 73.7, 73.4 (d, *J* = 4.2 Hz), 71.5, 50.4, 30.1. MS (FAB+) *m/z* 1074 [M⁺ (2)], 1038 [M⁺-Cl (9)], 601 (5), 438 (100).

(*R_p*,*R_s*)-2-(*tert*-Butylsulfenyl)-1-(dicyclohexylphosphino)ferrocene copper (I) chloride dimer [6d]

According to the general procedure, the reaction of (*R*)-**1d** with CuCl gave complex **6d** as an orange solid (99%). Mp >200 °C (decomp). [α]_D²⁰ = +231 (*c* 0.1, CHCl₃). ¹H NMR (300 MHz): δ 4.92 (m, 1H), 4.60 (t, 1H, *J* = 2.6 Hz), 4.32 (dd, 1H, *J* = 1.2, 2.6 Hz), 4.23 (s, 5H), 2.50-0.90 (m, 22H), 1.40 (s, 9H). ¹³C NMR (75 MHz): δ 86.0 (d, *J* = 29.3 Hz), 79.7 (d, *J* = 37.7 Hz), 75.4 (d, *J* = 3.1 Hz), 72.8 (d, *J* = 4.2 Hz), 72.5, 71.1, 50.1, 39.4 (d, *J* = 20.9 Hz), 34.3 (d, *J* = 19.9 Hz), 32.6 (d, *J* = 12.6 Hz), 31.8 (d, *J* = 9.4 Hz), 31.0, 30.8 (d, *J* = 3.1 Hz), 28.3 (d, *J* = 5.2 Hz), 28.0 (d, *J* = 16.7 Hz), 27.3, 27.2, 27.1, 27.0, 26.8, 26.6, 25.8 (d, *J* = 18.8 Hz). MS (FAB+) *m/z* 1139 [M⁺ (2)], 1103 [M⁺-Cl (64)], 533 (22), 476 (100), 470 (47).

(*R_p*,*R_s*)-2-(*tert*-Butylsulfenyl)-1-[bis(*o*-tolyl)phosphino]ferrocene copper (I) chloride dimer [6e]

According to the general procedure, the reaction of (*R*)-**1e** with CuCl gave complex **6e** as an orange solid (99%). Mp >200 °C (decomp). [α]_D²⁰ = -385 (*c* 0.1, CHCl₃). ¹H NMR (300 MHz): δ 7.45 (m, 1H), 7.32 (m, 2H), 7.23-7.00 (m, 5H), 4.92 (m, 1H), 4.62 (t, 1H, *J* = 2.6 Hz), 4.58 (dd, 1H, *J* = 1.2, 2.6 Hz), 3.90 (s, 5H), 3.08 (s, 3H), 2.35 (s, 3H), 1.20 (s, 9H). ¹³C NMR (75 MHz): δ 142.5, 142.3, 141.1, 141.0, 135.2 (d, *J* = 6.3 Hz), 133.0, 132.5, 131.3, 131.2, 131.1, 131.0, 130.9, 130.8, 130.7, 130.6, 130.3, 129.3, 126.3, 125.1 (d, *J* = 5.2 Hz), 85.3 (d, *J* = 37.7 Hz), 78.1, 78.0, 77.9, 74.5 (d, *J* = 4.2 Hz), 72.4, 71.1, 51.2, 30.6, 23.2 (d, *J* = 16.7 Hz), 21.4 (d, *J* = 15.7 Hz). MS (FAB+) *m/z* 1170 [M⁺ (2)], 1135 [M⁺-Cl (14)], 549 (39), 492 (100), 486 (42).

(*R_p*,*R_s*)-2-(*tert*-Butylsulfenyl)-1-[bis(1-naphthyl)phosphino]ferrocene copper (I) chloride dimer [6f]

According to the general procedure, the reaction of (*R*)-**1f** with CuCl gave complex **6f** as an orange solid (61%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -300$ (c 0.1, CHCl₃). ¹H NMR (300 MHz): δ 8.50 (m, 1H), 7.90 (m, 3H), 7.71 (m, 2H), 7.60-7.27 (m, 8H), 4.95 (m, 1H), 4.74 (t, 1H, *J* = 2.6 Hz), 4.65 (m, 1H), 3.65 (s, 5H), 1.17 (s, 9H). ¹³C NMR (75 MHz): δ 134.7 (d, *J* = 12.6 Hz), 133.8 (d, *J* = 6.3 Hz), 133.6 (d, *J* = 6.3 Hz), 133.1 (d, *J* = 16.7 Hz), 131.9, 131.3, 130.9, 130.8, 130.7, 129.5, 129.1, 129.0, 128.4, 127.7, 127.2, 126.6, 126.5, 126.2, 126.1, 125.9, 125.8, 125.2, 125.1 (d, *J* = 10.5 Hz), 124.3 (d, *J* = 6.3 Hz), 85.1 (d, *J* = 36.6 Hz), 78.4 (d, *J* = 3.1 Hz), 77.5 (d, *J* = 39.7 Hz), 74.5 (d, *J* = 4.2 Hz), 73.0, 71.2, 51.3, 30.7. MS (FAB+) *m/z* 1314 [*M*⁺ (1)], 1279 [*M*⁺+H-Cl (7)], 658 (7), 621 (26), 564 (57), 558 (20), 154 (100).

(*R_p*,*R_s*)-2-(*tert*-Butylsulfenyl)-1-(diphenylphosphino)ferrocene copper (I) bromide dimer [7a]

According to the general procedure, the reaction of (*R*)-**1a** with CuBr gave complex **7a** as an orange solid (94%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -283$ (c 0.1, CHCl₃). ¹H NMR (300 MHz): δ 8.15 (m, 2H), 7.70 (m, 2H), 7.42 (m, 3H), 7.25 (m, 3H), 4.42 (m, 1H), 4.63 (m, 1H), 4.50 (m, 1H), 4.00 (s, 5H), 1.12 (s, 9H). ¹³C NMR (75 MHz): δ 135.3, 135.0, 134.7, 134.5, 132.5 (d, *J*_{C-P} = 14.6 Hz), 130.1, 129.0, 128.4, 128.2, 128.1, 126.4, 85.2 (d, *J*_{C-P} = 36.6 Hz), 78.4 (d, *J*_{C-P} = 46.0 Hz), 77.6, 73.4, 71.9, 71.5, 50.3, 30.4. MS (FAB+) *m/z* 1204 [*M*⁺+H (6)], 1123 [*M*⁺-Br (32)], 458 (100).

(*R_p*,*R_s*)-2-(*tert*-Butylsulfenyl)-1-[bis(1-naphthyl)phosphino]ferrocene copper (I) bromide dimer [7f]

According to the general procedure, the reaction of (*R*)-**1f** with CuBr gave complex **7f** as an orange solid (90%). Mp >200 °C (decomp). $[\alpha]_D^{20} = -251$ (c 0.12, CHCl₃). ¹H NMR (300 MHz): δ 8.50 (m, 1H), 7.95 (d, 1H, *J* = 8.3 Hz), 7.90 (d, 1H, *J* = 8.3 Hz), 7.84 (d, 1H, *J* = 8.1 Hz), 7.74 (m, 2H), 7.60-7.32 (m, 8H), 4.96 (m, 1H), 4.77 (t, 1H, *J* = 2.5 Hz), 4.67 (m, 1H), 3.69 (s, 5H), 1.17 (s, 9H). ¹³C NMR (75 MHz): δ 134.8, 134.7, 133.8

(d, $J = 6.3$ Hz), 133.5 (d, $J = 6.3$ Hz), 133.2, 133.0, 131.9, 131.3, 131.0, 130.9, 130.8, 130.7, 130.6, 129.5, 129.1, 128.4, 127.7, 127.3, 126.6 (d, $J = 5.2$ Hz), 126.4 (d, $J = 4.2$ Hz), 126.1 (d, $J = 5.2$ Hz), 125.1 (d, $J = 11.5$ Hz), 124.3 (d, $J = 6.3$ Hz), 85.5 (d, $J = 40.8$ Hz), 78.4 (d, $J = 3.1$ Hz), 77.5 (d, $J = 43.9$ Hz), 74.7 (d, $J = 4.2$ Hz), 73.1, 71.2, 51.6, 30.8. HRMS (FAB+) calcd for monoisotopic ion $(C_{68}H_{62}(^{79}Br)(^{63}Cu)_2(^{56}Fe)_2P_2S_2)[M^+-Br]$ 1321.0242, found 1321.0249. Calcd for peak maximum isotopic ion $\{C_{68}H_{62}(^{81}Br)(^{63}Cu)_2(^{56}Fe)_2P_2S_2\} [M^+-Br]$ 1323.0222, found 1323.0232. Calcd for peak maximum isotopic ion $\{C_{68}H_{62}(^{79}Br)(^{63}Cu)(^{65}Cu)(^{56}Fe)_2P_2S_2\} [M^+-Br]$ 1323.0224, found 1323.0232

General procedure for the formal aza Diels-Alder reactions: A solution of **7f** (0.0056 mmol) and $AgClO_4$ (0.011 mmol) in CH_2Cl_2 (0.6 mL) was stirred in the dark at room temperature under argon for 2 h and treated with a solution of imine **3** (0.11 mmol) in CH_2Cl_2 (1 mL). The reaction mixture was stirred at room temperature for 5 min before it was treated with diene **2a** or **2b** (0.15 mmol) at the temperature indicated in Table 2. Once the starting material was consumed (reaction time indicated in each case), TFA (0.1-0.2 mL) was added and the mixture was stirred at room temperature for 30-60 min. The reaction mixture was neutralised with saturated aqueous $NaHCO_3$, extracted with CH_2Cl_2 , dried over $MgSO_4$ and filtered. After evaporation of the solvent, the residue was purified by flash chromatography (*n*-hexane-EtOAc 4:1, except for **5i-j**, for which *n*-hexane-EtOAc 6:1 was used). Enantiomeric excesses were determined by HPLC analysis, using the chiral columns indicated in each case.

(*R*)-2-Phenyl-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5a**]⁵**

The reaction of **3a** with diene **2a** at -20 °C for 1 h gave **5a** as a white solid (87%, 97% ee). The same reaction carried out at room temperature afforded **5a** with 93% ee in 90% yield. The enantiopurity of a 93% ee sample of **5a** (obtained at room temperature) was increased to >99.5% ee by recrystallization from *n*-hexanes- CH_2Cl_2 (68% yield of the recrystallization). Mp = 122-123 °C (CH_2Cl_2/n -Hexane). $[\alpha]_D^{20} = +110$ (c 0.5, $CHCl_3$) [$>99.5\%$ ee]; Lit.⁵ [(*S*)-**5a**]: $[\alpha]_D^{20} = -54$ (c 0.5, $CHCl_3$) [48% ee]. HPLC: Daicel Chiralpak AD [hexane/*i*-PrOH 90:10; 0.5 mL/min; 290 nm;

(*R*)-**5a** t_R = 48.3 min; (*S*)-**5a** t_R = 55.8 min]. ^1H NMR (300 MHz): δ 7.80 (dd, 1H, J = 1.4, 8.3 Hz), 7.60 (d, 2H, J = 8.3 Hz), 7.30-7.10 (m, 7H), 5.52 (m, 1H), 5.40 (dd, 1H, J = 1.2, 8.3 Hz), 2.84 (dd, 1H, J = 7.1, 16.6 Hz), 2.66 (ddd, 1H, J = 1.2, 1.8, 16.4 Hz), 2.40 (s, 3H). ^{13}C NMR (75 MHz): δ 190.5, 145.0, 142.5, 137.0, 135.5, 130.0, 128.7, 128.1, 127.0, 126.2, 108.3, 57.6, 41.7, 21.5. MS (EI+) m/z 327 [M^+ (55)], 250 [M^+ -Ph (18)], 172 [M^+ -Ts (46)], 104 (100), 91 (78).

