Supporting Information for

Iron(II) Active Species in Iron-Bisphosphine Catalyzed Kumada and Suzuki-Miyaura Cross-Couplings of Phenyl Nucleophiles and Secondary Alkyl Halides

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Table of Contents

1. Supplementary Spectral Data .................................................. S2
   1.1 Mössbauer ................................................................. S2
   1.2 UV-Vis MCD ............................................................. S16
   1.3 EPR ................................................................. S17
   1.4 NMR ............................................................ S18

2. Reaction/GC Data ................................................................. S19

3. X-ray Crystal Structure Details ................................................ S20
   3.1 Fe(η^6-biphenyl)(SciOPP) (2) ........................................ S21
   3.2 Fe(Ph)Br(SciOPP) (5-Br) ............................................ S66
1. Supplementary Spectral Data

1.1 Mössbauer

![Mössbauer spectrum](image)

**Figure S1.** The 80 K $^{57}$Fe Mössbauer spectrum of the in-situ iron species from reaction of $^{57}$Fe-1-Cl$_2$ with 20 equiv PhMgBr in 1:1 THF:2-MeTHF at 25 °C. Data (black dots), total fit (black line) and individual components are shown. The individual components exhibit Mössbauer parameters of δ = 0.44 mm/s and ΔE$_Q$ = 1.75 mm/s (94%, purple) and δ = 0.46 mm/s and ΔE$_Q$ = 0.65 mm/s (6%, orange).

**Table S1.** Mössbauer parameters of the in-situ iron species during the reaction of 2 with 20 equiv chlorocycloheptane in 1:1 THF:2-MeTHF at 25 °C. The colors of the components below match those in Figure 2. Times are relative to the addition of chlorocycloheptane.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|-----------|-----------------------|--------------------------|
| 0         | δ = 0.44 mms, ΔE$_Q$ = 1.75 mm/s<br>δ = 0.46 mms, ΔE$_Q$ = 0.65 mm/s | 95<br>5 |
| 5         | δ = 0.44 mms, ΔE$_Q$ = 1.75 mm/s<br>δ = 0.46 mms, ΔE$_Q$ = 0.65 mm/s<br>δ = 0.94 mms, ΔE$_Q$ = 2.80 mm/s | 87<br>5<br>8 |
| 15        | δ = 0.44 mms, ΔE$_Q$ = 1.75 mm/s<br>δ = 0.46 mms, ΔE$_Q$ = 0.65 mm/s<br>δ = 0.94 mms, ΔE$_Q$ = 2.80 mm/s | 78<br>5<br>17 |
| 45        | δ = 0.44 mms, ΔE$_Q$ = 1.75 mm/s<br>δ = 0.46 mms, ΔE$_Q$ = 0.65 mm/s<br>δ = 0.94 mms, ΔE$_Q$ = 2.80 mm/s | 62<br>5<br>33 |
Figure S2. Pseudo-first order kinetic data for the reaction of 2 with 20 equiv chlorocycloheptane in 1:1 THF:2-MeTHF at 25 °C using freeze-trapped $^{57}$Fe Mössbauer spectroscopy. The observed rate is $9.0(5) \times 10^{-3}$ min$^{-1}$. Errors are determined from the average of multiple measurements and the error for quantitation by Mössbauer ($\pm 3\%$).

Figure S3. The 5 K $^{57}$Fe Mössbauer spectrum of the in-situ generated iron species from reaction of $^{57}$Fe-1-Cl$_2$ with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C for 5 min. Data (black dots), total fit (black line) and individual components are shown. The individual components exhibit Mössbauer parameters of $\delta = 0.33$ mm/s and $\Delta E_Q = 1.50$ mm/s (63%, red), $\delta = 0.32$ mm/s and $\Delta E_Q = 3.13$ mm/s (33%, blue) and $\delta = 0.46$ mm/s and $\Delta E_Q = 0.65$ mm/s (4%, orange). The parameters of these components are identical to those obtained for the same sample at 80 K and all quantitations are within 2 % of those for the 80 K data, within the error for quantitation ($\pm 3\%$).
Figure S4. The 80 K $^{57}$Fe Mössbauer spectrum of the in-situ generated iron species from reaction of $^{57}$Fe-1-Cl$_2$ + 1 equiv free SciOPP ligand with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C for 5 min. Data (black dots), total fit (black line) and individual components are shown. The individual components exhibit Mössbauer parameters of $\delta = 0.33$ mm/s and $\Delta E_Q = 1.50$ mm/s (59%, red), $\delta = 0.32$ mm/s and $\Delta E_Q = 3.13$ mm/s (35%, blue) and $\delta = 0.46$ mm/s and $\Delta E_Q = 0.65$ mm/s (6%, orange). The parameters of these components are identical to those obtained for the same sample at 80 K without added ligand and all quantitations are within the error (± 3 %).

Table S2. Mössbauer Parameters of the In-Situ Iron Species During the Reaction of $^{57}$Fe-1-Cl$_2$ with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 25 °C. The colors of the components below match those in Figure 4.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|-----------|----------------------|--------------------------|
| 0.5       | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 62                       |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 32                       |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
| 3         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 49                       |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 22                       |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
|           | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 23                       |
| 5         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 44                       |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 18                       |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
|           | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 32                       |
| 10        | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 27                       |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 10                       |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 7                        |
|           | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 56                       |
Figure S5. Pseudo-first order kinetic data for the formation of 2 from reaction of $^{57}\text{Fe-1-Cl}_2$ with 2 equiv PhMgBr at 25 °C using freeze-trapped $^{57}\text{Fe}$ Mössbauer spectroscopy. The observed rate is 0.12(2) min$^{-1}$. Errors are determined from the average of multiple measurements and the error for quantitation by Mössbauer (± 3 %).
Figure S6. The 80 K $^{57}$Fe Mössbauer spectrum of the in-situ iron species as a function of reaction time at 0 °C in 1:1 THF:2-MeTHF upon reaction of $^{57}$Fe-1-Cl$_2$ with 2 equiv PhMgBr. The Mössbauer parameters of the individual components are given in Table S3.
**Table S3.** Mössbauer parameters of the in-situ iron species during the reaction of $^{57}$Fe-$\text{I-Cl}_2$ with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C. The colors of the components below match those in Figure S6.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|------------|-----------------------|--------------------------|
| 1          | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s |
| 20         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s |
| 90         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s |
| 150        | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s |

**Figure S7.** 80 K $^{57}$Fe Mössbauer spectra of the in-situ generated iron species from reaction of $^{57}$Fe-$\text{I-Cl}_2$ with 2 equiv PhMgBr in (A) THF and (B) Et$_2$O at 0 °C for 5 min. Data (black dots), total fit (black line) and individual components are shown for each spectrum. In THF, two major components are observed with Mössbauer parameters of $\delta = 0.31$ mm/s and $\Delta E_Q = 1.45$ mm/s (74%, red), and $\delta = 0.33$ mm/s and $\Delta E_Q = 3.17$ mm/s (26%, blue). In Et$_2$O, a single species is observed with Mössbauer parameters of $\delta = 0.32$ mm/s and $\Delta E_Q = 1.38$ mm/s.
Figure S8. The 80 K $^{57}$Fe Mössbauer spectrum of the in-situ generated iron species from reaction of $^{57}$Fe-1-Cl$_2$ with 1 equiv PhMgBr in 1:1 THF:2-MeTHF at (A) 25 °C for 1 min and (B) 0 °C for 5 min. Data (black dots), total fit (black line) and individual components are shown for each spectrum. The individual components for spectrum A exhibit Mössbauer parameters of $\delta = 0.51$ mm/s and $\Delta E_Q = 2.33$ mm/s (72%, green), $\delta = 0.33$ mm/s and $\Delta E_Q = 1.50$ mm/s (18%, red), and $\delta = 0.32$ mm/s and $\Delta E_Q = 3.13$ mm/s (5%, blue) and $\delta = 0.94$ mm/s and $\Delta E_Q = 2.80$ mm/s (6%, brown). The same components with identical Mössbauer parameters are observed for spectrum B with the following quantitations: 75 % (green), 15 % (red), 4 % (blue) and 6 % (brown).
Figure S9. 80 K Mössbauer spectra of the in-situ iron species formed as a function of time at 25 °C in 1:1 THF:2-MeTHF following reaction of 3 mM $^{57}$Fe-1-Cl$_2$ with 1 equiv PhMgBr. The Mössbauer parameters of the individual components are given in Table S4.
Table S4. Mössbauer parameters of the in-situ iron species during the disproportionation of 5-X formed in-situ from the reaction of $^{57}$Fe-1-Cl$_2$ with 1 equiv PhMgBr in 1:1 THF:2-MeTHF at 25 °C. The colors of the components below match those in Figure S9. Note that the reductive elimination of the $\delta = 0.33, 0.32$ mm/s species at 25 °C at early reaction times contributes to initial formation of 2 as previously determined.

| Time (min) | Mössbauer Parameters                  | Amount of Total Iron (%) |
|------------|---------------------------------------|--------------------------|
| 1          | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 72                       |
|            | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 18                       |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 5                        |
|            | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 5                        |
| 15         | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 63                       |
|            | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 5                        |
|            | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 11                       |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 21                       |
| 40         | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 52                       |
|            | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 17                       |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 31                       |
| 60         | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 46                       |
|            | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 22                       |
|            | $\delta = 0.44$ mms, $\Delta E_Q = 1.75$ mm/s | 33                       |

Figure S10. Second order kinetic data for the disproportionation of 5-X at 25 °C in 1:1 THF:2-MeTHF using freeze-trapped $^{57}$Fe Mössbauer spectroscopy. The observed rate is $4.7(6) \times 10^{-3}$ mM$^{-1}$min$^{-1}$. Errors are determined from the average of multiple measurements and the error for quantitation by Mössbauer (± 3 %).
Figure S11. 80 K $^{57}$Fe Mössbauer spectra of the in-situ generated iron species from reaction of $^{57}$Fe-1-Cl$_2$ with 1 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C demonstrating the stability of 5-X at 0 °C.
Figure S12. 80 K Mössbauer spectra of the in-situ iron species formed at 0 °C in 1:1 THF:2-MeTHF upon addition of 1 equiv PhMgBr to 3 mM $^{57}$Fe-1-Cl$_2$ and subsequent reaction with 20 equiv chlorocycloheptane as a function of time at 0 °C. Initial reaction with 1 equiv PhMgBr was for 5 min prior to electrophile addition. All times given in the figure are relative to the addition of chlorocycloheptane. The Mössbauer parameters of the individual components are given in Table S5.
Figure S13. 80 K Mössbauer spectra of the in-situ iron species formed at 0 °C in 1:1 THF:2-MeTHF upon addition of 2 equiv PhMgBr to 3 mM $^{57}$Fe-1-Cl$_2$ and subsequent reaction with 2 equiv chlorocycloheptane as a function of time at 0 °C. Initial reaction with 2 equiv PhMgBr was for 5 min prior to electrophile addition. All times given in the figure are relative to the addition of chlorocycloheptane. The Mössbauer parameters of the individual components are given in Table S6.
Figure S14. 5 K Mössbauer spectra of the in-situ iron species formed at 0 °C in 1:1 THF:2-MeTHF upon addition of 2 equiv PhMgBr to 3 mM $^{57}$Fe-1-Cl$_2$ and subsequent reaction with 2 equiv chlorocycloheptane as a function of time at 0 °C. Initial reaction with 2 equiv PhMgBr was for 5 min prior to electrophile addition. All times given in the figure are relative to the addition of chlorocycloheptane. The Mössbauer parameters of the individual components are given in Table S7.
**Table S5.** Mössbauer parameters of the in-situ iron species during the reaction of $^{57}$Fe-1-Cl$_2$ with 1 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C and subsequent reaction as a function of time at 0 °C with 20 equiv chlorocycloheptane. The colors of the components below match those in Figure S12.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|-----------|----------------------|--------------------------|
| 0         | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 75                        |
|           | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 15                        |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 4                         |
|           | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 6                         |
| 10        | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 44                        |
|           | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 56                        |
| 20        | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 35                        |
|           | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 65                        |
| 60        | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 20                        |
|           | $\delta = 0.94$ mms, $\Delta E_Q = 2.80$ mm/s | 80                        |