(*R*)-2-(*o*-Tolyl)-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5b**]**

The reaction of **3b** with diene **2a** at room temperature for 3 h gave **5b** as a white solid (82%, 93% ee). Mp = 137-138 °C. $[\alpha]_D^{20}$ = -203 (c 0.4, CHCl_3). HPLC: Daicel Chiralpak AD [n -hexane/ i -PrOH 80:20; 0.6 mL/min; 290 nm; (*S*)-**5b** t_R = 14.6 min; (*R*)-**5b** t_R = 15.7 min]. ^1H NMR (300 MHz): δ 7.96 (dd, 1H, J = 1.2, 8.5 Hz), 7.42 (d, 2H, J = 8.4 Hz), 7.10 (d, 2H, J = 8.4 Hz), 6.99-7.06 (m, 2H), 6.87 (d, 1H, J = 7.9 Hz), 6.72 (dt, 1H, J = 1.6, 7.5 Hz), 5.77 (dt, 1H, J = 1.4, 8.3 Hz), 5.43 (dd, 1H, J = 1.2, 8.3 Hz), 3.05 (dd, 1H, J = 8.3, 16.2 Hz), 2.66 (ddd, 1H, J = 1.2, 1.8, 16.2 Hz), 2.31 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (75 MHz): δ 190.1, 144.9, 143.7, 135.3, 135.2, 133.7, 131.0, 129.8, 127.8, 127.1, 126.2, 125.2, 106.7, 54.5, 41.5, 21.5, 19.1. MS (EI+) m/z 341 [M^+ (27)], 284 (65), 250 [M^+ -*o*-Tol (23)], 186 [M^+ -Ts (34)], 155 (31), 118 (84). HRMS (EI+) calcd for $\text{C}_{19}\text{H}_{19}\text{NO}_3\text{S}$: 341.1086, found 341.1091.

(*R*)-2-[(*p*-Fluoro)phenyl]-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5c**]**

The reaction of **3c** with diene **2a** at -20 °C for 3 h gave **5c** as a white solid (50%, 93% ee). The same reaction carried out at room temperature afforded **5c** with 88% ee in 78% yield. Mp = 120-121 °C. $[\alpha]_D^{20}$ = +82 (c 0.3, CHCl_3). HPLC: Daicel Chiralpak AD [n -hexane/ i -PrOH 80:20; 0.6 mL/min; 290 nm; (*S*)-**5c** t_R = 22.5 min; (*R*)-**5c** t_R = 24.6 min]. ^1H NMR (300 MHz): δ 7.85 (dd, 1H, J = 1.2, 8.3 Hz), 7.62 (d, 2H, J = 8.5 Hz), 7.30 (d, 2H, J = 8.5 Hz), 7.28 (dd, 2H, J = 5.3, 8.5 Hz), 6.92 (t, 2H, J = 8.5 Hz), 5.55 (d, 1H, J = 7.0 Hz), 5.45 (dd, 1H, J = 1.0, 8.3 Hz), 2.88 (dd, 1H, J = 7.0, 16.4 Hz), 2.65 (dt, 1H, J = 1.2, 16.4 Hz), 2.45 (s, 3H). ^{13}C NMR (75 MHz): δ 190.3, 164.0, 160.8, 145.2, 142.3, 135.5, 132.9, 130.1, 128.2, 128.1, 127.0,

115.8, 115.4, 108.3, 56.9, 41.6, 21.6. MS (EI+) m/z 345 [M^+ (41)], 250 [$M^+ - p\text{-FC}_6\text{H}_4$ (19)], 190 [$M^+ - \text{Ts}$ (39)], 155 (26), 122 (100). HRMS (EI+) calcd for $\text{C}_{18}\text{H}_{16}\text{FNO}_3\text{S}$: 345.0835, found 345.0839.

(*R*)-2-[(*p*-Methoxy)phenyl]-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5d]

The reaction of **3d** with diene **2a** at room temperature for 3 h gave **5d** as a pale yellow solid (76%, 91% ee). Mp = 111-113 °C. $[\alpha]_{\text{D}}^{20} = +47$ (c 0.35, CHCl_3). HPLC: Daicel Chiralcel OD [n -hexane/ i -PrOH 90:10; 0.7 mL/min;

290 nm; (*S*)-**5d** t_R = 37.9 min; (*R*)-**5d** t_R = 42.4 min]. ^1H NMR (300 MHz): δ 7.75 (dd, 1H, J = 1.2, 8.3 Hz), 7.60 (d, 2H, J = 8.3 Hz), 7.24 (d, 2H, J = 8.3 Hz), 7.11 (d, 2H, J = 8.9 Hz), 6.72 (d, 2H, J = 8.9 Hz), 5.47 (d, 1H, J = 6.9 Hz), 5.40 (dd, 1H, J = 1.0, 8.3 Hz), 3.75 (s, 3H), 2.79 (dd, 1H, J = 6.9, 16.4 Hz), 2.64 (ddd, 1H, J = 1.2, 2.0, 16.4 Hz), 2.40 (s, 3H). ^{13}C NMR (75 MHz): δ 190.8, 159.4, 144.9, 142.4, 135.8, 130.0, 127.7, 127.0, 126.4, 114.0, 108.3, 57.2, 55.2, 41.7, 21.5. MS (EI+) m/z 357 [M^+ (23)], 250 [$M^+ - p\text{-OMeC}_6\text{H}_4$ (16)], 202 [$M^+ - \text{Ts}$ (33)], 174 (11), 134 (100). HRMS (EI+) calcd for $\text{C}_{19}\text{H}_{19}\text{NO}_4\text{S}$: 357.1035, found 357.1031.

(*R*)-2-[(*p*-Dimethylamino)phenyl]-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5e]

The reaction of **3e** with diene **2a** at room temperature for 3 h gave **5e** as a yellow solid (39%, 93% ee). Mp = 111-113 °C. $[\alpha]_{\text{D}}^{20} = +2$ (c 0.4, CHCl_3). HPLC: Daicel Chiralpak AD [n -hexane/ i -PrOH 80:20; 0.6 mL/min; 290

nm; (*S*)-**5e** t_R = 42.4 min; (*R*)-**5e** t_R = 46.8 min]. ^1H NMR (300 MHz): δ 7.85 (dd, 1H, J = 1.4, 8.3 Hz), 7.70 (d, 2H, J = 8.5 Hz), 7.24 (d, 2H, J = 8.5 Hz), 7.05 (d, 2H, J = 8.5 Hz), 6.50 (d, 2H, J = 8.5 Hz), 5.42 (d, 1H, J = 6.7 Hz), 5.40 (dd, 1H, J = 1.0, 8.3 Hz), 2.90 (s, 6H), 2.76 (dd, 1H, J = 6.7, 16.5 Hz), 2.65 (ddd, 1H, J = 1.2, 2.2, 16.5 Hz), 2.40 (s, 3H). ^{13}C NMR (75 MHz): δ 191.2, 150.3, 144.6, 142.4, 136.0, 129.9, 127.5, 127.0, 124.5, 112.3, 108.3, 71.6, 57.4, 41.6, 40.4, 21.6. MS (EI+) m/z 370 [M^+ (34)], 215 [$M^+ - \text{Ts}$ (21)], 147 (100). HRMS (EI+) calcd for $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_3\text{S}$: 370.1351, found 370.1368.

(*R*)-2-(2-Naphthyl)-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5f]

The reaction of **3f** with diene **2a** at $-20\text{ }^{\circ}\text{C}$ for 3 h gave **5f** as a pale yellow solid (58%, 93% ee). The same reaction carried out at room temperature afforded **5f** with 86% ee in 85% yield. Mp = 142-143 $^{\circ}\text{C}$. $[\alpha]_{\text{D}}^{20} = +22$ (c

0.4, CHCl_3). HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 80:20; 0.5 mL/min; 290 nm; (*S*)-**5f** $t_{\text{R}} = 21.2$ min; (*R*)-**5f** $t_{\text{R}} = 23.3$ min]. ^1H NMR (300 MHz): δ 8.10 (d, 1H, $J = 8.3$ Hz), 7.85 (d, 2H, $J = 8.6$ Hz), 7.75-7.55 (m, 3H), 7.52 (d, 2H, $J = 8.6$ Hz), 7.10 (m, 4H), 6.40 (d, 2H, $J = 7.9$ Hz), 5.45 (d, 1H, $J = 8.3$ Hz), 3.18 (dd, 1H, $J = 7.9, 16.4$ Hz), 2.80 (d, 1H, $J = 16.4$ Hz), 2.34 (s, 3H). ^{13}C NMR (75 MHz): δ 190.0, 145.0, 143.5, 135.0, 134.1, 131.1, 129.8, 129.3, 129.1, 128.5, 127.2, 126.8, 125.8, 124.7, 123.4, 121.7, 106.7, 54.5, 41.8, 21.4. MS (EI+) m/z 377 [M^+ (57)], 250 [M^+ -Naph (33)], 222 [M^+ -Ts (46)], 180 (41), 154 (100). HRMS (EI+) calcd for $\text{C}_{22}\text{H}_{19}\text{NO}_3\text{S}$: 377.1086, found 377.1091.

(*R*)-2-[(2-Phenyl)ethenyl]-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-1H-pyridone [(*R*)-5g]

The reaction of **3g** with diene **2a** at $-20\text{ }^{\circ}\text{C}$ for 1.5 h gave **5g** as a pale yellow solid (82%, 96% ee). The same reaction carried out at room temperature

afforded **5g** with 83% ee in 66% yield. Recrystallization from *n*-hexane- CH_2Cl_2 gave **5g** with >99.5% ee. Mp = 129-130 $^{\circ}\text{C}$ (CH_2Cl_2 /*n*-Hexane). $[\alpha]_{\text{D}}^{20} = -47$ (c 0.3, CHCl_3). HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 80:20; 0.6 mL/min; 290 nm; (*S*)-**5g** $t_{\text{R}} = 27.8$ min; (*R*)-**5g** $t_{\text{R}} = 43.4$ min]. ^1H NMR (300 MHz): δ 7.75 (d, 2H, $J = 8.3$ Hz), 7.70 (m, 1H), 7.25 (m, 5H), 7.12 (m, 2H), 6.40 (d, 1H, $J = 15.9$ Hz), 5.95 (dd, 1H, $J = 7.0, 15.9$ Hz), 5.40 (dd, 1H, $J = 1.1, 8.3$ Hz), 5.05 (t, 1H, $J = 6.4$ Hz), 2.82 (dd, 1H, $J = 6.4, 16.4$ Hz), 2.50 (dt, 1H, $J = 1.6, 16.4$ Hz), 2.33 (s, 3H). ^{13}C NMR (75 MHz): δ 190.8, 145.2, 141.7, 135.8, 135.4, 133.9, 130.2, 128.5, 128.3, 127.4, 126.6, 122.7, 107.6, 57.0, 41.2, 21.5. MS (EI+) m/z 353 [M^+ (34)], 235 [M^+ -(PhCH=CH)-(Me) (27)], 198 [M^+ -Ts (34)], 170 (50), 129 (66). HRMS (EI+) calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_3\text{S}$: 353.1086, found 353.1094.

(*R*)-2-Propyl-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-1H-pyridone [(*S*)-5h]

The reaction of **3h** with diene **2a** at $-78\text{ }^{\circ}\text{C}$ for 5 h gave **5h** as a pale yellow solid (51%, 82% ee). The same reaction carried out at $-20\text{ }^{\circ}\text{C}$ afforded **5h** with 73% ee in

65% yield. Mp = 67-68 °C. $[\alpha]_D^{20} = +495$ (*c* 0.25, CHCl₃). HPLC: Daicel Chiralpak AS [*n*-hexane/*i*-PrOH 40:60; 0.4 mL/min; 290 nm; (*R*)-**5h** t_R = 25.7 min; (*S*)-**5h** t_R = 31.4 min]. ¹H NMR (300 MHz): δ 7.75 (d, 2H, *J* = 8.3 Hz), 7.62 (dd, 1H, *J* = 1.4, 8.3 Hz), 7.39 (d, 2H, *J* = 8.3 Hz), 5.38 (d, 1H, *J* = 8.3 Hz), 4.25 (m, 1H), 2.45 (s, 3H), 2.30 (m, 2H), 1.65 (m, 2H), 1.35 (m, 2H), 0.90 (t, 3H, *J* = 7.3 Hz). ¹³C NMR (75 MHz): δ 191.5, 145.0, 141.5, 136.2, 130.3, 126.8, 108.0, 55.1, 39.1, 32.9, 21.6, 19.0, 13.7. MS (EI+) *m/z* 293 [*M*⁺ (10)], 250 [*M*⁺-*n*-Pr (33)], 236 (20), 155 (77), 138 [*M*⁺-Ts (24)] 91 (100). HRMS (EI+) calcd for C₁₅H₁₉NO₃S: 293.1085, found 293.1094.

(*R*)-5-Methyl-2-phenyl-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5i**]**

The reaction of **3a** with diene **2b** at 0 °C for 5 h gave **5i** as a pale yellow gummy solid (47%, 92% ee). The same reaction carried out at room temperature afforded **5i** with 87% ee in 64% yield. $[\alpha]_D^{20} = +141$ (*c* 0.4, CHCl₃). HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 90:10; 0.7 mL/min; 290 nm; (*R*)-**5i** t_R = 24.8 min; (*S*)-**5i** t_R = 30.0 min]. ¹H NMR (300 MHz): δ 7.69 (d, 2H, *J* = 8.5 Hz), 7.64 (m, 1H), 7.35-7.15 (m, 7H), 5.54 (m, 1H), 2.78 (m, 2H), 2.45 (s, 3H), 1.75 (d, 3H, *J* = 1.0 Hz). ¹³C NMR (75 MHz): δ 191.0, 144.7, 138.2, 137.2, 136.0, 130.1, 128.6, 128.0, 126.9, 126.3, 116.4, 57.5, 41.2, 21.6, 12.9. MS (EI+) *m/z* 341 [*M*⁺ (81)], 250 [*M*⁺-Ph (53)], 186 [*M*⁺-Ts (74)], 155 (31), 91 (100). HRMS (EI+) calcd for C₁₉H₁₉NO₃S: 341.1086, found 341.1091.

(*R*)-5-Methyl-2-[(2-phenyl)ethenyl]-1-(*p*-tolylsulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5j**]**

The reaction of **3g** with diene **2b** at -20 °C for 5 h gave **5j** as a pale yellow solid (57%, 88% ee). $[\alpha]_D^{20} = +20$ (*c* 0.3, CHCl₃). HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 80:20; 0.7 mL/min; 290 nm; (*R*)-**5j** t_R = 17.0 min; (*S*)-**5j** t_R = 35.5 min]. ¹H NMR (300 MHz): δ 7.80 (d, 2H, *J* = 8.3 Hz), 7.58 (m, 1H), 7.30 (m, 5H), 7.18 (d, 2H, *J* = 8.3 Hz), 6.44 (d, 1H, *J* = 16.0 Hz), 5.98 (dd, 1H, *J* = 6.9, 16.0 Hz), 5.06 (m, 1H), 2.81 (dd, 1H, *J* = 6.5, 16.4 Hz), 2.58 (dd, 1H, *J* = 2.2, 16.4 Hz), 2.40 (s, 3H), 1.80 (d, 3H, *J* = 1.2 Hz). ¹³C NMR (75 MHz): δ 191.3, 144.9, 137.7, 136.1, 135.6, 133.6, 130.1, 128.5, 128.2, 127.3, 126.6, 123.4, 115.3, 57.0, 41.0, 21.5, 13.0.

(*R*)-1-(*p*-Methoxybenzenesulfonyl)-2-phenyl-2,3-dihydro-4-*1H*-pyridone [(*R*)-5k**]**

The reaction of **3k** with diene **2a** at room temperature for 3 h gave **5k** as a white solid (61%, 94% ee). Mp = 152-153 °C. $[\alpha]_D^{20} = +70$ (*c* 0.4, CHCl₃).

HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 80:20; 0.5 mL/min; 290 nm; (*S*)-**5k** t_R = 34.7 min; (*R*)-**5k** t_R = 37.0 min]. ¹H NMR (300 MHz): δ 7.82 (dd, 1H, *J* = 1.4, 8.3 Hz), 7.63 (d, 2H, *J* = 9.1 Hz), 7.22-7.10 (m, 5H), 6.88 (d, 2H, *J* = 9.1 Hz), 5.56 (m, 1H), 5.40 (dd, 1H, *J* = 1.2, 8.3 Hz), 3.84 (s, 3H), 2.88 (dd, 1H, *J* = 7.1, 16.6 Hz), 2.67 (ddd, 1H, *J* = 1.4, 2.0, 16.6 Hz). ¹³C NMR (75 MHz): δ 190.5, 163.8, 142.6, 139.9, 137.0, 129.3, 128.7, 128.1, 114.6, 108.0, 57.6, 55.7, 41.9.

(*R*)-2-[(*p*-Fluoro)phenyl]-1-(*p*-methoxybenzenesulfonyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5m]

The reaction of **3m** with diene **2a** at room temperature for 3 h gave **5m** as a white solid (78%, 90% ee). Mp = 131-132 °C. $[\alpha]_D^{20} = +70$ (*c* 0.4, CHCl₃).

HPLC: Daicel Chiralpak AD [hexane/*i*-PrOH 80:20; 0.5 mL/min; 290 nm; (*S*)-**5m** t_R = 33.4 min; (*R*)-**5m** t_R = 38.1 min]. ¹H NMR (300 MHz): δ 7.83 (m, 1H), 7.64 (d, 2H, *J* = 9.1 Hz), 7.19 (dd, 2H, *J* = 5.3, 8.5 Hz), 6.98-6.85 (m, 4H), 5.49 (d, 1H, *J* = 7.1 Hz), 5.41 (dd, 1H, *J* = 1.2, 8.3 Hz), 3.89 (s, 3H), 2.85 (dd, 1H, *J* = 7.1, 16.4 Hz), 2.63 (dt, 1H, *J* = 1.4, 16.4 Hz). ¹³C NMR (75 MHz): δ 190.2, 163.9, 142.4, 129.3, 128.6, 128.2, 128.1, 115.8, 115.5, 114.7, 114.2, 108.1, 57.0, 55.8, 41.8. MS (EI+) *m/z* 361 [*M*⁺ (48)], 266 [*M*⁺-*p*-FC₆H₄ (7)], 190 [*M*⁺-*p*-OMeC₆H₄SO₂ (43)], 171 [*M*⁺-(*p*-OMeC₆H₄SO₂)-F (43)], (100). HRMS (EI+) calcd for C₁₈H₁₆FNO₄S: 361.0784, found 361.0793.

(*R*)-1-(*p*-Methoxybenzenesulfonyl)-2-(2-naphthyl)-2,3-dihydro-4-*1H*-pyridone [(*R*)-5n]

The reaction of **3n** with diene **2a** at room temperature for 3 h gave **5n** as a pale yellow solid (56%, 82% ee). Mp = 144-145 °C. $[\alpha]_D^{20} = -11$ (*c* 0.4, CHCl₃).

HPLC: Daicel Chiralpak AD [*n*-hexane/*i*-PrOH 70:30; 0.7 mL/min; 290 nm; (*S*)-**5n** t_R = 21.4 min; (*R*)-**5n** t_R = 35.3 min]. ¹H NMR (300 MHz): δ 7.90 (dd, 1H, *J* = 1.3, 8.3 Hz), 7.80-7.27 (m, 9H), 6.70 (d, 2H, *J* = 9.1 Hz), 5.70 (d, 1H,

$J = 7.3$ Hz), 5.45 (d, 1H, $J = 8.3$ Hz), 3.67 (s, 3H), 3.0 (dd, 1H, $J = 7.3, 16.4$ Hz), 2.66 (d, 1H, $J = 16.4$ Hz). ^{13}C NMR (75 MHz): δ 190.4, 163.7, 142.7, 134.2, 132.9, 129.3, 128.8, 128.6, 128.0, 127.5, 126.4, 125.6, 124.0, 114.4, 114.2, 108.0, 57.9, 55.6, 41.9. MS (EI+) m/z 393 [M^+ (39)], 350 (5), 266 [$\text{M}^+ - p\text{-OMeC}_6\text{H}_4\text{SO}_2$ (43)], 195 (43), 171 (41), 154 (100). HRMS (EI+) calcd for $\text{C}_{22}\text{H}_{19}\text{NO}_4\text{S}$: 393.1035, found 393.1034.

(*R*)-1-(*p*-Methoxybenzenesulfonyl)-2-[(2-phenyl)ethenyl]-2,3-dihydro-4-*1H*-pyridone [(*R*)-5o]

The reaction of **3o** with diene **2a** at room temperature for 3 h gave **5o** as a pale yellow solid (58%, 76% ee). Mp = 102-104 °C. $[\alpha]_{\text{D}}^{20} = -43$ (c 0.4, CHCl_3). HPLC: Daicel Chiralpak AD [n -hexane/ i -PrOH 70:30; 0.7 mL/min; 290 nm; (*S*)-**5o** $t_R = 18.3$ min; (*R*)-**5o** $t_R = 27.8$ min]. ^1H NMR (300 MHz): δ 7.80 (d, 2H, $J = 8.9$ Hz), 7.70 (dd, 1H, $J = 1.6, 8.3$ Hz), 7.25 (m, 3H), 7.25 (m, 2H), 6.90 (d, 2H, $J = 8.9$ Hz), 6.41 (d, 1H, $J = 16.0$ Hz), 5.95 (dd, 1H, $J = 7.3, 16.0$ Hz), 5.40 (dd, 1H, $J = 1.2, 8.3$ Hz), 5.04 (t, 1H, $J = 6.5$ Hz), 3.64 (s, 3H), 2.83 (dd, 1H, $J = 6.5, 16.4$ Hz), 2.51 (ddd, 1H, $J = 1.2, 2.2, 16.4$ Hz). ^{13}C NMR (75 MHz): δ 190.8, 163.9, 141.8, 135.5, 133.8, 130.0, 129.7, 128.5, 128.3, 126.6, 122.8, 114.7, 107.4, 57.0, 55.6, 41.3. MS (EI+) m/z 369 [M^+ (69)], 327 (9), 251 [$\text{M}^+ - (\text{PhCH}=\text{CH}) - \text{Me}$ (47)], 198 [$\text{M}^+ - p\text{-OMeC}_6\text{H}_4\text{SO}_2$ (43)], 170 (97), 129 (100). HRMS (EI+) calcd for $\text{C}_{20}\text{H}_{19}\text{NO}_4\text{S}$: 369.1035, found 393.1041.