**Table S6.** 80 K Mössbauer parameters of the in-situ iron species during the reaction of $^{57}$Fe-1-Cl$_2$ with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C and subsequent reaction as a function of time at 0 °C with 2 equiv chlorocycloheptane. The colors of the components below match those in Figure S13.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|-----------|----------------------|--------------------------|
| 0         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 62                        |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 32                        |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                         |
| 1         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 38                        |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 18                        |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                         |
|           | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 40                        |
| 5         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 32                        |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 11                        |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                         |
|           | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 53                        |
| 15        | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 18                        |
|           | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 2                         |
|           | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                         |
|           | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 65                        |
Table S7. 5 K Mössbauer parameters of the in-situ iron species during the reaction of $^{57}$Fe-1-Cl$_2$ with 2 equiv PhMgBr in 1:1 THF:2-MeTHF at 0 °C and subsequent reaction as a function of time at 0 °C with 2 equiv chlorocycloheptane. The colors of the components below match those in Figure S14.

| Time (min) | Mössbauer Parameters | Amount of Total Iron (%) |
|------------|----------------------|--------------------------|
| 0          | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 62                       |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 32                       |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
| 1          | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 38                       |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 18                       |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
|            | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 40                       |
| 5          | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 32                       |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 11                       |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
|            | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 53                       |
| 15         | $\delta = 0.33$ mms, $\Delta E_Q = 1.50$ mm/s | 18                       |
|            | $\delta = 0.32$ mms, $\Delta E_Q = 3.13$ mm/s | 2                        |
|            | $\delta = 0.46$ mms, $\Delta E_Q = 0.65$ mm/s | 6                        |
|            | $\delta = 0.51$ mms, $\Delta E_Q = 2.33$ mm/s | 65                       |

1.2 UV-Vis MCD

Figure S15. 5 K, 7 T UV-Vis MCD spectrum of the iron species in solution upon reaction of 1-Cl$_2$ with 2 equiv PhMgBr at 0 °C for 5 min in 1:1 THF:2-MeTHF.
1.3 EPR

**Figure S16.** 10 K EPR Spectrum of the $S = 1/2$ species $3$ present in solution after addition of 2 equiv PhMgBr to 1-Cl$_2$ at 0 °C in 1:1 THF-2-MeTHF. The orange spectrum is 3 min after PhMgBr addition and the black spectrum is 120 min after addition. Spin quantitation indicates no change within error of the amount of $3$ present over this time frame ($\sim 5\%$), where significant reductive elimination to form 2 has occurred (see Figure S5).

**Figure S17.** 10 K EPR Spectrum of $3$ present in solution after addition of 2 equiv PhMgBr to 1-Cl$_2$ at 0 °C in 1:1 THF-2-MeTHF (orange) and following reaction with 2 equiv cycloheptylchloride at 0 °C for 1 min (blue) and 5 min (black). Spin quantitation indicates no change in the amount of $3$ present over this time frame ($\sim 3-4\%$), where significant consumption of $4a/4b$ to form 5-X has occurred (see Figure S13).
1.4 NMR

Figure S18. In-situ (A) $^1$H-NMR and (B) $^{31}$P-NMR spectra (500 MHz) of the formation of 2 from the reaction of 1-Cl$_2$ with 2 equiv PhMgBr at 0 °C followed by slow warming to 25 °C. The inset in (A) shows the growth with time of the 5 protons associated with $\eta^6$-aryl coordination. The observed $^{31}$P NMR resonance (88.98 ppm) and $^1$H resonances at 4.48 and 5.66 ppm are in a range consistent with previously reported values for ($\eta^6$-napthalene)Fe$^0$(bisphosphine) complexes, where the presence of multiple $\eta^6$-aryl $^1$H resonances is consistent with asymmetric $\eta^6$-aryl coordination. Note: The in-situ $^1$H NMR spectrum also contains contributions from unreacted PhMgBr, THF (from PhMgBr solution that is added) and paramagnetic intermediates that are consumed with time. A minor amount of free SciOPP ligand is also observed to form with time in both spectra.

1. Kubo, H.; Hirano, M.; Komiya, S. *J. Organomet. Chem.* 1998, 556, 89-95.
2. Reaction/GC Data

Table S8. GC data for reactions on in-situ generated phenylated iron(II)-SciOPP species with chlorocycloheptane (ChpCl) at 25 °C. All yields are with respect to iron.

| PhMgBr (equiv) | time | Chp-Ph | cycloheptene |
|---------------|------|--------|--------------|
| 1             | 60 s | 35 %   | 13 %         |
| 1             | 150 s| 48 %   | 14 %         |
| 1             | 300 s| 58 %   | 14 %         |
| 2             | 10 s | 87 %   | 67 %         |
| 2             | 30 s | 104 %  | 67 %         |
| 2             | 60 s | 104 %  | 65 %         |

Note: 1-Cl shows no reactivity towards bromocycloheptane at 25 °C (i.e. no ChpBr consumption or product generation following reaction for 10 min) as determined by GC analysis.

Table S9. GC data for reactions on in-situ generated phenylated iron(II)-SciOPP species with chlorocycloheptane and bromocycloheptane at 0 °C. Results are also given for quenching the phenylated iron(II)-SciOPP species without added electrophile which results in formation of biphenyl due to the quenching process. All yields are with respect to iron.

| PhMgBr (equiv) | ChpX (equiv) | time (min) | Chp-Ph | cycloheptene | biphenyl |
|---------------|--------------|------------|--------|--------------|----------|
| 2             | -            | 5 min      | 0 %    | 0 %          | 51 %     |
| 2             | Cl           | 60 min     | 24 %   | 52 %         | 37 %     |
| 2             | Cl           | 30 min     | 58 %   | 51 %         | 16 %     |
| 2             | Cl           | 10 min     | 108 %  | 96 %         | 9 %      |
| 2             | Br           | 20 min     | 56 %   | 46 %         | 14 %     |
| 2             | Br           | 20 min     | 105 %  | 71 %         | 8 %      |
| 2             | Br           | 5 min      | 88 %   | 96 %         | 9 %      |
| 1             | -            | 5 min      | 0 %    | 0 %          | 15 %     |
| 1             | Cl           | 60 min     | 96 %   | 32 %         | 6 %      |
| 1             | Br           | 20 min     | 85 %   | 22 %         | 3 %      |

Identical GC results were obtained using either dilute HCl or aqueous NaHSO₄ for quenching.

For the reaction of Fe(η⁶-biphenyl)(SciOPP) with chlorocycloheptane at 25 °C, the following product distributions were observed by GC: cycloheptene (41 %), biphenyl (71 %) and phenylcycloheptane (4 %). All yields are with respect to iron.
3. X-ray Crystal Structure Details

General Comments: For the Fe(η⁶-biphenyl)(SciOPP) (2) crystal structure there are two independent iron molecules in the asymmetric unit, which lie in general positions. Additionally there is a cocrystallized isopropanol molecule that lies in a crystallographic inversion center, over which it is modeled as disordered (0.50:0.50). The π-ligand disorder on molecule Fe1 is a site disorder of biphenyl and benzene with an occupancy ratio of 0.67:0.33. There appears to be a cocrystallized n-hexane solvent molecule that is only present when the ligand is benzene, presumably to fill the void. Although there is a similar disorder on molecule Fe2, the biphenyl ligand is present much more of the time (> 90 % by mass) and no solvent could be identified for the minor component of the disorder (which was not modeled anyway because no significant improvement to the overall model was achieved). While the quality of the structure determination is less than desirable due to the disorder and ligand exchange with solvent, the results provide unambiguous information on the connectivity and geometry of 2. For the Fe(Ph)Br(SciOPP) (5-Br) structure, the phenyl ligand and tert-butyl groups C35-C38 and C55-C58 are modeled as disordered over two positions each (0.70:0.30, 0.78:0.22, and 0.72:0.28, respectively). Extensive efforts to obtain less disordered crystals for both species were unsuccessful, including the use of alternative solvents for crystallization. Both structure determinations are consistent with the formulations proposed from the synthesis and spectroscopic studies.
3.1 Fe(η^6-biphenyl)(SciOPP) (2)

CRYSTAL STRUCTURE REPORT

C_{74.75} H_{101.66} Fe O_{0.25} P_{2}

or

[(PP)Fe(η^6-biphenyl)]_{0.834} · [(PP)Fe(η^6-benzene)]_{0.166} · ¼ iPrOH

Report prepared for:
B. Snyder, Prof. M. Neidig

July 14, 2012

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Rochester, NY 14627
Data collection
A crystal (0.18 x 0.10 x 0.06 mm³) was placed onto the tip of a 0.1 mm diameter glass capillary tube or fiber and mounted on a Bruker SMART APEX II CCD Platform diffractometer for a data collection at 100.0(5) K.¹ A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 120 seconds and a detector distance of 4.01 cm. A randomly oriented region of reciprocal space was surveyed: five major sections of frames were collected with 0.50º steps in ω at five different φ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.² Final cell constants were calculated from the xyz centroids of 2152 strong reflections from the actual data collection after integration.³ See Table 1 for additional crystal and refinement information.

Structure solution and refinement
The structure was solved using SIR97⁴ and refined using SHELXL-97.⁵ The space group P-1 was determined based on intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to \( R_1 = 0.0880 \) (\( F^2, I > 2\sigma(I) \)) and \( wR_2 = 0.2103 \) (\( F^2, \text{all data} \)).

Structure description
The structure is similar to the one suggested. All atoms of the iron molecules lie in general positions, but the cocrystallized isopropanol molecule lies in a crystallographic inversion center, over which it is modeled as disordered (50:50). The pi-ligand disorder on molecule Fe1 is a site disorder of biphenyl and benzene/n-hexane (67:33). The cocrystallized n-hexane solvent molecule is only present when the ligand is benzene. Although there is a similar disorder on molecule Fe2, the biphenyl ligand is present much more of the time (> 90 % by mass) and no solvent could be identified for the minor component of the disorder (which was not modeled because no significant improvement to the overall model was achieved).

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.
Some equations of interest:

\[ R_{\text{int}} = \Sigma |F_o^2 - F_c^2| / \Sigma F_o^2 \]
\[ R1 = \Sigma |F_o| - |F_c| / \Sigma F_o \]
\[ wR2 = [\Sigma w(F_o^2-F_c^2)^2] / \Sigma [w(F_o^2)^2] ]^{1/2} \]

where \( w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP] \) and \( P = 1/3 \max (0, F_o^2) + 2/3 F_c^2 \)
\[ \text{GOF} = S = \{ \Sigma [w(F_o^2-F_c^2)^2] / (m-n) \} ^{1/2} \]

where \( m = \) number of reflections and \( n = \) number of parameters
| **Identification code**       | neibs06               |
|------------------------------|-----------------------|
| **Empirical formula**        | C74.75 H101.66 Fe O0.25 P2 |
| **Formula weight**           | 1122.01               |
| **Temperature**              | 100.0(5) K            |
| **Wavelength**               | 0.71073 Å             |
| **Crystal system**           | Triclinic             |
| **Space group**              | P-1                   |
| **Unit cell dimensions**     |                       |
| \(a\)                       | 14.922(3) Å           |
| \(\alpha\)                  | 77.487(3)°            |
| \(b\)                       | 21.309(4) Å           |
| \(\beta\)                   | 80.874(3)°            |
| \(c\)                       | 22.714(4) Å           |
| \(\gamma\)                  | 71.734(3)°            |
| **Volume**                   | 6664(2) Å³            |
| **Z**                        | 4                     |
| **Density (calculated)**     | 1.118 Mg/m³           |
| **Absorption coefficient**   | 0.315 mm⁻¹            |
| \(F(000)\)                  | 2433                  |
| **Crystal color, morphology**| red-purple, plate     |
| **Crystal size**             | 0.18 x 0.10 x 0.06 mm³|
| **Theta range for data collection** | 1.79 to 25.03° |
| **Index ranges**             | -17 ≤ \(h\) ≤ 17, -25 ≤ \(k\) ≤ 25, -27 ≤ \(l\) ≤ 27 |
| **Reflections collected**    | 87423                 |
| **Independent reflections**  | 23523 \([R(\text{int}) = 0.3618]\) |
| **Observed reflections**     | 7831                  |
| **Completeness to theta = 25.03°** | 100.0%                |
| **Absorption correction**    | Multi-scan            |
| **Max. and min. transmission** | 0.9814 and 0.9455     |
| **Refinement method**        | Full-matrix least-squares on \(F^2\) |
| **Data / restraints / parameters** | 23523 / 44 / 1502 |
| **Goodness-of-fit on \(F^2\)** | 0.931                |
| **Final \(R\) indices** \([I>2\sigma(I)]\) | \(R_1 = 0.0880, wR_2 = 0.1455\) |
| **\(R\) indices (all data)** | \(R_1 = 0.2742, wR_2 = 0.2103\) |
| **Largest diff. peak and hole** | 0.427 and -0.448 e.Å⁻³ |
Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3). \( U_{eq} \) is defined as one third of the trace of the orthogonalized \( U_{ij} \) tensor.

|     | x     | y     | z     | \( U_{eq} \) |
|-----|-------|-------|-------|-------------|
| Fe1 | 843(1)| 2006(1)| 3110(1) | 29(1)       |
| P1  | 1234(1)| 979(1)| 3007(1) | 24(1)       |
| P2  | 1103(1)| 2213(1)| 2143(1)| 27(1)       |
| C1  | 1160(8)| 2747(5)| 3404(4) | 58(3)       |
| C2  | 272(9)| 2988(4)| 3239(4) | 58(3)       |
| C3  | -403(7)| 2646(5)| 3453(4) | 52(3)       |
| C4  | -167(7)| 2058(5)| 3854(4) | 49(3)       |
| C5  | 739(7)| 1810(4)| 4052(3) | 42(2)       |
| C6  | 1443(6)| 2143(5)| 3824(4) | 47(3)       |
| C7  | 2379(11)| 1978(7)| 4052(6) | 59(3)       |
| C8  | 2510(11)| 1682(8)| 4635(6) | 74(5)       |
| C9  | 3378(17)| 1540(14)| 4864(12)| 106(5)     |
| C10 | 4119(13)| 1709(9)| 4487(6) | 59(3)       |
| C11 | 3977(13)| 2029(11)| 3903(8) | 80(5)       |
| C12 | 3112(12)| 2161(8)| 3677(7) | 80(6)       |
| C211| 2850(20)| 2413(16)| 5579(15)| 106(5)     |
| C212| 2580(20)| 2066(18)| 5211(16)| 106(5)     |
| C213| 3370(30)| 1500(20)| 4980(20)| 106(5)     |
| C214| 4200(20)| 1728(18)| 4798(13)| 59(3)       |
| C215| 4140(30)| 2130(20)| 4150(15)| 80(5)       |
| C216| 5050(20)| 2105(16)| 3836(12)| 80(5)       |
| C21 | 1828(5)| 860(4)| 2252(3) | 25(2)       |
| C22 | 2283(5)| 251(4)| 2070(3) | 29(2)       |
| C23 | 2759(5)| 221(4)| 1503(4) | 32(2)       |
| C24 | 2793(5)| 805(4)| 1105(4) | 37(2)       |
| C25 | 2324(5)| 1427(4)| 1275(4) | 33(2)       |
| C26 | 1832(5)| 1454(4)| 1846(3) | 25(2)       |
| C27 | 2102(5)| 374(3)| 3505(3) | 26(2)       |
| C28 | 1843(5)| 57(4)| 4072(3) | 27(2)       |
| C29 | 2519(6)| -345(4)| 4459(3) | 29(2)       |
| C30 | 3467(5)| -420(4)| 4258(3) | 29(2)       |
|   | C31      | C32      | C33      | C34      | C35      | C36      | C37      | C38      | C39      | C40      | C41      | C42      | C43      | C44      | C45      | C46      | C47      | C48      | C49      | C50      | C51      | C52      | C53      | C54      | C55      | C56      | C57      | C58      | C59      | C60      | C61      | C62      | C63      | C64      | C65      | C66      | S27      |
|---|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| C67  | 1328(14) | 4628(9)  | 920(13) | 55(3) |
|------|----------|----------|---------|-------|
| C68  | 285(15)  | 4909(10) | 1142(14)| 55(3) |
| C69  | 1850(30) | 5120(30) | 970(20) | 98(9) |
| C70  | 1410(30) | 4550(20) | 258(15) | 84(13)|
| C67' | 1235(16) | 4643(10) | 988(14) | 55(3) |
| C68' | 372(18)  | 4910(11) | 1424(14)| 55(3) |
| C69' | 1780(30) | 5160(30) | 810(30) | 98(9) |
| C70' | 900(40)  | 4550(20) | 418(18) | 84(13)|
| C71  | 4245(7)  | 2971(4)  | 1837(5) | 58(3) |
| C72  | 4834(7)  | 3084(5)  | 1204(5) | 87(4) |
| C73  | 4343(6)  | 3468(5)  | 2206(4) | 71(3) |
| C74  | 4658(6)  | 2270(5)  | 2117(5) | 71(3) |
| C75  | -586(6)  | 2393(4)  | 173(3)  | 31(2) |
| C76  | -1470(6) | 2754(4)  | -171(4) | 46(2) |
| C77  | 269(6)   | 2541(5)  | -238(3) | 57(3) |
| C78  | -483(7)  | 1648(4)  | 295(4)  | 54(3) |
| C79  | -2277(6) | 3916(4)  | 1708(4) | 41(2) |
| C80  | -3193(6) | 3736(4)  | 1746(4) | 56(3) |
| C81  | -2316(6) | 4550(4)  | 1192(4) | 53(3) |
| C82  | -2190(6) | 4101(5)  | 2303(4) | 72(3) |
| Fe2  | 3865(1)  | 6336(1)  | 1983(1) | 26(1) |
| P3   | 3728(1)  | 6330(1)  | 2933(1) | 26(1) |
| P4   | 3252(1)  | 7393(1)  | 1906(1) | 25(1) |
| C101 | 4169(6)  | 6347(4)  | 1051(3) | 35(2) |
| C102 | 3398(6)  | 6087(4)  | 1274(3) | 31(2) |
| C103 | 3483(6)  | 5556(4)  | 1765(3) | 32(2) |
| C104 | 4341(6)  | 5300(4)  | 2028(4) | 34(2) |
| C105 | 5097(6)  | 5579(4)  | 1833(4) | 35(2) |
| C106 | 5016(6)  | 6115(4)  | 1326(4) | 33(2) |
| C107 | 5820(7)  | 6379(5)  | 1092(5) | 58(3) |
| C108 | 6514(8)  | 6353(5)  | 1471(5) | 79(3) |
| C109 | 7325(8)  | 6574(6)  | 1198(7) | 98(5) |
| C110 | 7453(10) | 6799(7)  | 578(8)  | 112(6)|
| C111 | 6782(9)  | 6841(7)  | 208(7)  | 105(5)|
| C112 | 5996(8)  | 6632(5)  | 447(5)  | 80(4) |
| C121 | 3568(5)  | 7166(4)  | 3092(3) | 24(2)|
| C122 | 3726(5) | 7317(4) | 3625(4) | 36(2) |
| C123 | 3553(5) | 7975(4) | 3685(4) | 37(2) |
| C124 | 3217(5) | 8489(4) | 3210(4) | 34(2) |
| C125 | 3074(5) | 8346(4) | 2675(4) | 34(2) |
| C126 | 3274(5) | 7680(4) | 2599(3) | 25(2) |
| C127 | 4731(5) | 5797(4) | 3352(3) | 26(2) |
| C128 | 5528(5) | 6029(4) | 3300(3) | 30(2) |
| C129 | 6346(6) | 5640(4) | 3573(4) | 37(2) |
| C130 | 6359(6) | 4995(4) | 3860(3) | 39(2) |
| C131 | 5605(6) | 4738(4) | 3913(4) | 36(2) |
| C132 | 4793(5) | 5160(4) | 3649(3) | 29(2) |
| C133 | 2744(5) | 6077(4) | 3424(3) | 24(2) |
| C134 | 2233(5) | 6408(4) | 3883(3) | 28(2) |
| C135 | 1511(6) | 6189(4) | 4251(4) | 32(2) |
| C136 | 1312(6) | 5622(4) | 4154(3) | 33(2) |
| C137 | 1834(5) | 5274(4) | 3690(3) | 29(2) |
| C138 | 2525(5) | 5518(4) | 3323(3) | 28(2) |
| C139 | 3862(5) | 7922(3) | 1357(3) | 23(2) |
| C140 | 4632(5) | 8044(4) | 1529(3) | 31(2) |
| C141 | 5148(5) | 8436(4) | 1139(4) | 32(2) |
| C142 | 4881(6) | 8678(4) | 550(4)  | 39(2) |
| C143 | 4133(6) | 8541(4) | 352(4)  | 37(2) |
| C144 | 3625(5) | 8158(4) | 762(3)  | 31(2) |
| C145 | 1990(5) | 7770(4) | 1769(3) | 24(2) |
| C146 | 1406(5) | 7357(4) | 1966(3) | 27(2) |
| C147 | 441(5)  | 7584(4) | 1922(3) | 25(2) |
| C148 | 63(5)   | 8254(4) | 1669(3) | 24(2) |
| C149 | 607(5)  | 8705(4) | 1467(3) | 24(2) |
| C150 | 1584(5) | 8448(3) | 1525(3) | 26(2) |
| C151 | 7210(6) | 5902(5) | 3540(4) | 45(2) |
| C152 | 7009(6) | 6649(4) | 3245(4) | 56(3) |
| C153 | 8042(6) | 5487(5) | 3163(4) | 65(3) |
| C154 | 7454(6) | 5824(4) | 4182(4) | 59(3) |
| C155 | 5636(6) | 4022(4) | 4236(4) | 43(2) |
| C156 | 4776(13)| 3820(9) | 4220(10)| 62(4) |
| C157 | 6522(13)| 3537(8) | 3935(9) | 56(4) |
| Atom  | X     | Y     | Z     | U1   | U2   | U3   | U4   | U5   |
|-------|-------|-------|-------|------|------|------|------|------|
| C158  | 5820(15) | 3953(9) | 4903(9) | 61(4) |
| C56"  | 6528(13) | 3617(9) | 4509(10) | 62(4) |
| C57"  | 4836(14) | 4042(8) | 4782(9) | 56(4) |
| C58"  | 5421(15) | 3659(9) | 3777(9) | 61(4) |
| C159  | 910(6) | 6568(4) | 4757(3) | 34(2) |
| C160  | 987(6) | 6079(4) | 5368(3) | 47(2) |
| C161  | 1243(6) | 7145(4) | 4823(4) | 43(2) |
| C162  | -134(5) | 6829(4) | 4632(4) | 43(2) |
| C163  | 1594(6) | 4654(4) | 3601(4) | 35(2) |
| C164  | 2236(10)| 4342(6) | 3083(7) | 70(4) |
| C165  | 546(7) | 4867(5) | 3443(5) | 49(3) |
| C166  | 1732(9) | 4132(5) | 4169(5) | 50(3) |
| C64"  | 830(40)| 4490(30)| 3980(30)| 70(4) |
| C65"  | 2550(30)| 4050(20)| 3760(20)| 49(3) |
| C66"  | 1590(40)| 4670(20)| 2990(20)| 50(3) |
| C167  | 5922(6) | 8634(4) | 1362(4) | 38(2) |
| C168  | 5498(6) | 9356(4) | 1471(4) | 52(3) |
| C169  | 6781(6) | 8584(4) | 874(4) | 50(3) |
| C170  | 6256(6) | 8194(4) | 1952(4) | 50(3) |
| C171  | 3872(7) | 8829(4) | -291(4) | 46(2) |
| C172  | 3221(7) | 8514(6) | -490(4) | 83(4) |
| C173  | 3314(7) | 9592(5) | -314(4) | 68(3) |
| C174  | 4745(6) | 8779(4) | -757(3) | 47(2) |
| C175  | -153(5) | 7099(4) | 2186(3) | 29(2) |
| C176  | -1194(5)| 7422(4) | 2083(3) | 34(2) |
| C177  | 223(5) | 6468(4) | 1891(4) | 37(2) |
| C178  | -85(5) | 6883(4) | 2868(3) | 36(2) |
| C179  | 194(5) | 9441(4) | 1208(3) | 26(2) |
| C180  | -835(5)| 9610(4) | 1070(4) | 47(2) |
| C181  | 793(5) | 9647(3) | 625(3) | 31(2) |
| C182  | 230(6) | 9861(4) | 1672(3) | 42(2) |
| O1    | 4388(13)| 4711(9) | 686(7) | 128(5) |
| C201  | 4780(15)| 4764(14)| 73(8) | 128(5) |
| C202  | 5744(18)| 4880(17)| 49(13) | 128(5) |
| C203  | 4251(18)| 5452(13)| -261(12)| 128(5) |
Table S12. Bond lengths [Å] and angles [°].