(*R*)-1-(*p*-Nitrobenzenesulfonyl)-2-phenyl-2,3-dihydro-4-*1H*-pyridone [(*R*)-5p]

The reaction of **3p** with diene **2a** at room temperature for 3h gave **5p** as a white solid (58%, 90% ee). Mp = 164-166 °C. $[\alpha]_{\text{D}}^{20} = -136$ (c 0.25, CHCl_3). HPLC: Daicel Chiralpak AD [n -hexane/ i -PrOH 80:20; 0.5 mL/min; 290 nm; (*S*)-**5p** $t_R = 50.0$ min; (*R*)-**5p** $t_R = 57.8$ min]. ^1H NMR (300 MHz): δ 8.18 (d, 2H, $J = 8.9$ Hz), 7.86-7.70 (m, 3H), 7.25-7.05 (m, 5H), 5.62 (d, 1H, $J = 7.5$ Hz), 5.50 (dd, 1H, $J = 1.2, 8.3$ Hz), 3.05 (dd, 1H, $J = 7.5, 16.4$ Hz), 2.70 (dt, 1H, $J = 1.6, 16.4$ Hz). ^{13}C NMR (75 MHz): δ 189.7, 144.0, 141.5, 136.7, 129.0, 128.7, 128.4, 126.3, 124.4, 109.2, 58.6, 42.4. MS (EI+) m/z 358 [M^+ (23)], 328

[M⁺-NO (5)], 281 [M⁺-Ph (21)], 172 [M⁺-*p*-NO₂C₆H₄SO₂ (13)], 156 [M⁺-(*p*-NO₂C₆H₄SO₂)-O (15)], 104 (100). HRMS (EI⁺) calcd for C₁₇H₁₄N₂O₅S: 358.0623, found 358.0632.

(*R*)-2-Phenyl-4-piperidinone [(*R*)-8a]⁶

To a solution of **5a** (32.5 mg, 0.10 mmol) in AcOH (1.0 mL), at room temperature, was added zinc dust (98 mg, 1.5 mmol) in one portion. The mixture was stirred at room temperature for 20 h, filtered through Celite, and concentrated under reduced pressure. The residue was purified by flash chromatography (*n*-hexane-EtOAc) to afford **8a** (10 mg, 58%) as a pale yellow oil. ¹H NMR (200 MHz): δ 7.40-7.25 (m, 5H), 3.93 (t, 1H, *J*=7.0 Hz), 3.50-3.44 (m, 1H), 3.03 (td, 1H, *J*=3.8, 11.8 Hz), 2.67-2.38 (m, 2H), 1.91 (bs, 1H). ¹³C NMR (50 MHz): δ 208.7, 142.5, 128.7, 127.8, 126.4, 62.0, 50.7, 45.8, 42.1.

(*R*)-2-[(2-Phenyl)ethenyl]-4-piperidinone [(*R*)-8g]

To a solution of **5g** (33 mg, 0.10 mmol) in AcOH (1.0 mL), at room temperature, was added zinc dust (98 mg, 1.5 mmol) in one portion. The mixture was stirred at room temperature for 20 h, filtered through Celite, and concentrated under reduced pressure. The residue was purified by flash chromatography (EtOAc) to afford **8g** (11 mg, 63%) as a pale yellow oil. ¹H NMR (200 MHz): δ 7.40-7.24 (m, 5H), 6.59 (d, 1H, *J*=16.1 Hz), 6.21 (dd, 1H, *J*=6.5, 16.1 Hz), 3.62 (ddd, 1H, *J*=3.8, 6.5, 10.2 Hz), 3.44 (ddd, 1H, *J*=3.2, 5.9, 11.5 Hz), 3.00 (td, 1H, *J*=4.3, 11.5 Hz), 2.59-2.37 (m, 4H), 1.88 (bs, 1H). ¹³C NMR (50 MHz): δ 208.3, 136.4, 130.9, 130.4, 128.6, 127.8, 126.4, 59.6, 48.8, 45.3, 42.3.

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X-RAY CRYSTALLOGRAPHIC DATA OF (+)-5a

Table 1. Crystal data and structure refinement for Comp5a.

Identification code	og7_m	
Empirical formula	C18 H17 N O3 S	
Formula weight	327.39	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.0002(8) Å	$\alpha = 90^\circ$.
	b = 10.4496(8) Å	$\beta = 90^\circ$.
	c = 16.0871(10) Å	$\gamma = 90^\circ$.
Volume	1681.1(2) Å ³	
Z	4	

Density (calculated)	1.294 Mg/m ³
Absorption coefficient	1.828 mm ⁻¹
F(000)	688
Crystal size	0.35 x 0.33 x 0.30 mm ³
Theta range for data collection	5.05 to 70.27°.
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 11, -19 ≤ l ≤ 19
Reflections collected	9382
Independent reflections	3109 [R(int) = 0.0256]
Completeness to theta = 70.27°	98.3 %
Absorption correction	YES, SADABS v. 2.03
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3109 / 0 / 277
Goodness-of-fit on F ²	1.073
Final R indices [I > 2σ(I)]	R1 = 0.0296, wR2 = 0.0849
R indices (all data)	R1 = 0.0304, wR2 = 0.0859
Absolute structure parameter	0.011(16)
Extinction coefficient	0.0039(4)
Largest diff. peak and hole	0.107 and -0.154 e.Å ⁻³

Table 2. Atomic coordinates (× 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for Comp5a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7342(2)	920(2)	6130(1)	70(1)
C(2)	7433(3)	1386(3)	6937(2)	89(1)
C(3)	6586(3)	949(3)	7534(2)	102(1)
C(4)	5633(2)	32(3)	7369(2)	88(1)
C(5)	5549(2)	-433(3)	6561(2)	89(1)
C(6)	6394(2)	12(2)	5946(1)	81(1)
C(7)	4699(4)	-473(5)	8028(2)	124(1)
C(8)	9652(2)	-772(2)	5176(1)	61(1)
C(9)	10642(2)	-1628(2)	5217(1)	63(1)
C(10)	11982(2)	-1244(2)	5438(1)	62(1)
C(11)	12197(2)	184(2)	5443(1)	68(1)
C(12)	11027(2)	943(2)	5813(1)	58(1)

C(13)	10987(2)	875(2)	6754(1)	60(1)
C(14)	11654(2)	1811(2)	7198(2)	82(1)
C(15)	11636(3)	1788(3)	8059(2)	106(1)
C(16)	10974(3)	839(3)	8478(2)	99(1)
C(17)	10335(4)	-86(3)	8043(2)	94(1)
C(18)	10324(2)	-84(2)	7188(1)	75(1)
N(1)	9787(1)	493(1)	5405(1)	58(1)
O(1)	7824(2)	1192(2)	4574(1)	92(1)
O(2)	8926(2)	2687(1)	5549(1)	96(1)
O(3)	12898(1)	-1997(1)	5546(1)	85(1)
S(1)	8446(1)	1440(1)	5352(1)	71(1)

Table 3. Bond lengths [Å] and angles [°] for Comp5a.

C(1)-C(6)	1.373(3)
C(1)-C(2)	1.390(3)
C(1)-S(1)	1.755(2)
C(2)-C(3)	1.361(4)
C(2)-H(2)	0.72(3)
C(3)-C(4)	1.377(4)
C(3)-H(3)	0.93(5)
C(4)-C(5)	1.390(3)
C(4)-C(7)	1.507(4)
C(5)-C(6)	1.382(4)
C(5)-H(5)	1.01(3)
C(6)-H(6)	0.95(3)
C(7)-H(17A)	1.03(5)
C(7)-H(17B)	1.16(5)
C(7)-H(17C)	1.12(4)
C(8)-C(9)	1.336(2)
C(8)-N(1)	1.378(2)
C(8)-H(8)	1.05(2)
C(9)-C(10)	1.443(3)
C(9)-H(9)	0.89(2)
C(10)-O(3)	1.221(2)

C(10)-C(11)	1.508(2)
C(11)-C(12)	1.533(3)
C(11)-H(11A)	0.89(2)
C(11)-H(11B)	1.03(2)
C(12)-N(1)	1.479(2)
C(12)-C(13)	1.517(3)
C(12)-H(12)	0.89(2)
C(13)-C(14)	1.382(3)
C(13)-C(18)	1.389(3)
C(14)-C(15)	1.387(4)
C(14)-H(14)	1.00(3)
C(15)-C(16)	1.370(5)
C(15)-H(15)	1.10(4)
C(16)-C(17)	1.354(4)
C(16)-H(16)	0.89(3)
C(17)-C(18)	1.376(3)
C(17)-H(17)	0.71(3)
C(18)-H(18)	0.97(3)
N(1)-S(1)	1.6685(13)
O(1)-S(1)	1.4220(15)
O(2)-S(1)	1.4245(16)

C(6)-C(1)-C(2)	119.3(2)
C(6)-C(1)-S(1)	119.64(15)
C(2)-C(1)-S(1)	121.1(2)
C(3)-C(2)-C(1)	120.1(3)
C(3)-C(2)-H(2)	124(2)
C(1)-C(2)-H(2)	116(2)
C(2)-C(3)-C(4)	121.9(2)
C(2)-C(3)-H(3)	121(3)
C(4)-C(3)-H(3)	117(3)
C(3)-C(4)-C(5)	117.7(2)
C(3)-C(4)-C(7)	122.4(3)
C(5)-C(4)-C(7)	119.8(3)
C(6)-C(5)-C(4)	121.0(2)
C(6)-C(5)-H(5)	120.9(16)

C(4)-C(5)-H(5)	117.9(16)
C(1)-C(6)-C(5)	120.00(19)
C(1)-C(6)-H(6)	124.1(16)
C(5)-C(6)-H(6)	115.8(16)
C(4)-C(7)-H(17A)	85(3)
C(4)-C(7)-H(17B)	113(2)
H(17A)-C(7)-H(17B)	152(4)
C(4)-C(7)-H(17C)	103(2)
H(17A)-C(7)-H(17C)	90(3)
H(17B)-C(7)-H(17C)	105(3)
C(9)-C(8)-N(1)	123.80(16)
C(9)-C(8)-H(8)	123.9(13)
N(1)-C(8)-H(8)	112.2(12)
C(8)-C(9)-C(10)	120.95(15)
C(8)-C(9)-H(9)	119.9(13)
C(10)-C(9)-H(9)	119.0(12)
O(3)-C(10)-C(9)	123.56(15)
O(3)-C(10)-C(11)	122.05(17)
C(9)-C(10)-C(11)	114.14(15)
C(10)-C(11)-C(12)	113.88(15)
C(10)-C(11)-H(11A)	109.2(15)
C(12)-C(11)-H(11A)	110.2(15)
C(10)-C(11)-H(11B)	109.3(13)
C(12)-C(11)-H(11B)	113.7(13)
H(11A)-C(11)-H(11B)	100(2)
N(1)-C(12)-C(13)	113.97(14)
N(1)-C(12)-C(11)	107.67(14)
C(13)-C(12)-C(11)	112.54(15)
N(1)-C(12)-H(12)	104.7(13)
C(13)-C(12)-H(12)	109.7(13)
C(11)-C(12)-H(12)	107.7(13)
C(14)-C(13)-C(18)	118.8(2)
C(14)-C(13)-C(12)	118.00(18)
C(18)-C(13)-C(12)	123.22(16)
C(13)-C(14)-C(15)	119.9(3)
C(13)-C(14)-H(14)	113.2(17)