| Bond                  | Length (Å) |
|-----------------------|------------|
| Fe(1)-C(1)            | 2.046(9)   |
| Fe(1)-C(2)            | 2.062(8)   |
| Fe(1)-C(4)            | 2.074(8)   |
| Fe(1)-C(5)            | 2.078(8)   |
| Fe(1)-C(3)            | 2.082(9)   |
| Fe(1)-C(6)            | 2.085(8)   |
| Fe(1)-P(1)            | 2.137(2)   |
| Fe(1)-P(2)            | 2.143(2)   |
| P(1)-C(21)            | 1.833(7)   |
| P(1)-C(27)            | 1.844(7)   |
| P(1)-C(33)            | 1.845(7)   |
| P(1)-C(45)            | 1.830(7)   |
| P(2)-C(26)            | 1.841(7)   |
| P(2)-C(39)            | 1.841(7)   |
| C(1)-C(2)             | 1.346(12)  |
| C(1)-C(6)             | 1.414(12)  |
| C(1)-H(1A)            | 0.9500     |
| C(2)-C(3)             | 1.389(12)  |
| C(2)-H(2A)            | 0.9500     |
| C(3)-C(4)             | 1.361(12)  |
| C(3)-H(3A)            | 0.9500     |
| C(4)-C(5)             | 1.398(11)  |
| C(4)-H(4A)            | 0.9500     |
| C(5)-C(6)             | 1.418(11)  |
| C(5)-H(5A)            | 0.9500     |
| C(6)-C(7)             | 1.477(16)  |
| C(6)-H(6A)            | 0.9500     |
| C(7)-C(8)             | 1.354(14)  |
| C(7)-C(12)            | 1.379(15)  |
| C(8)-C(9)             | 1.39(2)    |
| C(8)-H(8)             | 0.9500     |
| C(9)-C(10)            | 1.38(2)    |
| C(9)-H(9)             | 0.9500     |
| C(10)-C(11)           | 1.369(18)  |
C(10)-H(10) 0.9500
C(11)-C(12) 1.388(19)
C(11)-H(11) 0.9500
C(12)-H(12) 0.9500
C(211)-C(212) 1.40(3)
C(211)-H(21A) 0.9800
C(211)-H(21B) 0.9800
C(211)-H(21C) 0.9800
C(212)-C(213) 1.53(4)
C(212)-H(21D) 0.9900
C(212)-H(21E) 0.9900
C(213)-C(214) 1.45(5)
C(213)-H(21F) 0.9900
C(213)-H(21G) 0.9900
C(214)-C(215) 1.53(4)
C(214)-H(21H) 0.9900
C(214)-H(21I) 0.9900
C(215)-C(216) 1.43(3)
C(215)-H(21J) 0.9900
C(215)-H(21K) 0.9900
C(216)-H(21L) 0.9800
C(216)-H(21M) 0.9800
C(216)-H(21N) 0.9800
C(21)-C(22) 1.380(9)
C(21)-C(26) 1.396(9)
C(22)-C(23) 1.372(10)
C(22)-H(22A) 0.9500
C(23)-C(24) 1.380(10)
C(23)-H(23A) 0.9500
C(24)-C(25) 1.397(10)
C(24)-H(24A) 0.9500
C(25)-C(26) 1.389(9)
C(25)-H(25A) 0.9500
C(27)-C(28) 1.377(9)
C(27)-C(32) 1.401(10)
C(28)-C(29) 1.392(10)
C(28)-H(28A)   0.9500
C(29)-C(30)    1.385(9)
C(29)-C(51)    1.533(10)
C(30)-C(31)    1.401(10)
C(30)-H(30A)   0.9500
C(31)-C(32)    1.392(10)
C(31)-C(55)    1.539(10)
C(32)-H(32A)   0.9500
C(33)-C(38)    1.373(9)
C(33)-C(34)    1.399(9)
C(34)-C(35)    1.399(10)
C(34)-H(34A)   0.9500
C(35)-C(36)    1.392(9)
C(35)-C(59)    1.528(10)
C(36)-C(37)    1.389(9)
C(36)-H(36A)   0.9500
C(37)-C(38)    1.403(9)
C(37)-C(63)    1.534(9)
C(38)-H(38A)   0.9500
C(39)-C(44)    1.385(10)
C(39)-C(40)    1.393(10)
C(40)-C(41)    1.393(10)
C(40)-H(40A)   0.9500
C(41)-C(42)    1.388(11)
C(41)-C(67)    1.536(12)
C(41)-C(67')   1.539(12)
C(42)-C(43)    1.385(10)
C(42)-H(42A)   0.9500
C(43)-C(44)    1.389(10)
C(43)-C(71)    1.524(11)
C(44)-H(44A)   0.9500
C(45)-C(46)    1.377(9)
C(45)-C(50)    1.405(9)
C(46)-C(47)    1.393(9)
C(46)-H(46A)   0.9500
C(47)-C(48)    1.384(10)
C(47)-C(75) 1.529(10)
C(48)-C(49) 1.405(10)
C(48)-H(48A) 0.9500
C(49)-C(50) 1.391(10)
C(49)-C(79) 1.531(10)
C(50)-H(50A) 0.9500
C(51)-C(54) 1.532(9)
C(51)-C(53) 1.534(9)
C(51)-C(52) 1.539(10)
C(52)-H(52A) 0.9800
C(52)-H(52B) 0.9800
C(52)-H(52C) 0.9800
C(53)-H(53A) 0.9800
C(53)-H(53B) 0.9800
C(53)-H(53C) 0.9800
C(54)-H(54A) 0.9800
C(54)-H(54B) 0.9800
C(54)-H(54C) 0.9800
C(55)-C(56) 1.520(10)
C(55)-C(58) 1.529(10)
C(55)-C(57) 1.552(10)
C(56)-H(56A) 0.9800
C(56)-H(56B) 0.9800
C(56)-H(56C) 0.9800
C(57)-H(57A) 0.9800
C(57)-H(57B) 0.9800
C(57)-H(57C) 0.9800
C(58)-H(58A) 0.9800
C(58)-H(58B) 0.9800
C(58)-H(58C) 0.9800
C(59)-C(62) 1.506(10)
C(59)-C(61) 1.537(9)
C(59)-C(60) 1.539(10)
C(60)-H(60A) 0.9800
C(60)-H(60B) 0.9800
C(60)-H(60C) 0.9800
C(61)-H(61A) 0.9800
C(61)-H(61B) 0.9800
C(61)-H(61C) 0.9800
C(62)-H(62A) 0.9800
C(62)-H(62B) 0.9800
C(62)-H(62C) 0.9800
C(63)-C(65) 1.522(10)
C(63)-C(66) 1.531(9)
C(63)-C(64) 1.542(9)
C(64)-H(64A) 0.9800
C(64)-H(64B) 0.9800
C(64)-H(64C) 0.9800
C(65)-H(65A) 0.9800
C(65)-H(65B) 0.9800
C(65)-H(65C) 0.9800
C(66)-H(66A) 0.9800
C(66)-H(66B) 0.9800
C(66)-H(66C) 0.9800
C(67)-C(68) 1.527(9)
C(67)-C(69) 1.527(9)
C(67)-C(70) 1.529(10)
C(68)-H(68A) 0.9800
C(68)-H(68B) 0.9800
C(68)-H(68C) 0.9800
C(69)-H(69A) 0.9800
C(69)-H(69B) 0.9800
C(69)-H(69C) 0.9800
C(70)-H(70A) 0.9800
C(70)-H(70B) 0.9800
C(70)-H(70C) 0.9800
C(67')-C(69') 1.529(10)
C(67')-C(68') 1.530(10)
C(67')-C(70') 1.531(10)
C(68')-H(68D) 0.9800
C(68')-H(68E) 0.9800
C(68')-H(68F) 0.9800
C(69')-H(69D)          0.9800
C(69')-H(69E)          0.9800
C(69')-H(69F)          0.9800
C(70')-H(70D)          0.9800
C(70')-H(70E)          0.9800
C(70')-H(70F)          0.9800
C(71)-C(74)            1.467(11)
C(71)-C(73)            1.538(12)
C(71)-C(72)            1.575(13)
C(72)-H(72A)           0.9800
C(72)-H(72B)           0.9800
C(72)-H(72C)           0.9800
C(73)-H(73A)           0.9800
C(73)-H(73B)           0.9800
C(73)-H(73C)           0.9800
C(74)-H(74A)           0.9800
C(74)-H(74B)           0.9800
C(74)-H(74C)           0.9800
C(75)-C(78)            1.513(10)
C(75)-C(77)            1.532(10)
C(75)-C(76)            1.539(10)
C(76)-H(76A)           0.9800
C(76)-H(76B)           0.9800
C(76)-H(76C)           0.9800
C(77)-H(77A)           0.9800
C(77)-H(77B)           0.9800
C(77)-H(77C)           0.9800
C(78)-H(78A)           0.9800
C(78)-H(78B)           0.9800
C(78)-H(78C)           0.9800
C(79)-C(80)            1.516(10)
C(79)-C(82)            1.522(11)
C(79)-C(81)            1.578(11)
C(80)-H(80A)           0.9800
C(80)-H(80B)           0.9800
C(80)-H(80C)           0.9800
| Bond                  | Distance |
|----------------------|----------|
| C(81)-H(81A)         | 0.9800   |
| C(81)-H(81B)         | 0.9800   |
| C(81)-H(81C)         | 0.9800   |
| C(82)-H(82A)         | 0.9800   |
| C(82)-H(82B)         | 0.9800   |
| C(82)-H(82C)         | 0.9800   |
| Fe(2)-C(105)         | 2.069(7) |
| Fe(2)-C(102)         | 2.080(7) |
| Fe(2)-C(104)         | 2.080(8) |
| Fe(2)-C(101)         | 2.091(8) |
| Fe(2)-C(103)         | 2.091(7) |
| Fe(2)-C(106)         | 2.094(8) |
| Fe(2)-P(4)           | 2.128(2) |
| Fe(2)-P(3)           | 2.133(2) |
| P(3)-C(121)          | 1.830(7) |
| P(3)-C(127)          | 1.831(8) |
| P(3)-C(133)          | 1.845(7) |
| P(4)-C(126)          | 1.817(7) |
| P(4)-C(139)          | 1.824(7) |
| P(4)-C(145)          | 1.848(7) |