C(15)-C(14)-H(14)	126.3(17)
C(16)-C(15)-C(14)	120.7(2)
C(16)-C(15)-H(15)	125.6(18)
C(14)-C(15)-H(15)	112.3(18)
C(17)-C(16)-C(15)	119.3(3)
C(17)-C(16)-H(16)	117.8(19)
C(15)-C(16)-H(16)	122.8(18)
C(16)-C(17)-C(18)	121.4(3)
C(16)-C(17)-H(17)	117(2)
C(18)-C(17)-H(17)	121(2)
C(17)-C(18)-C(13)	120.0(2)
C(17)-C(18)-H(18)	117.5(15)
C(13)-C(18)-H(18)	121.4(15)
C(8)-N(1)-C(12)	120.30(13)
C(8)-N(1)-S(1)	118.45(12)
C(12)-N(1)-S(1)	120.52(11)
O(1)-S(1)-O(2)	120.61(10)
O(1)-S(1)-N(1)	106.74(8)
O(2)-S(1)-N(1)	105.11(9)
O(1)-S(1)-C(1)	107.22(10)
O(2)-S(1)-C(1)	109.72(10)
N(1)-S(1)-C(1)	106.62(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Comp5a. 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)	66(1)	70(1)	74(1)	-15(1)	-15(1)	23(1)
C(2)	84(1)	91(2)	91(1)	-34(1)	-9(1)	4(1)
C(3)	94(2)	132(2)	80(1)	-38(1)	-3(1)	16(2)
C(4)	71(1)	108(2)	86(1)	-16(1)	-7(1)	21(1)
C(5)	72(1)	105(2)	91(1)	-16(1)	-11(1)	4(1)
C(6)	75(1)	94(1)	75(1)	-23(1)	-14(1)	7(1)

C(7)	95(2)	172(4)	104(2)	-8(2)	14(2)	3(2)
C(8)	66(1)	51(1)	66(1)	-8(1)	-5(1)	-2(1)
C(9)	68(1)	45(1)	75(1)	-7(1)	6(1)	-1(1)
C(10)	67(1)	54(1)	66(1)	-2(1)	10(1)	6(1)
C(11)	60(1)	58(1)	85(1)	0(1)	6(1)	-8(1)
C(12)	67(1)	38(1)	70(1)	2(1)	-4(1)	-4(1)
C(13)	63(1)	46(1)	69(1)	-4(1)	-12(1)	8(1)
C(14)	84(1)	69(1)	94(1)	-22(1)	-21(1)	2(1)
C(15)	118(2)	100(2)	99(2)	-39(2)	-39(2)	17(2)
C(16)	120(2)	109(2)	69(1)	-17(1)	-26(1)	43(2)
C(17)	126(2)	87(2)	70(1)	12(1)	-6(1)	19(2)
C(18)	98(1)	61(1)	66(1)	3(1)	-10(1)	0(1)
N(1)	64(1)	45(1)	65(1)	-2(1)	-9(1)	4(1)
O(1)	96(1)	104(1)	77(1)	8(1)	-25(1)	24(1)
O(2)	117(1)	49(1)	121(1)	4(1)	-18(1)	21(1)
O(3)	70(1)	74(1)	110(1)	-7(1)	5(1)	21(1)
S(1)	81(1)	58(1)	75(1)	2(1)	-17(1)	20(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for Comp5a.

	x	y	z	U(eq)
H(2)	7910(30)	1890(30)	7000(15)	78(8)
H(3)	6640(50)	1250(50)	8080(30)	191(18)
H(5)	4810(30)	-1050(30)	6428(17)	96(7)
H(6)	6230(30)	-310(20)	5401(17)	99(7)
H(8)	8670(20)	-1000(20)	5001(13)	80(6)
H(9)	10495(18)	-2430(20)	5067(12)	60(5)
H(11A)	12940(20)	360(20)	5716(14)	77(6)
H(11B)	12470(20)	480(20)	4855(16)	85(6)
H(12)	11110(20)	1750(20)	5652(12)	69(5)
H(14)	12000(30)	2520(30)	6841(18)	113(9)
H(15)	12370(40)	2450(30)	8330(20)	138(11)

H(16)	10950(30)	790(30)	9031(19)	97(8)
H(17)	10110(30)	-620(30)	8267(18)	87(9)
H(17A)	5110(60)	230(50)	8400(30)	185(19)
H(17B)	3800(50)	-1020(50)	7750(30)	184(18)
H(17C)	5320(40)	-1220(40)	8350(20)	147(13)
H(18)	9700(30)	-650(30)	6913(16)	91(7)

Table 6. Torsion angles [°] for Comp5a.

C(6)-C(1)-C(2)-C(3)	-0.3(4)
S(1)-C(1)-C(2)-C(3)	-178.6(2)
C(1)-C(2)-C(3)-C(4)	0.8(4)
C(2)-C(3)-C(4)-C(5)	-0.6(4)
C(2)-C(3)-C(4)-C(7)	179.2(3)
C(3)-C(4)-C(5)-C(6)	-0.1(4)
C(7)-C(4)-C(5)-C(6)	-179.9(3)
C(2)-C(1)-C(6)-C(5)	-0.4(3)
S(1)-C(1)-C(6)-C(5)	177.93(18)
C(4)-C(5)-C(6)-C(1)	0.5(4)
N(1)-C(8)-C(9)-C(10)	-5.9(3)
C(8)-C(9)-C(10)-O(3)	174.16(18)
C(8)-C(9)-C(10)-C(11)	-11.4(2)
O(3)-C(10)-C(11)-C(12)	-145.11(19)
C(9)-C(10)-C(11)-C(12)	40.4(2)
C(10)-C(11)-C(12)-N(1)	-50.1(2)
C(10)-C(11)-C(12)-C(13)	76.3(2)
N(1)-C(12)-C(13)-C(14)	-145.77(16)
C(11)-C(12)-C(13)-C(14)	91.26(19)
N(1)-C(12)-C(13)-C(18)	34.7(2)
C(11)-C(12)-C(13)-C(18)	-88.3(2)
C(18)-C(13)-C(14)-C(15)	-0.8(3)
C(12)-C(13)-C(14)-C(15)	179.6(2)
C(13)-C(14)-C(15)-C(16)	0.6(4)
C(14)-C(15)-C(16)-C(17)	0.1(4)
C(15)-C(16)-C(17)-C(18)	-0.7(4)

C(16)-C(17)-C(18)-C(13)	0.5(4)
C(14)-C(13)-C(18)-C(17)	0.2(3)
C(12)-C(13)-C(18)-C(17)	179.8(2)
C(9)-C(8)-N(1)-C(12)	-7.5(3)
C(9)-C(8)-N(1)-S(1)	-177.77(14)
C(13)-C(12)-N(1)-C(8)	-90.97(19)
C(11)-C(12)-N(1)-C(8)	34.6(2)
C(13)-C(12)-N(1)-S(1)	79.05(16)
C(11)-C(12)-N(1)-S(1)	-155.37(13)
C(8)-N(1)-S(1)-O(1)	-45.60(16)
C(12)-N(1)-S(1)-O(1)	144.19(14)
C(8)-N(1)-S(1)-O(2)	-174.80(15)
C(12)-N(1)-S(1)-O(2)	15.00(16)
C(8)-N(1)-S(1)-C(1)	68.76(15)
C(12)-N(1)-S(1)-C(1)	-101.45(14)
C(6)-C(1)-S(1)-O(1)	23.03(18)
C(2)-C(1)-S(1)-O(1)	-158.70(18)
C(6)-C(1)-S(1)-O(2)	155.67(16)
C(2)-C(1)-S(1)-O(2)	-26.1(2)
C(6)-C(1)-S(1)-N(1)	-91.00(17)
C(2)-C(1)-S(1)-N(1)	87.27(18)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for Comp5a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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X-RAY CRYSTALLOGRAPHIC DATA OF (+)-6a

Table 1. Crystal data and structure refinement for Comp6a.

Identification code	og3_m
Empirical formula	C _{53.33} H _{55.33} Cl ₄ Cu ₂ Fe ₂ P ₂ S ₂
Formula weight	1202.95
Temperature	297(2) K
Wavelength	1.54178 Å
Crystal system	Trigonal
Space group	P3(2)21
Unit cell dimensions	a = 17.7079(2) Å α = 90°. b = 17.7079(2) Å β = 90°. c = 15.0264(2) Å γ = 120°.
Volume	4080.56(8) Å ³
Z	3
Density (calculated)	1.469 Mg/m ³
Absorption coefficient	8.413 mm ⁻¹
F(000)	1846
Crystal size	0.38 x 0.36 x 0.34 mm ³

Theta range for data collection	2.88 to 70.62°.
Index ranges	-21<= <i>h</i> <=20, -21<= <i>k</i> <=20, -18<= <i>l</i> <=18
Reflections collected	24724
Independent reflections	5090 [R(int) = 0.0718]
Completeness to theta = 70.62°	97.9 %
Absorption correction	YES, SADABS v. 2.03
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5090 / 0 / 304
Goodness-of-fit on F ²	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0911
R indices (all data)	R1 = 0.0374, wR2 = 0.0921
Absolute structure parameter	0.001(4)
Extinction coefficient	0.00233(14)
Largest diff. peak and hole	0.477 and -0.564 e.Å ⁻³

Table 2. Atomic coordinates (× 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for Comp6a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-223(2)	2231(2)	673(2)	32(1)
C(2)	-189(2)	2992(2)	285(2)	27(1)
C(3)	-517(2)	2760(2)	-608(2)	41(1)
C(4)	-724(2)	1896(2)	-774(2)	50(1)
C(5)	-550(2)	1559(2)	8(2)	46(1)
C(6)	-2714(3)	1277(7)	-40(4)	129(4)
C(7)	-2476(3)	2138(5)	256(4)	88(2)
C(8)	-2187(2)	2205(3)	1114(3)	51(1)
C(9)	-2222(3)	1446(3)	1365(3)	60(1)
C(10)	-2545(3)	852(3)	656(4)	90(2)
C(11)	1278(2)	4714(2)	484(2)	29(1)
C(12)	1564(2)	4637(3)	-352(2)	49(1)
C(13)	2406(3)	5217(3)	-634(3)	66(1)
C(14)	2976(2)	5879(3)	-77(3)	63(1)
C(15)	2699(3)	5968(2)	748(3)	53(1)
C(16)	1858(2)	5391(2)	1028(2)	41(1)

C(17)	-450(2)	4451(2)	489(2)	30(1)
C(18)	-364(2)	4755(3)	-384(2)	44(1)
C(19)	-894(3)	5060(3)	-700(3)	63(1)
C(20)	-1520(3)	5064(3)	-141(3)	66(1)
C(21)	-1587(3)	4791(3)	718(3)	54(1)
C(22)	-1060(2)	4485(2)	1041(2)	39(1)
C(23)	1107(3)	2255(3)	1756(3)	58(1)
C(24)	1313(4)	2228(5)	2739(4)	94(2)
C(25)	1065(5)	1489(5)	1271(5)	110(3)
C(26)	1749(3)	3128(5)	1360(4)	100(2)
C(27)	4017(10)	4481(6)	9995(11)	157(8)
Cl(1)	1128(1)	4286(1)	3421(1)	38(1)
Cl(2)	3672(3)	4150(2)	9160(2)	167(1)
Cu(1)	90(1)	3563(1)	2314(1)	36(1)
Fe(1)	-1429(1)	1946(1)	282(1)	34(1)
P(1)	185(1)	3980(1)	914(1)	23(1)
S(1)	4(1)	2135(1)	1790(1)	38(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for Comp6a.

C(1)-C(5)	1.435(4)
C(1)-C(2)	1.441(4)
C(1)-S(1)	1.753(3)
C(1)-Fe(1)	2.021(3)
C(2)-C(3)	1.437(4)
C(2)-P(1)	1.799(3)
C(2)-Fe(1)	2.046(3)
C(3)-C(4)	1.406(5)
C(3)-Fe(1)	2.037(3)
C(4)-C(5)	1.420(5)
C(4)-Fe(1)	2.049(3)
C(5)-Fe(1)	2.033(4)
C(6)-C(10)	1.405(11)
C(6)-C(7)	1.435(12)
C(6)-Fe(1)	2.029(4)
C(7)-C(8)	1.370(7)

C(7)-Fe(1)	2.044(5)
C(8)-C(9)	1.366(6)
C(8)-Fe(1)	2.046(4)
C(9)-C(10)	1.403(7)
C(9)-Fe(1)	2.039(4)
C(10)-Fe(1)	2.036(4)
C(11)-C(12)	1.386(4)
C(11)-C(16)	1.389(4)
C(11)-P(1)	1.826(3)
C(12)-C(13)	1.388(5)
C(13)-C(14)	1.382(7)
C(14)-C(15)	1.371(7)
C(15)-C(16)	1.385(5)
C(17)-C(22)	1.386(4)
C(17)-C(18)	1.398(4)
C(17)-P(1)	1.819(3)
C(18)-C(19)	1.379(5)
C(19)-C(20)	1.394(6)
C(20)-C(21)	1.364(6)
C(21)-C(22)	1.381(5)
C(23)-C(25)	1.508(7)
C(23)-C(26)	1.509(8)
C(23)-C(24)	1.527(6)
C(23)-S(1)	1.859(4)
C(27)-Cl(2)	1.391(16)
C(27)-C(27)#1	1.42(3)
C(27)-Cl(2)#1	2.014(17)
Cl(1)-Cu(1)	2.3303(7)
Cl(1)-Cu(1)#2	2.3621(8)
Cl(2)-C(27)#1	2.014(18)
Cu(1)-P(1)	2.2075(7)
Cu(1)-Cl(1)#2	2.3621(8)
Cu(1)-S(1)	2.5785(9)
C(5)-C(1)-C(2)	107.7(3)
C(5)-C(1)-S(1)	127.1(2)

C(2)-C(1)-S(1)	125.0(2)
C(5)-C(1)-Fe(1)	69.70(19)
C(2)-C(1)-Fe(1)	70.16(16)
S(1)-C(1)-Fe(1)	121.21(15)
C(3)-C(2)-C(1)	106.8(3)
C(3)-C(2)-P(1)	131.9(2)
C(1)-C(2)-P(1)	121.3(2)
C(3)-C(2)-Fe(1)	69.07(17)
C(1)-C(2)-Fe(1)	68.34(16)
P(1)-C(2)-Fe(1)	125.97(13)
C(4)-C(3)-C(2)	108.9(3)
C(4)-C(3)-Fe(1)	70.33(19)
C(2)-C(3)-Fe(1)	69.70(16)
C(3)-C(4)-C(5)	108.5(3)
C(3)-C(4)-Fe(1)	69.42(18)
C(5)-C(4)-Fe(1)	69.03(19)
C(4)-C(5)-C(1)	108.0(3)
C(4)-C(5)-Fe(1)	70.3(2)
C(1)-C(5)-Fe(1)	68.84(17)
C(10)-C(6)-C(7)	108.1(4)
C(10)-C(6)-Fe(1)	70.1(3)
C(7)-C(6)-Fe(1)	69.9(3)
C(8)-C(7)-C(6)	106.4(6)
C(8)-C(7)-Fe(1)	70.5(2)
C(6)-C(7)-Fe(1)	68.8(3)
C(9)-C(8)-C(7)	110.1(5)
C(9)-C(8)-Fe(1)	70.2(2)
C(7)-C(8)-Fe(1)	70.4(3)
C(8)-C(9)-C(10)	109.2(5)
C(8)-C(9)-Fe(1)	70.7(2)
C(10)-C(9)-Fe(1)	69.7(2)
C(9)-C(10)-C(6)	106.2(5)
C(9)-C(10)-Fe(1)	70.0(2)
C(6)-C(10)-Fe(1)	69.5(3)
C(12)-C(11)-C(16)	117.9(3)
C(12)-C(11)-P(1)	124.1(2)

C(16)-C(11)-P(1)	118.0(2)
C(11)-C(12)-C(13)	121.0(4)
C(14)-C(13)-C(12)	120.1(4)
C(15)-C(14)-C(13)	119.6(3)
C(14)-C(15)-C(16)	120.3(4)
C(15)-C(16)-C(11)	121.1(3)
C(22)-C(17)-C(18)	118.9(3)
C(22)-C(17)-P(1)	118.9(2)
C(18)-C(17)-P(1)	122.2(2)
C(19)-C(18)-C(17)	120.6(3)
C(18)-C(19)-C(20)	119.6(3)
C(21)-C(20)-C(19)	119.8(3)
C(20)-C(21)-C(22)	121.0(3)
C(21)-C(22)-C(17)	120.1(3)
C(25)-C(23)-C(26)	113.8(5)
C(25)-C(23)-C(24)	110.2(4)
C(26)-C(23)-C(24)	110.1(5)
C(25)-C(23)-S(1)	109.5(4)
C(26)-C(23)-S(1)	109.7(3)
C(24)-C(23)-S(1)	102.9(3)
Cl(2)-C(27)-C(27)#1	91.5(11)
Cl(2)-C(27)-Cl(2)#1	116.8(6)
C(27)#1-C(27)-Cl(2)#1	43.6(11)
Cu(1)-Cl(1)-Cu(1)#2	81.94(3)
C(27)-Cl(2)-C(27)#1	44.9(9)
P(1)-Cu(1)-Cl(1)	126.09(3)
P(1)-Cu(1)-Cl(1)#2	124.87(3)
Cl(1)-Cu(1)-Cl(1)#2	95.31(3)
P(1)-Cu(1)-S(1)	89.67(3)
Cl(1)-Cu(1)-S(1)	113.64(3)
Cl(1)#2-Cu(1)-S(1)	106.63(3)
C(1)-Fe(1)-C(6)	162.0(3)
C(1)-Fe(1)-C(5)	41.46(13)
C(6)-Fe(1)-C(5)	125.3(3)
C(1)-Fe(1)-C(10)	124.0(2)
C(6)-Fe(1)-C(10)	40.4(3)

C(5)-Fe(1)-C(10)	106.1(2)
C(1)-Fe(1)-C(3)	69.44(13)
C(6)-Fe(1)-C(3)	121.2(2)
C(5)-Fe(1)-C(3)	68.62(14)
C(10)-Fe(1)-C(3)	154.6(2)
C(1)-Fe(1)-C(9)	106.79(16)
C(6)-Fe(1)-C(9)	67.0(2)
C(5)-Fe(1)-C(9)	119.48(17)
C(10)-Fe(1)-C(9)	40.3(2)
C(3)-Fe(1)-C(9)	164.05(16)
C(1)-Fe(1)-C(7)	153.8(2)
C(6)-Fe(1)-C(7)	41.2(3)
C(5)-Fe(1)-C(7)	164.3(2)
C(10)-Fe(1)-C(7)	68.6(3)
C(3)-Fe(1)-C(7)	109.5(2)
C(9)-Fe(1)-C(7)	66.6(2)
C(1)-Fe(1)-C(2)	41.50(11)
C(6)-Fe(1)-C(2)	155.8(3)
C(5)-Fe(1)-C(2)	69.42(12)
C(10)-Fe(1)-C(2)	162.3(2)
C(3)-Fe(1)-C(2)	41.23(11)
C(9)-Fe(1)-C(2)	125.89(15)
C(7)-Fe(1)-C(2)	120.2(2)
C(1)-Fe(1)-C(8)	119.78(14)
C(6)-Fe(1)-C(8)	66.9(2)
C(5)-Fe(1)-C(8)	153.88(16)
C(10)-Fe(1)-C(8)	67.15(19)
C(3)-Fe(1)-C(8)	128.30(15)
C(9)-Fe(1)-C(8)	39.08(18)
C(7)-Fe(1)-C(8)	39.1(2)
C(2)-Fe(1)-C(8)	108.93(13)
C(1)-Fe(1)-C(4)	69.16(13)
C(6)-Fe(1)-C(4)	108.63(19)
C(5)-Fe(1)-C(4)	40.71(16)
C(10)-Fe(1)-C(4)	119.65(18)
C(3)-Fe(1)-C(4)	40.25(14)

C(9)-Fe(1)-C(4)	154.34(18)
C(7)-Fe(1)-C(4)	128.0(2)
C(2)-Fe(1)-C(4)	68.79(12)
C(8)-Fe(1)-C(4)	164.82(17)
C(2)-P(1)-C(17)	104.49(13)
C(2)-P(1)-C(11)	104.48(12)
C(17)-P(1)-C(11)	103.13(13)
C(2)-P(1)-Cu(1)	104.26(9)
C(17)-P(1)-Cu(1)	121.78(9)
C(11)-P(1)-Cu(1)	116.87(9)
C(1)-S(1)-C(23)	103.99(17)
C(1)-S(1)-Cu(1)	95.82(9)
C(23)-S(1)-Cu(1)	110.67(15)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+2 #2 -x,-x+y,-z+2/3

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Comp6a. 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)	36(1)	34(1)	29(2)	-4(1)	5(1)	20(1)
C(2)	28(1)	39(1)	14(1)	0(1)	4(1)	16(1)
C(3)	46(2)	52(2)	17(1)	-1(1)	3(1)	18(1)
C(4)	50(2)	57(2)	26(2)	-17(1)	4(1)	14(2)
C(5)	52(2)	44(2)	41(2)	-12(2)	4(2)	23(2)
C(6)	32(2)	219(9)	62(3)	-64(5)	-12(2)	6(3)
C(7)	53(2)	149(6)	76(4)	17(4)	-2(2)	61(3)
C(8)	35(2)	59(2)	56(2)	-1(2)	13(2)	20(2)
C(9)	51(2)	73(3)	48(2)	10(2)	24(2)	25(2)
C(10)	60(3)	55(2)	108(5)	-23(3)	42(3)	-6(2)
C(11)	32(1)	36(1)	24(1)	5(1)	2(1)	21(1)
C(12)	42(2)	63(2)	34(2)	-3(2)	11(1)	20(2)
C(13)	55(2)	76(3)	52(2)	5(2)	30(2)	22(2)
C(14)	38(2)	57(2)	80(3)	20(2)	20(2)	13(2)