| C(101)-C(106)        | 1.400(10) |
| C(101)-C(102)        | 1.409(10) |
| C(101)-H(10D)        | 0.9500   |
| C(102)-C(103)        | 1.396(10) |
| C(102)-H(10E)        | 0.9500   |
| C(103)-C(104)        | 1.400(10) |
| C(103)-H(10F)        | 0.9500   |
| C(104)-C(105)        | 1.403(10) |
| C(104)-H(10G)        | 0.9500   |
| C(105)-C(106)        | 1.425(10) |
| C(105)-H(10H)        | 0.9500   |
| C(106)-C(107)        | 1.457(12) |
| C(107)-C(108)        | 1.429(13) |
| C(107)-C(112)        | 1.461(13) |
| C(108)-C(109)        | 1.436(14) |
| C(108)-H(108)        | 0.9500   |
C(109)-C(110) 1.389(17)
C(109)-H(109) 0.9500
C(110)-C(111) 1.377(17)
C(110)-H(110) 0.9500
C(111)-C(112) 1.374(13)
C(111)-H(111) 0.9500
C(112)-H(112) 0.9500
C(121)-C(122) 1.391(10)
C(121)-C(126) 1.403(9)
C(122)-C(123) 1.376(10)
C(122)-H(12B) 0.9500
C(123)-C(124) 1.389(10)
C(123)-H(12C) 0.9500
C(124)-C(125) 1.379(10)
C(124)-H(12D) 0.9500
C(125)-C(126) 1.399(9)
C(125)-H(12E) 0.9500
C(127)-C(132) 1.362(9)
C(127)-C(128) 1.403(9)
C(128)-C(129) 1.394(10)
C(128)-H(12F) 0.9500
C(129)-C(130) 1.384(10)
C(129)-C(151) 1.543(11)
C(130)-C(131) 1.376(10)
C(130)-H(13A) 0.9500
C(131)-C(132) 1.396(9)
C(131)-C(155) 1.534(10)
C(132)-H(13B) 0.9500
C(133)-C(134) 1.376(9)
C(133)-C(138) 1.403(9)
C(134)-C(135) 1.393(10)
C(134)-H(13C) 0.9500
C(135)-C(136) 1.397(10)
C(135)-C(159) 1.549(10)
C(136)-C(137) 1.409(10)
C(136)-H(13D) 0.9500
| Bond                  | Distance  |
|----------------------|-----------|
| C(137)-C(138)        | 1.380(9)  |
| C(137)-C(163)        | 1.535(10) |
| C(138)-H(13E)        | 0.9500    |
| C(139)-C(140)        | 1.382(9)  |
| C(139)-C(144)        | 1.397(9)  |
| C(140)-C(141)        | 1.394(10) |
| C(140)-H(14A)        | 0.9500    |
| C(141)-C(142)        | 1.399(10) |
| C(141)-C(167)        | 1.533(10) |
| C(142)-C(143)        | 1.399(10) |
| C(142)-H(14B)        | 0.9500    |
| C(143)-C(144)        | 1.394(10) |
| C(143)-C(171)        | 1.517(10) |
| C(144)-H(14C)        | 0.9500    |
| C(145)-C(146)        | 1.385(9)  |
| C(145)-C(150)        | 1.405(9)  |
| C(146)-C(147)        | 1.381(9)  |
| C(146)-H(14D)        | 0.9500    |
| C(147)-C(148)        | 1.389(9)  |
| C(147)-C(175)        | 1.533(10) |
| C(148)-C(149)        | 1.405(9)  |
| C(148)-H(14E)        | 0.9500    |
| C(149)-C(150)        | 1.403(9)  |
| C(149)-C(179)        | 1.515(9)  |
| C(150)-H(15A)        | 0.9500    |
| C(151)-C(154)        | 1.520(11) |
| C(151)-C(153)        | 1.536(11) |
| C(151)-C(152)        | 1.540(11) |
| C(152)-H(15B)        | 0.9800    |
| C(152)-H(15C)        | 0.9800    |
| C(152)-H(15D)        | 0.9800    |
| C(153)-H(15E)        | 0.9800    |
| C(153)-H(15F)        | 0.9800    |
| C(153)-H(15G)        | 0.9800    |
| C(154)-H(15H)        | 0.9800    |
| C(154)-H(15I)        | 0.9800    |
C(154)-H(15J)  0.9800
C(155)-C(156)  1.484(18)
C(155)-C(56")  1.486(18)
C(155)-C(158)  1.551(19)
C(155)-C(58")  1.551(19)
C(155)-C(157)  1.564(19)
C(155)-C(57")  1.577(19)
C(156)-H(15K)  0.9800
C(156)-H(15L)  0.9800
C(156)-H(15M)  0.9800
C(157)-H(15N)  0.9800
C(157)-H(15O)  0.9800
C(157)-H(15P)  0.9800
C(158)-H(15Q)  0.9800
C(158)-H(15R)  0.9800
C(158)-H(15S)  0.9800
C(56")-H(56D)  0.9800
C(56")-H(56E)  0.9800
C(56")-H(56F)  0.9800
C(57")-H(57D)  0.9800
C(57")-H(57E)  0.9800
C(57")-H(57F)  0.9800
C(58")-H(58D)  0.9800
C(58")-H(58E)  0.9800
C(58")-H(58F)  0.9800
C(159)-C(161)  1.507(10)
C(159)-C(162)  1.531(10)
C(159)-C(160)  1.542(10)
C(160)-H(16A)  0.9800
C(160)-H(16B)  0.9800
C(160)-H(16C)  0.9800
C(161)-H(16D)  0.9800
C(161)-H(16E)  0.9800
C(161)-H(16F)  0.9800
C(162)-H(16G)  0.9800
C(162)-H(16H)  0.9800
C(162)-H(16I)  0.9800
C(163)-C(66")  1.37(5)
C(163)-C(64")  1.41(5)
C(163)-C(166)  1.504(12)
C(163)-C(164)  1.525(13)
C(163)-C(165)  1.562(12)
C(163)-C(65")  1.62(4)
C(164)-H(16J)  0.9800
C(164)-H(16K)  0.9800
C(164)-H(16L)  0.9800
C(165)-H(16M)  0.9800
C(165)-H(16N)  0.9800
C(165)-H(16O)  0.9800
C(166)-H(16P)  0.9800
C(166)-H(16Q)  0.9800
C(166)-H(16R)  0.9800
C(64")-H(64D)  0.9800
C(64")-H(64E)  0.9800
C(64")-H(64F)  0.9800
C(65")-H(65D)  0.9800
C(65")-H(65E)  0.9800
C(65")-H(65F)  0.9800
C(66")-H(66D)  0.9800
C(66")-H(66E)  0.9800
C(66")-H(66F)  0.9800
C(167)-C(170)  1.516(10)
C(167)-C(168)  1.528(10)
C(167)-C(169)  1.548(10)
C(168)-H(16S)  0.9800
C(168)-H(16T)  0.9800
C(168)-H(16U)  0.9800
C(169)-H(16V)  0.9800
C(169)-H(16W)  0.9800
C(169)-H(16X)  0.9800
C(170)-H(17A)  0.9800
C(170)-H(17B)  0.9800
| Bond                  | Distance (Å) |
|----------------------|--------------|
| C(170)-H(17C)        | 0.9800       |
| C(171)-C(172)        | 1.511(11)    |
| C(171)-C(174)        | 1.535(10)    |
| C(171)-C(173)        | 1.570(11)    |
| C(172)-H(17D)        | 0.9800       |
| C(172)-H(17E)        | 0.9800       |
| C(172)-H(17F)        | 0.9800       |
| C(173)-H(17G)        | 0.9800       |
| C(173)-H(17H)        | 0.9800       |
| C(173)-H(17I)        | 0.9800       |
| C(174)-H(17J)        | 0.9800       |
| C(174)-H(17K)        | 0.9800       |
| C(174)-H(17L)        | 0.9800       |
| C(175)-C(176)        | 1.523(9)     |
| C(175)-C(178)        | 1.528(9)     |
| C(175)-C(177)        | 1.539(10)    |
| C(176)-H(17M)        | 0.9800       |
| C(176)-H(17N)        | 0.9800       |
| C(176)-H(17O)        | 0.9800       |
| C(177)-H(17P)        | 0.9800       |
| C(177)-H(17Q)        | 0.9800       |
| C(177)-H(17R)        | 0.9800       |
| C(178)-H(17S)        | 0.9800       |
| C(178)-H(17T)        | 0.9800       |
| C(178)-H(17U)        | 0.9800       |
| C(179)-C(180)        | 1.530(10)    |
| C(179)-C(181)        | 1.536(9)     |
| C(179)-C(182)        | 1.539(9)     |
| C(180)-H(18A)        | 0.9800       |
| C(180)-H(18B)        | 0.9800       |
| C(180)-H(18C)        | 0.9800       |
| C(181)-H(18D)        | 0.9800       |
| C(181)-H(18E)        | 0.9800       |
| C(181)-H(18F)        | 0.9800       |
| C(182)-H(18G)        | 0.9800       |
| C(182)-H(18H)        | 0.9800       |
| Bond                      | Distance |
|---------------------------|----------|
| C(182)-H(18I)            | 0.9800   |
| O(1)-C(201)              | 1.417(10) |
| O(1)-H(1)                | 0.8400   |
| C(201)-C(202)            | 1.525(10) |
| C(201)-C(203)            | 1.526(10) |
| C(201)-H(201)            | 1.0000   |
| C(202)-H(20A)            | 0.9800   |
| C(202)-H(20B)            | 0.9800   |
| C(202)-H(20C)            | 0.9800   |