C(15)	46(2)	39(2)	61(2)	5(2)	2(2)	11(1)
C(16)	43(2)	37(2)	39(2)	1(1)	1(1)	17(1)
C(17)	33(1)	36(1)	25(1)	5(1)	3(1)	21(1)
C(18)	52(2)	71(2)	28(2)	23(2)	13(1)	45(2)
C(19)	79(3)	100(3)	42(2)	33(2)	17(2)	69(3)
C(20)	66(2)	96(3)	69(3)	35(3)	15(2)	66(3)
C(21)	52(2)	70(2)	64(2)	18(2)	23(2)	47(2)
C(22)	49(2)	50(2)	29(2)	8(1)	12(1)	33(1)
C(23)	65(2)	83(3)	57(2)	2(2)	-8(2)	59(2)
C(24)	115(4)	148(5)	69(3)	3(4)	-25(3)	103(4)
C(25)	137(6)	150(6)	115(5)	-47(5)	-31(4)	125(5)
C(26)	51(2)	138(5)	131(6)	46(4)	18(3)	62(3)
C(27)	220(16)	50(5)	142(12)	-10(6)	69(12)	23(6)
Cl(1)	26(1)	56(1)	19(1)	1(1)	-1(1)	11(1)
Cl(2)	224(3)	149(2)	172(2)	-17(2)	-22(2)	126(2)
Cu(1)	38(1)	55(1)	13(1)	2(1)	-1(1)	22(1)
Fe(1)	30(1)	41(1)	21(1)	-5(1)	1(1)	11(1)
P(1)	28(1)	32(1)	13(1)	3(1)	2(1)	17(1)
S(1)	49(1)	43(1)	32(1)	6(1)	1(1)	31(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for Comp6a.

	x	y	z	U(eq)
H(3)	-589	3141	-1030	49
H(4)	-967	1574	-1328	60
H(5)	-644	969	83	56
H(6)	-2956	1027	-624	155
H(7)	-2526	2584	-82	106
H(8)	-1973	2726	1488	61
H(9)	-2045	1337	1947	72
H(10)	-2652	253	654	108
H(12)	1186	4191	-729	59
H(13)	2588	5160	-1198	79

H(14)	3544	6262	-260	76
H(15)	3078	6417	1122	64
H(16)	1678	5459	1589	49
H(18)	55	4753	-756	53
H(19)	-834	5260	-1282	75
H(20)	-1890	5253	-354	79
H(21)	-1995	4811	1093	65
H(22)	-1113	4301	1629	47
H(24A)	888	1679	2990	141
H(24B)	1296	2694	3049	141
H(24C)	1883	2294	2795	141
H(25A)	1581	1460	1396	166
H(25B)	1024	1559	642	166
H(25C)	561	961	1466	166
H(26A)	1608	3559	1555	150
H(26B)	1718	3089	723	150
H(26C)	2328	3290	1551	150
H(27)	4320	5111	10107	170(50)

Table 6. Torsion angles [°] for Comp6a.

C(5)-C(1)-C(2)-C(3)	1.3(3)
S(1)-C(1)-C(2)-C(3)	-173.4(2)
Fe(1)-C(1)-C(2)-C(3)	-58.5(2)
C(5)-C(1)-C(2)-P(1)	179.7(2)
S(1)-C(1)-C(2)-P(1)	5.1(4)
Fe(1)-C(1)-C(2)-P(1)	119.88(19)
C(5)-C(1)-C(2)-Fe(1)	59.8(2)
S(1)-C(1)-C(2)-Fe(1)	-114.8(2)
C(1)-C(2)-C(3)-C(4)	-1.5(3)
P(1)-C(2)-C(3)-C(4)	-179.7(2)
Fe(1)-C(2)-C(3)-C(4)	-59.6(2)
C(1)-C(2)-C(3)-Fe(1)	58.09(19)
P(1)-C(2)-C(3)-Fe(1)	-120.1(2)
C(2)-C(3)-C(4)-C(5)	1.2(4)
Fe(1)-C(3)-C(4)-C(5)	-58.1(2)

C(2)-C(3)-C(4)-Fe(1)	59.2(2)
C(3)-C(4)-C(5)-C(1)	-0.4(4)
Fe(1)-C(4)-C(5)-C(1)	-58.7(2)
C(3)-C(4)-C(5)-Fe(1)	58.3(2)
C(2)-C(1)-C(5)-C(4)	-0.6(4)
S(1)-C(1)-C(5)-C(4)	173.9(2)
Fe(1)-C(1)-C(5)-C(4)	59.5(3)
C(2)-C(1)-C(5)-Fe(1)	-60.14(19)
S(1)-C(1)-C(5)-Fe(1)	114.4(2)
C(10)-C(6)-C(7)-C(8)	-0.9(5)
Fe(1)-C(6)-C(7)-C(8)	-60.9(3)
C(10)-C(6)-C(7)-Fe(1)	59.9(4)
C(6)-C(7)-C(8)-C(9)	0.7(5)
Fe(1)-C(7)-C(8)-C(9)	-59.1(3)
C(6)-C(7)-C(8)-Fe(1)	59.8(3)
C(7)-C(8)-C(9)-C(10)	-0.1(4)
Fe(1)-C(8)-C(9)-C(10)	-59.3(3)
C(7)-C(8)-C(9)-Fe(1)	59.2(3)
C(8)-C(9)-C(10)-C(6)	-0.5(5)
Fe(1)-C(9)-C(10)-C(6)	-60.4(3)
C(8)-C(9)-C(10)-Fe(1)	59.9(3)
C(7)-C(6)-C(10)-C(9)	0.8(5)
Fe(1)-C(6)-C(10)-C(9)	60.7(3)
C(7)-C(6)-C(10)-Fe(1)	-59.8(3)
C(16)-C(11)-C(12)-C(13)	0.4(6)
P(1)-C(11)-C(12)-C(13)	-179.6(3)
C(11)-C(12)-C(13)-C(14)	0.5(7)
C(12)-C(13)-C(14)-C(15)	-1.1(7)
C(13)-C(14)-C(15)-C(16)	0.9(7)
C(14)-C(15)-C(16)-C(11)	0.0(6)
C(12)-C(11)-C(16)-C(15)	-0.6(5)
P(1)-C(11)-C(16)-C(15)	179.4(3)
C(22)-C(17)-C(18)-C(19)	-2.0(6)
P(1)-C(17)-C(18)-C(19)	176.0(4)
C(17)-C(18)-C(19)-C(20)	0.1(7)
C(18)-C(19)-C(20)-C(21)	1.8(8)

C(19)-C(20)-C(21)-C(22)	-1.8(8)
C(20)-C(21)-C(22)-C(17)	-0.1(6)
C(18)-C(17)-C(22)-C(21)	1.9(5)
P(1)-C(17)-C(22)-C(21)	-176.1(3)
Cl(2)#1-C(27)-Cl(2)-C(27)#1	-37.0(10)
Cu(1)#2-Cl(1)-Cu(1)-P(1)	158.66(3)
Cu(1)#2-Cl(1)-Cu(1)-Cl(1)#2	17.55(4)
Cu(1)#2-Cl(1)-Cu(1)-S(1)	-93.21(3)
C(5)-C(1)-Fe(1)-C(6)	48.8(6)
C(2)-C(1)-Fe(1)-C(6)	167.4(6)
S(1)-C(1)-Fe(1)-C(6)	-73.0(6)
C(2)-C(1)-Fe(1)-C(5)	118.6(2)
S(1)-C(1)-Fe(1)-C(5)	-121.8(3)
C(5)-C(1)-Fe(1)-C(10)	75.0(3)
C(2)-C(1)-Fe(1)-C(10)	-166.4(2)
S(1)-C(1)-Fe(1)-C(10)	-46.8(3)
C(5)-C(1)-Fe(1)-C(3)	-80.6(2)
C(2)-C(1)-Fe(1)-C(3)	37.98(16)
S(1)-C(1)-Fe(1)-C(3)	157.6(2)
C(5)-C(1)-Fe(1)-C(9)	115.8(2)
C(2)-C(1)-Fe(1)-C(9)	-125.66(19)
S(1)-C(1)-Fe(1)-C(9)	-6.0(2)
C(5)-C(1)-Fe(1)-C(7)	-173.2(4)
C(2)-C(1)-Fe(1)-C(7)	-54.6(5)
S(1)-C(1)-Fe(1)-C(7)	65.0(5)
C(5)-C(1)-Fe(1)-C(2)	-118.6(2)
S(1)-C(1)-Fe(1)-C(2)	119.6(2)
C(5)-C(1)-Fe(1)-C(8)	156.2(2)
C(2)-C(1)-Fe(1)-C(8)	-85.3(2)
S(1)-C(1)-Fe(1)-C(8)	34.4(2)
C(5)-C(1)-Fe(1)-C(4)	-37.4(2)
C(2)-C(1)-Fe(1)-C(4)	81.14(19)
S(1)-C(1)-Fe(1)-C(4)	-159.2(2)
C(10)-C(6)-Fe(1)-C(1)	34.4(8)
C(7)-C(6)-Fe(1)-C(1)	153.3(5)
C(10)-C(6)-Fe(1)-C(5)	72.0(4)

C(7)-C(6)-Fe(1)-C(5)	-169.0(3)
C(7)-C(6)-Fe(1)-C(10)	118.9(5)
C(10)-C(6)-Fe(1)-C(3)	156.7(3)
C(7)-C(6)-Fe(1)-C(3)	-84.4(4)
C(10)-C(6)-Fe(1)-C(9)	-38.7(3)
C(7)-C(6)-Fe(1)-C(9)	80.2(3)
C(10)-C(6)-Fe(1)-C(7)	-118.9(5)
C(10)-C(6)-Fe(1)-C(2)	-166.3(3)
C(7)-C(6)-Fe(1)-C(2)	-47.3(6)
C(10)-C(6)-Fe(1)-C(8)	-81.4(3)
C(7)-C(6)-Fe(1)-C(8)	37.6(3)
C(10)-C(6)-Fe(1)-C(4)	114.2(3)
C(7)-C(6)-Fe(1)-C(4)	-126.9(3)
C(4)-C(5)-Fe(1)-C(1)	-119.4(3)
C(4)-C(5)-Fe(1)-C(6)	77.1(4)
C(1)-C(5)-Fe(1)-C(6)	-163.5(3)
C(4)-C(5)-Fe(1)-C(10)	117.0(3)
C(1)-C(5)-Fe(1)-C(10)	-123.5(3)
C(4)-C(5)-Fe(1)-C(3)	-36.7(2)
C(1)-C(5)-Fe(1)-C(3)	82.7(2)
C(4)-C(5)-Fe(1)-C(9)	158.5(2)
C(1)-C(5)-Fe(1)-C(9)	-82.0(2)
C(4)-C(5)-Fe(1)-C(7)	49.4(8)
C(1)-C(5)-Fe(1)-C(7)	168.8(7)
C(4)-C(5)-Fe(1)-C(2)	-81.0(2)
C(1)-C(5)-Fe(1)-C(2)	38.44(17)
C(4)-C(5)-Fe(1)-C(8)	-172.2(3)
C(1)-C(5)-Fe(1)-C(8)	-52.8(4)
C(1)-C(5)-Fe(1)-C(4)	119.4(3)
C(9)-C(10)-Fe(1)-C(1)	75.1(4)
C(6)-C(10)-Fe(1)-C(1)	-167.9(4)
C(9)-C(10)-Fe(1)-C(6)	-117.0(5)
C(9)-C(10)-Fe(1)-C(5)	116.9(3)
C(6)-C(10)-Fe(1)-C(5)	-126.1(4)
C(9)-C(10)-Fe(1)-C(3)	-169.2(4)
C(6)-C(10)-Fe(1)-C(3)	-52.3(7)