| C(203)-H(20D)            | 0.9800   |
| C(203)-H(20E)            | 0.9800   |
| C(203)-H(20F)            | 0.9800   |
| C(1)-Fe(1)-C(2)          | 38.2(3)  |
| C(1)-Fe(1)-C(4)          | 84.4(4)  |
| C(2)-Fe(1)-C(4)          | 70.0(4)  |
| C(1)-Fe(1)-C(5)          | 71.2(3)  |
| C(2)-Fe(1)-C(5)          | 82.8(3)  |
| C(4)-Fe(1)-C(5)          | 39.4(3)  |
| C(1)-Fe(1)-C(3)          | 70.8(4)  |
| C(2)-Fe(1)-C(3)          | 39.2(3)  |
| C(4)-Fe(1)-C(3)          | 38.2(3)  |
| C(5)-Fe(1)-C(3)          | 70.1(3)  |
| C(1)-Fe(1)-C(6)          | 40.0(3)  |
| C(2)-Fe(1)-C(6)          | 70.9(4)  |
| C(4)-Fe(1)-C(6)          | 72.4(4)  |
| C(5)-Fe(1)-C(6)          | 39.8(3)  |
| C(3)-Fe(1)-C(6)          | 85.1(3)  |
| C(1)-Fe(1)-P(1)          | 148.4(3) |
| C(2)-Fe(1)-P(1)          | 171.9(4) |
| C(4)-Fe(1)-P(1)          | 103.8(3) |
| C(5)-Fe(1)-P(1)          | 95.6(2)  |
| C(3)-Fe(1)-P(1)          | 132.9(3) |
| C(6)-Fe(1)-P(1)          | 112.8(3) |
| C(1)-Fe(1)-P(2)          | 105.1(3) |
| C(2)-Fe(1)-P(2)          | 97.4(3)  |
| C(4)-Fe(1)-P(2)          | 146.4(3) |
| Bond                        | Angle (°) |
|-----------------------------|-----------|
| C(5)-Fe(1)-P(2)             | 173.8(3)  |
| C(3)-Fe(1)-P(2)             | 113.9(3)  |
| C(6)-Fe(1)-P(2)             | 134.4(3)  |
| P(1)-Fe(1)-P(2)             | 85.05(9)  |
| C(21)-P(1)-C(27)            | 102.0(3)  |
| C(21)-P(1)-C(33)            | 102.0(3)  |
| C(27)-P(1)-C(33)            | 104.2(3)  |
| C(21)-P(1)-Fe(1)            | 111.8(3)  |
| C(27)-P(1)-Fe(1)            | 116.8(2)  |
| C(33)-P(1)-Fe(1)            | 118.0(2)  |
| C(45)-P(2)-C(26)            | 103.0(3)  |
| C(45)-P(2)-C(39)            | 100.1(3)  |
| C(26)-P(2)-C(39)            | 102.9(3)  |
| C(45)-P(2)-Fe(1)            | 119.9(3)  |
| C(26)-P(2)-Fe(1)            | 111.3(2)  |
| C(39)-P(2)-Fe(1)            | 117.4(2)  |
| C(2)-C(1)-C(6)              | 121.4(9)  |
| C(2)-C(1)-Fe(1)             | 71.5(5)   |
| C(6)-C(1)-Fe(1)             | 71.5(5)   |
| C(2)-C(1)-H(1A)             | 119.3     |
| C(6)-C(1)-H(1A)             | 119.3     |
| Fe(1)-C(1)-H(1A)            | 130.4     |
| C(1)-C(2)-C(3)              | 122.0(9)  |
| C(1)-C(2)-Fe(1)             | 70.2(6)   |
| C(3)-C(2)-Fe(1)             | 71.2(5)   |
| C(1)-C(2)-H(2A)             | 119.0     |
| C(3)-C(2)-H(2A)             | 119.0     |
| Fe(1)-C(2)-H(2A)            | 132.9     |
| C(4)-C(3)-C(2)              | 119.2(10) |
| C(4)-C(3)-Fe(1)             | 70.6(5)   |
| C(2)-C(3)-Fe(1)             | 69.6(5)   |
| C(4)-C(3)-H(3A)             | 120.4     |
| C(2)-C(3)-H(3A)             | 120.4     |
| Fe(1)-C(3)-H(3A)            | 132.3     |
| C(3)-C(4)-C(5)              | 120.0(9)  |
| C(3)-C(4)-Fe(1)             | 71.2(5)   |
| Bond                        | Angle (°) |
|-----------------------------|-----------|
| C(5)-C(4)-Fe(1)             | 70.5(5)   |
| C(3)-C(4)-H(4A)             | 120.0     |
| C(5)-C(4)-H(4A)             | 120.0     |
| Fe(1)-C(4)-H(4A)            | 131.1     |
| C(4)-C(5)-C(6)              | 121.4(8)  |
| C(4)-C(5)-Fe(1)             | 70.2(5)   |
| C(6)-C(5)-Fe(1)             | 70.4(5)   |
| C(4)-C(5)-H(5A)             | 119.3     |
| C(6)-C(5)-H(5A)             | 119.3     |
| Fe(1)-C(5)-H(5A)            | 133.6     |
| C(1)-C(6)-C(5)              | 115.9(8)  |
| C(1)-C(6)-C(7)              | 117.2(10) |
| C(5)-C(6)-C(7)              | 126.1(10) |
| C(1)-C(6)-Fe(1)             | 68.5(5)   |
| C(5)-C(6)-Fe(1)             | 69.8(5)   |
| C(7)-C(6)-Fe(1)             | 140.0(8)  |
| C(1)-C(6)-H(6A)             | 122.0     |
| C(5)-C(6)-H(6A)             | 122.0     |
| Fe(1)-C(6)-H(6A)            | 132.1     |
| C(8)-C(7)-C(12)             | 119.6(15) |
| C(8)-C(7)-C(6)              | 120.7(13) |
| C(12)-C(7)-C(6)             | 119.7(11) |
| C(7)-C(8)-C(9)              | 121.6(16) |
| C(7)-C(8)-H(8)              | 119.2     |
| C(9)-C(8)-H(8)              | 119.2     |
| C(10)-C(9)-C(8)             | 119(2)    |
| C(10)-C(9)-H(9)             | 120.5     |
| C(8)-C(9)-H(9)              | 120.5     |
| C(11)-C(10)-C(9)            | 119(2)    |
| C(11)-C(10)-H(10)           | 120.4     |
| C(9)-C(10)-H(10)            | 120.4     |
| C(10)-C(11)-C(12)           | 121.2(16) |
| C(10)-C(11)-H(11)           | 119.4     |
| C(12)-C(11)-H(11)           | 119.4     |
| C(7)-C(12)-C(11)            | 119.3(15) |
| C(7)-C(12)-H(12)            | 120.4     |
C(11)-C(12)-H(12) 120.4
C(212)-C(211)-H(21A) 109.5
C(212)-C(211)-H(21B) 109.5
H(21A)-C(211)-H(21B) 109.5
C(212)-C(211)-H(21C) 109.5
H(21A)-C(211)-H(21C) 109.5
H(21B)-C(211)-H(21C) 109.5
C(211)-C(212)-C(213) 116(3)
C(211)-C(212)-H(21D) 108.4
C(213)-C(212)-H(21D) 108.4
C(211)-C(212)-H(21E) 108.4
C(213)-C(212)-H(21E) 108.4
H(21D)-C(212)-H(21E) 107.4
C(214)-C(213)-C(212) 107(3)
C(214)-C(213)-H(21F) 110.2
C(212)-C(213)-H(21F) 110.2
C(214)-C(213)-H(21G) 110.2
C(212)-C(213)-H(21G) 110.2
H(21F)-C(213)-H(21G) 108.5
C(213)-C(214)-C(215) 108(2)
C(213)-C(214)-H(21H) 110.0
C(215)-C(214)-H(21H) 110.0
C(213)-C(214)-H(21I) 110.0
C(215)-C(214)-H(21I) 110.0
H(21H)-C(214)-H(21I) 108.4
C(216)-C(215)-C(214) 112(3)
C(216)-C(215)-H(21J) 109.2
C(214)-C(215)-H(21J) 109.2
C(216)-C(215)-H(21K) 109.2
C(214)-C(215)-H(21K) 109.2
H(21J)-C(215)-H(21K) 107.9
C(215)-C(216)-H(21L) 109.5
C(215)-C(216)-H(21M) 109.5
H(21L)-C(216)-H(21M) 109.5
C(215)-C(216)-H(21N) 109.5
H(21L)-C(216)-H(21N) 109.5
| Bond/Distance          | Angle (°) |
|------------------------|-----------|
| H(21M)-C(216)-H(21N)  | 109.5     |
| C(22)-C(21)-C(26)     | 119.4(7)  |
| C(22)-C(21)-P(1)      | 126.0(6)  |
| C(26)-C(21)-P(1)      | 114.6(6)  |
| C(23)-C(22)-C(21)     | 121.0(7)  |
| C(23)-C(22)-H(22A)    | 119.5     |
| C(21)-C(22)-H(22A)    | 119.5     |
| C(22)-C(23)-C(24)     | 120.2(8)  |
| C(22)-C(23)-H(23A)    | 119.9     |
| C(24)-C(23)-H(23A)    | 119.9     |
| C(23)-C(24)-C(25)     | 119.8(8)  |
| C(23)-C(24)-H(24A)    | 120.1     |
| C(25)-C(24)-H(24A)    | 120.1     |
| C(26)-C(25)-C(24)     | 119.7(7)  |
| C(26)-C(25)-H(25A)    | 120.1     |
| C(24)-C(25)-H(25A)    | 120.1     |
| C(25)-C(26)-C(21)     | 119.9(7)  |
| C(25)-C(26)-P(2)      | 126.9(6)  |
| C(21)-C(26)-P(2)      | 113.2(6)  |
| C(28)-C(27)-C(32)     | 119.1(7)  |
| C(28)-C(27)-P(1)      | 122.9(6)  |
| C(32)-C(27)-P(1)      | 117.3(6)  |
| C(27)-C(28)-C(29)     | 121.3(7)  |
| C(27)-C(28)-H(28A)    | 119.3     |
| C(29)-C(28)-H(28A)    | 119.3     |