C(6)-C(10)-Fe(1)-C(9)	117.0(5)
C(9)-C(10)-Fe(1)-C(7)	-78.7(3)
C(6)-C(10)-Fe(1)-C(7)	38.3(4)
C(9)-C(10)-Fe(1)-C(2)	44.3(8)
C(6)-C(10)-Fe(1)-C(2)	161.3(6)
C(9)-C(10)-Fe(1)-C(8)	-36.3(3)
C(6)-C(10)-Fe(1)-C(8)	80.7(4)
C(9)-C(10)-Fe(1)-C(4)	158.8(3)
C(6)-C(10)-Fe(1)-C(4)	-84.2(4)
C(4)-C(3)-Fe(1)-C(1)	81.7(2)
C(2)-C(3)-Fe(1)-C(1)	-38.22(16)
C(4)-C(3)-Fe(1)-C(6)	-82.2(4)
C(2)-C(3)-Fe(1)-C(6)	158.0(4)
C(4)-C(3)-Fe(1)-C(5)	37.1(2)
C(2)-C(3)-Fe(1)-C(5)	-82.77(19)
C(4)-C(3)-Fe(1)-C(10)	-45.3(6)
C(2)-C(3)-Fe(1)-C(10)	-165.2(5)
C(4)-C(3)-Fe(1)-C(9)	160.7(6)
C(2)-C(3)-Fe(1)-C(9)	40.8(7)
C(4)-C(3)-Fe(1)-C(7)	-126.3(3)
C(2)-C(3)-Fe(1)-C(7)	113.8(3)
C(4)-C(3)-Fe(1)-C(2)	119.9(3)
C(4)-C(3)-Fe(1)-C(8)	-166.0(2)
C(2)-C(3)-Fe(1)-C(8)	74.1(2)
C(2)-C(3)-Fe(1)-C(4)	-119.9(3)
C(8)-C(9)-Fe(1)-C(1)	116.8(2)
C(10)-C(9)-Fe(1)-C(1)	-123.1(4)
C(8)-C(9)-Fe(1)-C(6)	-81.1(4)
C(10)-C(9)-Fe(1)-C(6)	38.9(5)
C(8)-C(9)-Fe(1)-C(5)	160.1(2)
C(10)-C(9)-Fe(1)-C(5)	-79.9(4)
C(8)-C(9)-Fe(1)-C(10)	-120.0(5)
C(8)-C(9)-Fe(1)-C(3)	43.0(7)
C(10)-C(9)-Fe(1)-C(3)	163.1(6)
C(8)-C(9)-Fe(1)-C(7)	-36.1(3)
C(10)-C(9)-Fe(1)-C(7)	83.9(4)

C(8)-C(9)-Fe(1)-C(2)	75.2(3)
C(10)-C(9)-Fe(1)-C(2)	-164.8(4)
C(10)-C(9)-Fe(1)-C(8)	120.0(5)
C(8)-C(9)-Fe(1)-C(4)	-166.5(3)
C(10)-C(9)-Fe(1)-C(4)	-46.5(6)
C(8)-C(7)-Fe(1)-C(1)	-44.5(6)
C(6)-C(7)-Fe(1)-C(1)	-161.7(4)
C(8)-C(7)-Fe(1)-C(6)	117.3(5)
C(8)-C(7)-Fe(1)-C(5)	152.4(6)
C(6)-C(7)-Fe(1)-C(5)	35.1(10)
C(8)-C(7)-Fe(1)-C(10)	79.7(3)
C(6)-C(7)-Fe(1)-C(10)	-37.6(4)
C(8)-C(7)-Fe(1)-C(3)	-127.3(3)
C(6)-C(7)-Fe(1)-C(3)	115.4(4)
C(8)-C(7)-Fe(1)-C(9)	36.0(3)
C(6)-C(7)-Fe(1)-C(9)	-81.3(4)
C(8)-C(7)-Fe(1)-C(2)	-83.1(3)
C(6)-C(7)-Fe(1)-C(2)	159.6(4)
C(6)-C(7)-Fe(1)-C(8)	-117.3(5)
C(8)-C(7)-Fe(1)-C(4)	-168.7(2)
C(6)-C(7)-Fe(1)-C(4)	74.0(5)
C(3)-C(2)-Fe(1)-C(1)	119.0(2)
P(1)-C(2)-Fe(1)-C(1)	-113.7(2)
C(3)-C(2)-Fe(1)-C(6)	-51.5(5)
C(1)-C(2)-Fe(1)-C(6)	-170.5(5)
P(1)-C(2)-Fe(1)-C(6)	75.8(5)
C(3)-C(2)-Fe(1)-C(5)	80.7(2)
C(1)-C(2)-Fe(1)-C(5)	-38.40(17)
P(1)-C(2)-Fe(1)-C(5)	-152.1(2)
C(3)-C(2)-Fe(1)-C(10)	158.9(6)
C(1)-C(2)-Fe(1)-C(10)	39.9(6)
P(1)-C(2)-Fe(1)-C(10)	-73.8(6)
C(1)-C(2)-Fe(1)-C(3)	-119.0(2)
P(1)-C(2)-Fe(1)-C(3)	127.2(3)
C(3)-C(2)-Fe(1)-C(9)	-167.2(2)
C(1)-C(2)-Fe(1)-C(9)	73.8(2)

P(1)-C(2)-Fe(1)-C(9)	-39.9(3)
C(3)-C(2)-Fe(1)-C(7)	-85.6(3)
C(1)-C(2)-Fe(1)-C(7)	155.4(2)
P(1)-C(2)-Fe(1)-C(7)	41.7(3)
C(3)-C(2)-Fe(1)-C(8)	-127.1(2)
C(1)-C(2)-Fe(1)-C(8)	113.88(19)
P(1)-C(2)-Fe(1)-C(8)	0.2(2)
C(3)-C(2)-Fe(1)-C(4)	36.9(2)
C(1)-C(2)-Fe(1)-C(4)	-82.1(2)
P(1)-C(2)-Fe(1)-C(4)	164.2(2)
C(9)-C(8)-Fe(1)-C(1)	-79.8(3)
C(7)-C(8)-Fe(1)-C(1)	159.1(3)
C(9)-C(8)-Fe(1)-C(6)	81.5(4)
C(7)-C(8)-Fe(1)-C(6)	-39.6(5)
C(9)-C(8)-Fe(1)-C(5)	-42.4(4)
C(7)-C(8)-Fe(1)-C(5)	-163.5(4)
C(9)-C(8)-Fe(1)-C(10)	37.4(3)
C(7)-C(8)-Fe(1)-C(10)	-83.7(4)
C(9)-C(8)-Fe(1)-C(3)	-166.2(2)
C(7)-C(8)-Fe(1)-C(3)	72.8(4)
C(7)-C(8)-Fe(1)-C(9)	-121.1(4)
C(9)-C(8)-Fe(1)-C(7)	121.1(4)
C(9)-C(8)-Fe(1)-C(2)	-124.1(3)
C(7)-C(8)-Fe(1)-C(2)	114.8(4)
C(9)-C(8)-Fe(1)-C(4)	157.2(5)
C(7)-C(8)-Fe(1)-C(4)	36.2(7)
C(3)-C(4)-Fe(1)-C(1)	-82.4(2)
C(5)-C(4)-Fe(1)-C(1)	38.09(19)
C(3)-C(4)-Fe(1)-C(6)	116.5(4)
C(5)-C(4)-Fe(1)-C(6)	-122.9(4)
C(3)-C(4)-Fe(1)-C(5)	-120.5(3)
C(3)-C(4)-Fe(1)-C(10)	159.5(3)
C(5)-C(4)-Fe(1)-C(10)	-80.0(3)
C(5)-C(4)-Fe(1)-C(3)	120.5(3)
C(3)-C(4)-Fe(1)-C(9)	-167.9(4)
C(5)-C(4)-Fe(1)-C(9)	-47.4(4)

C(3)-C(4)-Fe(1)-C(7)	74.6(3)
C(5)-C(4)-Fe(1)-C(7)	-164.9(3)
C(3)-C(4)-Fe(1)-C(2)	-37.80(19)
C(5)-C(4)-Fe(1)-C(2)	82.7(2)
C(3)-C(4)-Fe(1)-C(8)	46.4(6)
C(5)-C(4)-Fe(1)-C(8)	166.9(5)
C(3)-C(2)-P(1)-C(17)	30.9(3)
C(1)-C(2)-P(1)-C(17)	-147.1(2)
Fe(1)-C(2)-P(1)-C(17)	-62.39(19)
C(3)-C(2)-P(1)-C(11)	-77.1(3)
C(1)-C(2)-P(1)-C(11)	104.9(2)
Fe(1)-C(2)-P(1)-C(11)	-170.39(16)
C(3)-C(2)-P(1)-Cu(1)	159.7(3)
C(1)-C(2)-P(1)-Cu(1)	-18.2(2)
Fe(1)-C(2)-P(1)-Cu(1)	66.43(17)
C(22)-C(17)-P(1)-C(2)	112.2(3)
C(18)-C(17)-P(1)-C(2)	-65.8(3)
C(22)-C(17)-P(1)-C(11)	-138.8(3)
C(18)-C(17)-P(1)-C(11)	43.2(3)
C(22)-C(17)-P(1)-Cu(1)	-5.2(3)
C(18)-C(17)-P(1)-Cu(1)	176.8(2)
C(12)-C(11)-P(1)-C(2)	23.3(3)
C(16)-C(11)-P(1)-C(2)	-156.8(2)
C(12)-C(11)-P(1)-C(17)	-85.7(3)
C(16)-C(11)-P(1)-C(17)	94.2(2)
C(12)-C(11)-P(1)-Cu(1)	137.9(3)
C(16)-C(11)-P(1)-Cu(1)	-42.2(3)
Cl(1)-Cu(1)-P(1)-C(2)	136.77(9)
Cl(1)#2-Cu(1)-P(1)-C(2)	-92.87(9)
S(1)-Cu(1)-P(1)-C(2)	17.30(9)
Cl(1)-Cu(1)-P(1)-C(17)	-105.77(12)
Cl(1)#2-Cu(1)-P(1)-C(17)	24.59(12)
S(1)-Cu(1)-P(1)-C(17)	134.76(12)
Cl(1)-Cu(1)-P(1)-C(11)	22.06(11)
Cl(1)#2-Cu(1)-P(1)-C(11)	152.43(10)
S(1)-Cu(1)-P(1)-C(11)	-97.40(10)

C(5)-C(1)-S(1)-C(23)	82.3(3)
C(2)-C(1)-S(1)-C(23)	-104.1(3)
Fe(1)-C(1)-S(1)-C(23)	169.35(19)
C(5)-C(1)-S(1)-Cu(1)	-164.7(3)
C(2)-C(1)-S(1)-Cu(1)	8.9(3)
Fe(1)-C(1)-S(1)-Cu(1)	-77.63(15)
C(25)-C(23)-S(1)-C(1)	-66.3(4)
C(26)-C(23)-S(1)-C(1)	59.3(4)
C(24)-C(23)-S(1)-C(1)	176.5(3)
C(25)-C(23)-S(1)-Cu(1)	-168.2(4)
C(26)-C(23)-S(1)-Cu(1)	-42.6(4)
C(24)-C(23)-S(1)-Cu(1)	74.6(4)
P(1)-Cu(1)-S(1)-C(1)	-15.00(10)
Cl(1)-Cu(1)-S(1)-C(1)	-144.83(10)
Cl(1)#2-Cu(1)-S(1)-C(1)	111.51(10)
P(1)-Cu(1)-S(1)-C(23)	92.34(15)
Cl(1)-Cu(1)-S(1)-C(23)	-37.49(15)
Cl(1)#2-Cu(1)-S(1)-C(23)	-141.15(15)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z+2 #2 -x,-x+y,-z+2/3

Table 7. Hydrogen bonds for Comp6a [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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