| C(29)-C(29)-C(28)     | 118.2(7)  |
| C(30)-C(29)-C(51)     | 118.1(7)  |
| C(28)-C(29)-C(51)     | 123.7(7)  |
| C(29)-C(30)-C(31)     | 122.7(7)  |
| C(29)-C(30)-H(30A)    | 118.7     |
| C(31)-C(30)-H(30A)    | 118.7     |
| C(32)-C(31)-C(30)     | 117.1(7)  |
| C(32)-C(31)-C(55)     | 121.6(7)  |
| C(30)-C(31)-C(55)     | 121.3(7)  |
| C(31)-C(32)-C(27)     | 121.5(7)  |
| C(31)-C(32)-H(32A)    | 119.3     |
| Bond | Angle    |
|------|----------|
| C(27)-C(32)-H(32A) | 119.3    |
| C(38)-C(33)-C(34)  | 118.8(7) |
| C(38)-C(33)-P(1)   | 126.9(6) |
| C(34)-C(33)-P(1)   | 114.1(5) |
| C(33)-C(34)-C(35)  | 122.1(7) |
| C(33)-C(34)-H(34A) | 118.9    |
| C(35)-C(34)-H(34A) | 118.9    |
| C(36)-C(35)-C(34)  | 116.8(7) |
| C(36)-C(35)-C(59)  | 123.4(7) |
| C(34)-C(35)-C(59)  | 119.8(7) |
| C(37)-C(36)-C(35)  | 122.9(7) |
| C(37)-C(36)-H(36A) | 118.5    |
| C(35)-C(36)-H(36A) | 118.5    |
| C(36)-C(37)-C(38)  | 118.0(7) |
| C(36)-C(37)-C(63)  | 121.4(7) |
| C(38)-C(37)-C(63)  | 120.6(7) |
| C(33)-C(38)-C(37)  | 121.4(7) |
| C(33)-C(38)-H(38A) | 119.3    |
| C(37)-C(38)-H(38A) | 119.3    |
| C(44)-C(39)-C(40)  | 119.0(7) |
| C(44)-C(39)-P(2)   | 119.0(6) |
| C(40)-C(39)-P(2)   | 121.9(6) |
| C(41)-C(40)-C(39)  | 121.6(7) |
| C(41)-C(40)-H(40A) | 119.2    |
| C(39)-C(40)-H(40A) | 119.2    |
| C(42)-C(41)-C(40)  | 117.0(8) |
| C(42)-C(41)-C(67)  | 121.8(11) |
| C(40)-C(41)-C(67)  | 121.1(12) |
| C(42)-C(41)-C(67') | 125.4(13) |
| C(40)-C(41)-C(67') | 117.5(13) |
| C(43)-C(42)-C(41)  | 123.4(8) |
| C(43)-C(42)-H(42A) | 118.3    |
| C(41)-C(42)-H(42A) | 118.3    |
| C(42)-C(43)-C(44)  | 117.6(8) |
| C(42)-C(43)-C(71)  | 120.9(8) |
| C(44)-C(43)-C(71)  | 121.5(7) |
C(39)-C(44)-C(43)  121.4(7)
C(39)-C(44)-H(44A)  119.3
C(43)-C(44)-H(44A)  119.3
C(46)-C(45)-C(50)  117.7(7)
C(46)-C(45)-P(2)  124.8(6)
C(50)-C(45)-P(2)  117.3(6)
C(45)-C(46)-C(47)  123.0(7)
C(45)-C(46)-H(46A)  118.5
C(47)-C(46)-H(46A)  118.5
C(48)-C(47)-C(46)  117.7(7)
C(48)-C(47)-C(75)  122.8(7)
C(46)-C(47)-C(75)  119.4(7)
C(47)-C(48)-C(49)  121.9(7)
C(47)-C(48)-H(48A)  119.1
C(49)-C(48)-H(48A)  119.1
C(50)-C(49)-C(48)  118.0(7)
C(50)-C(49)-C(79)  121.6(7)
C(48)-C(49)-C(79)  120.4(7)
C(49)-C(50)-C(45)  121.6(7)
C(49)-C(50)-H(50A)  119.2
C(45)-C(50)-H(50A)  119.2
C(54)-C(51)-C(29)  109.0(6)
C(54)-C(51)-C(53)  109.6(6)
C(29)-C(51)-C(53)  111.1(6)
C(54)-C(51)-C(52)  107.8(6)
C(29)-C(51)-C(52)  112.1(6)
C(53)-C(51)-C(52)  107.2(6)
C(51)-C(52)-H(52A)  109.5
C(51)-C(52)-H(52B)  109.5
H(52A)-C(52)-H(52B)  109.5
C(51)-C(52)-H(52C)  109.5
H(52A)-C(52)-H(52C)  109.5
H(52B)-C(52)-H(52C)  109.5
C(51)-C(53)-H(53A)  109.5
C(51)-C(53)-H(53B)  109.5
H(53A)-C(53)-H(53B)  109.5
C(51)-C(53)-H(53C) 109.5
H(53A)-C(53)-H(53C) 109.5
H(53B)-C(53)-H(53C) 109.5
C(51)-C(54)-H(54A) 109.5
C(51)-C(54)-H(54B) 109.5
H(54A)-C(54)-H(54B) 109.5
C(51)-C(54)-H(54C) 109.5
H(54A)-C(54)-H(54C) 109.5
H(54B)-C(54)-H(54C) 109.5
C(56)-C(55)-C(58) 110.5(7)
C(56)-C(55)-C(31) 112.9(7)
C(58)-C(55)-C(31) 109.2(6)
C(56)-C(55)-C(57) 107.5(7)
C(58)-C(55)-C(57) 108.7(7)
C(31)-C(55)-C(57) 107.9(7)
C(55)-C(56)-H(56A) 109.5
C(55)-C(56)-H(56B) 109.5
H(56A)-C(56)-H(56B) 109.5
C(55)-C(56)-H(56C) 109.5
H(56A)-C(56)-H(56C) 109.5
H(56B)-C(56)-H(56C) 109.5
C(55)-C(57)-H(57A) 109.5
C(55)-C(57)-H(57B) 109.5
H(57A)-C(57)-H(57B) 109.5
C(55)-C(57)-H(57C) 109.5
H(57A)-C(57)-H(57C) 109.5
H(57B)-C(57)-H(57C) 109.5
C(55)-C(58)-H(58A) 109.5
C(55)-C(58)-H(58B) 109.5
H(58A)-C(58)-H(58B) 109.5
C(55)-C(58)-H(58C) 109.5
H(58A)-C(58)-H(58C) 109.5
H(58B)-C(58)-H(58C) 109.5
C(62)-C(59)-C(35) 111.5(6)
C(62)-C(59)-C(61) 109.0(7)
C(35)-C(59)-C(61) 109.2(6)
| Bond                  | Angles (°) |
|----------------------|------------|
| C(62)-C(59)-C(60)    | 109.4(6)   |
| C(35)-C(59)-C(60)    | 109.0(6)   |
| C(61)-C(59)-C(60)    | 108.7(6)   |
| C(59)-C(60)-H(60A)   | 109.5      |
| C(59)-C(60)-H(60B)   | 109.5      |
| H(60A)-C(60)-H(60B)  | 109.5      |
| C(59)-C(60)-H(60C)   | 109.5      |
| H(60A)-C(60)-H(60C)  | 109.5      |
| H(60B)-C(60)-H(60C)  | 109.5      |
| C(59)-C(61)-H(61A)   | 109.5      |
| C(59)-C(61)-H(61B)   | 109.5      |
| H(61A)-C(61)-H(61B)  | 109.5      |
| C(59)-C(61)-H(61C)   | 109.5      |
| H(61A)-C(61)-H(61C)  | 109.5      |
| H(61B)-C(61)-H(61C)  | 109.5      |
| C(59)-C(62)-H(62A)   | 109.5      |
| C(59)-C(62)-H(62B)   | 109.5      |
| H(62A)-C(62)-H(62B)  | 109.5      |
| C(59)-C(62)-H(62C)   | 109.5      |
| H(62A)-C(62)-H(62C)  | 109.5      |
| H(62B)-C(62)-H(62C)  | 109.5      |
| C(65)-C(63)-C(66)    | 109.0(6)   |
| C(65)-C(63)-C(37)    | 113.0(6)   |
| C(66)-C(63)-C(37)    | 110.5(6)   |
| C(65)-C(63)-C(64)    | 107.4(6)   |
| C(66)-C(63)-C(64)    | 108.3(6)   |
| C(37)-C(63)-C(64)    | 108.5(6)   |
| C(63)-C(64)-H(64A)   | 109.5      |
| C(63)-C(64)-H(64B)   | 109.5      |
| H(64A)-C(64)-H(64B)  | 109.5      |
| C(63)-C(64)-H(64C)   | 109.5      |
| H(64A)-C(64)-H(64C)  | 109.5      |
| H(64B)-C(64)-H(64C)  | 109.5      |
| C(63)-C(65)-H(65A)   | 109.5      |
| C(63)-C(65)-H(65B)   | 109.5      |
| H(65A)-C(65)-H(65B)  | 109.5      |
C(63)-C(65)-H(65C) 109.5
H(65A)-C(65)-H(65C) 109.5
H(65B)-C(65)-H(65C) 109.5
C(63)-C(66)-H(66A) 109.5
C(63)-C(66)-H(66B) 109.5
H(66A)-C(66)-H(66B) 109.5
C(63)-C(66)-H(66C) 109.5
H(66A)-C(66)-H(66C) 109.5
H(66B)-C(66)-H(66C) 109.5
C(68)-C(67)-C(69) 108.2(10)
C(68)-C(67)-C(70) 109.1(9)
C(69)-C(67)-C(70) 110.0(10)
C(68)-C(67)-C(41) 112.8(14)
C(69)-C(67)-C(41) 108(3)
C(70)-C(67)-C(41) 109(3)
C(69')-C(67')-C(68') 108.0(10)
C(69')-C(67')-C(70') 109.0(10)
C(68')-C(67')-C(70') 109.4(10)
C(69')-C(67')-C(41) 115(3)
C(68')-C(67')-C(41) 108.4(16)
C(70')-C(67')-C(41) 107(3)
C(74)-C(71)-C(43) 114.1(8)
C(74)-C(71)-C(73) 112.1(9)
C(43)-C(71)-C(73) 108.7(8)
C(74)-C(71)-C(72) 106.4(9)
C(43)-C(71)-C(72) 107.9(8)
C(73)-C(71)-C(72) 107.4(8)
C(71)-C(72)-H(72A) 109.5
C(71)-C(72)-H(72B) 109.5
H(72A)-C(72)-H(72B) 109.5
C(71)-C(72)-H(72C) 109.5
H(72A)-C(72)-H(72C) 109.5
H(72B)-C(72)-H(72C) 109.5
C(71)-C(73)-H(73A) 109.5
C(71)-C(73)-H(73B) 109.5
H(73A)-C(73)-H(73B) 109.5
| Bond                  | Angle      |
|----------------------|------------|
| C(71)-C(73)-H(73C)   | 109.5      |
| H(73A)-C(73)-H(73C)  | 109.5      |
| H(73B)-C(73)-H(73C)  | 109.5      |
| C(71)-C(74)-H(74A)   | 109.5      |
| C(71)-C(74)-H(74B)   | 109.5      |
| H(74A)-C(74)-H(74B)  | 109.5      |
| C(71)-C(74)-H(74C)   | 109.5      |
| H(74A)-C(74)-H(74C)  | 109.5      |
| H(74B)-C(74)-H(74C)  | 109.5      |
| C(78)-C(75)-C(47)    | 109.5(6)   |
| C(78)-C(75)-C(77)    | 110.5(7)   |
| C(47)-C(75)-C(77)    | 108.7(6)   |
| C(78)-C(75)-C(76)    | 107.8(7)   |
| C(47)-C(75)-C(76)    | 113.0(7)   |
| C(77)-C(75)-C(76)    | 107.5(6)   |
| C(75)-C(76)-H(76A)   | 109.5      |
| C(75)-C(76)-H(76B)   | 109.5      |
| H(76A)-C(76)-H(76B)  | 109.5      |
| C(75)-C(76)-H(76C)   | 109.5      |
| H(76A)-C(76)-H(76C)  | 109.5      |
| H(76B)-C(76)-H(76C)  | 109.5      |
| C(75)-C(77)-H(77A)   | 109.5      |
| C(75)-C(77)-H(77B)   | 109.5      |
| H(77A)-C(77)-H(77B)  | 109.5      |
| C(75)-C(77)-H(77C)   | 109.5      |
| H(77A)-C(77)-H(77C)  | 109.5      |
| H(77B)-C(77)-H(77C)  | 109.5      |
| C(75)-C(78)-H(78A)   | 109.5      |
| C(75)-C(78)-H(78B)   | 109.5      |
| H(78A)-C(78)-H(78B)  | 109.5      |
| C(75)-C(78)-H(78C)   | 109.5      |
| H(78A)-C(78)-H(78C)  | 109.5      |
| H(78B)-C(78)-H(78C)  | 109.5      |
| C(80)-C(79)-C(82)    | 110.1(8)   |
| C(80)-C(79)-C(49)    | 110.7(7)   |
| C(82)-C(79)-C(49)    | 113.7(7)   |
C(80)-C(79)-C(81)  108.0(7)
C(82)-C(79)-C(81)  108.3(7)
C(49)-C(79)-C(81)  105.8(7)
C(79)-C(80)-H(80A)  109.5
C(79)-C(80)-H(80B)  109.5
H(80A)-C(80)-H(80B)  109.5
C(79)-C(80)-H(80C)  109.5
H(80A)-C(80)-H(80C)  109.5
H(80B)-C(80)-H(80C)  109.5
C(79)-C(81)-H(81A)  109.5
C(79)-C(81)-H(81B)  109.5
H(81A)-C(81)-H(81B)  109.5
C(79)-C(81)-H(81C)  109.5
H(81A)-C(81)-H(81C)  109.5
H(81B)-C(81)-H(81C)  109.5
C(79)-C(82)-H(82A)  109.5
C(79)-C(82)-H(82B)  109.5
H(82A)-C(82)-H(82B)  109.5
C(79)-C(82)-H(82C)  109.5
H(82A)-C(82)-H(82C)  109.5
H(82B)-C(82)-H(82C)  109.5
C(105)-Fe(2)-C(102)  85.4(3)
C(105)-Fe(2)-C(104)  39.5(3)
C(102)-Fe(2)-C(104)  70.6(3)
C(105)-Fe(2)-C(101)  71.1(3)
C(102)-Fe(2)-C(101)  39.5(3)
C(104)-Fe(2)-C(101)  83.1(3)
C(105)-Fe(2)-C(103)  72.3(3)
C(102)-Fe(2)-C(103)  39.1(3)
C(104)-Fe(2)-C(103)  39.2(3)
C(101)-Fe(2)-C(103)  71.0(3)
C(105)-Fe(2)-C(106)  40.0(3)
C(102)-Fe(2)-C(106)  72.2(3)
C(104)-Fe(2)-C(106)  71.6(3)
C(101)-Fe(2)-C(106)  39.1(3)
C(103)-Fe(2)-C(106)  85.8(3)
| Bond                        | Angle (°) |
|-----------------------------|-----------|
| C(105)-Fe(2)-P(4)           | 144.9(3)  |
| C(102)-Fe(2)-P(4)           | 104.8(2)  |
| C(104)-Fe(2)-P(4)           | 174.3(2)  |
| C(101)-Fe(2)-P(4)           | 95.3(2)   |
| C(103)-Fe(2)-P(4)           | 135.1(2)  |
| C(106)-Fe(2)-P(4)           | 110.5(2)  |
| C(105)-P(4)-Fe(2)           | 85.16(9)  |
| C(121)-P(3)-C(127)          | 103.6(3)  |
| C(121)-P(3)-C(133)          | 102.4(3)  |
| C(127)-P(3)-C(133)          | 100.2(3)  |
| C(121)-P(3)-Fe(2)           | 111.5(3)  |
| C(127)-P(3)-Fe(2)           | 117.0(2)  |
| C(133)-P(3)-Fe(2)           | 119.9(2)  |
| C(126)-P(4)-C(139)          | 100.7(3)  |
| C(126)-P(4)-C(145)          | 101.2(3)  |
| C(139)-P(4)-C(145)          | 104.2(3)  |
| C(126)-P(4)-Fe(2)           | 111.8(3)  |
| C(139)-P(4)-Fe(2)           | 116.8(2)  |
| C(145)-P(4)-Fe(2)           | 119.6(2)  |
| C(106)-C(101)-C(102)        | 122.1(8)  |
| C(106)-C(101)-Fe(2)         | 70.6(4)   |
| C(102)-C(101)-Fe(2)         | 69.8(4)   |
| C(106)-C(101)-H(10D)        | 118.9     |
| C(102)-C(101)-H(10D)        | 118.9     |
| Fe(2)-C(101)-H(10D)         | 134.4     |
| C(103)-C(102)-C(101)        | 119.9(8)  |
| C(103)-C(102)-Fe(2)         | 70.9(4)   |
| C(101)-C(102)-Fe(2)         | 70.7(4)   |
| C(103)-C(102)-H(10E)        | 120.1     |
| C(101)-C(102)-H(10E)        | 120.1     |
Fe(2)-C(102)-H(10E) 131.1
C(102)-C(103)-C(104) 118.5(8)
C(102)-C(103)-Fe(2) 70.0(4)
C(104)-C(103)-Fe(2) 70.0(4)
C(102)-C(103)-H(10F) 120.8
C(104)-C(103)-H(10F) 120.8
Fe(2)-C(103)-H(10F) 132.0
C(103)-C(104)-C(105) 122.2(7)
C(103)-C(104)-Fe(2) 70.8(4)
C(105)-C(104)-Fe(2) 69.8(4)
C(103)-C(104)-H(10G) 118.9
C(105)-C(104)-H(10G) 118.9
Fe(2)-C(104)-H(10G) 134.2
C(104)-C(105)-C(106) 119.4(7)
C(104)-C(105)-Fe(2) 70.7(4)
C(106)-C(105)-Fe(2) 70.9(5)
C(104)-C(105)-H(10H) 120.3
C(106)-C(105)-H(10H) 120.3
Fe(2)-C(105)-H(10H) 130.6
C(101)-C(106)-C(105) 117.8(7)
C(101)-C(106)-C(107) 122.2(8)
C(105)-C(106)-C(107) 119.9(8)
C(101)-C(106)-Fe(2) 70.3(4)
C(105)-C(106)-Fe(2) 69.0(4)
C(107)-C(106)-Fe(2) 135.0(6)
C(108)-C(107)-C(106) 121.9(10)
C(108)-C(107)-C(112) 116.5(10)
C(106)-C(107)-C(112) 121.3(9)
C(107)-C(108)-C(109) 118.7(12)
C(107)-C(108)-H(108) 120.7
C(109)-C(108)-H(108) 120.7
C(110)-C(109)-C(108) 121.6(13)
C(110)-C(109)-H(109) 119.2
C(108)-C(109)-H(109) 119.2
C(111)-C(110)-C(109) 120.6(13)
C(111)-C(110)-H(110) 119.7
C(109)-C(110)-H(110) 119.7
C(112)-C(111)-C(110) 120.0(14)
C(112)-C(111)-H(111) 120.0
C(110)-C(111)-H(111) 120.0
C(111)-C(112)-C(107) 122.6(12)
C(111)-C(112)-H(112) 118.7
C(107)-C(112)-H(112) 118.7
C(122)-C(121)-C(126) 120.4(7)
C(122)-C(121)-P(3) 126.7(6)
C(126)-C(121)-P(3) 112.8(6)
C(123)-C(122)-C(121) 120.3(8)
C(123)-C(122)-H(12B) 119.9
C(121)-C(122)-H(12B) 119.9
C(122)-C(123)-C(124) 119.7(8)
C(122)-C(123)-H(12C) 120.2
C(124)-C(123)-H(12C) 120.2
C(125)-C(124)-C(123) 120.7(8)
C(125)-C(124)-H(12D) 119.7
C(123)-C(124)-H(12D) 119.7
C(124)-C(125)-C(126) 120.5(7)
C(124)-C(125)-H(12E) 119.8
C(126)-C(125)-H(12E) 119.8
C(125)-C(126)-C(121) 118.3(7)
C(125)-C(126)-P(4) 126.8(6)
C(121)-C(126)-P(4) 114.9(6)
C(132)-C(127)-C(128) 118.1(7)
C(132)-C(127)-P(3) 123.6(6)
C(128)-C(127)-P(3) 117.8(6)
C(129)-C(128)-C(127) 121.8(7)
C(129)-C(128)-H(12F) 119.1
C(127)-C(128)-H(12F) 119.1
C(130)-C(129)-C(128) 116.6(7)
C(130)-C(129)-C(151) 121.3(7)
C(128)-C(129)-C(151) 122.1(7)
C(131)-C(130)-C(129) 123.8(7)
C(131)-C(130)-H(13A) 118.1
C(129)-C(130)-H(13A)  118.1
C(130)-C(131)-C(132)  116.9(7)
C(130)-C(131)-C(155)  122.8(7)
C(132)-C(131)-C(155)  120.2(7)
C(127)-C(132)-C(131)  122.6(7)
C(127)-C(132)-H(13B)  118.7
C(131)-C(132)-H(13B)  118.7
C(134)-C(133)-C(138)  119.5(7)
C(134)-C(133)-P(3)    122.8(6)
C(138)-C(133)-P(3)    117.7(6)
C(133)-C(134)-C(135)  120.7(7)
C(133)-C(134)-H(13C)  119.7
C(135)-C(134)-H(13C)  119.7
C(134)-C(135)-C(136)  119.4(7)
C(134)-C(135)-C(159)  121.3(7)
C(136)-C(135)-C(159)  119.3(8)
C(135)-C(136)-C(137)  120.6(7)
C(135)-C(136)-H(13D)  119.7
C(137)-C(136)-H(13D)  119.7
C(138)-C(137)-C(136)  118.4(7)
C(138)-C(137)-C(163)  122.6(7)
C(136)-C(137)-C(163)  118.9(7)
C(137)-C(138)-C(133)  121.3(7)
C(137)-C(138)-H(13E)  119.3
C(133)-C(138)-H(13E)  119.3
C(140)-C(139)-C(144)  119.6(7)
C(140)-C(139)-P(4)    118.0(6)
C(144)-C(139)-P(4)    122.2(6)
C(139)-C(140)-C(141)  122.2(7)
C(139)-C(140)-H(14A)  118.9
C(141)-C(140)-H(14A)  118.9
C(140)-C(141)-C(142)  116.8(7)
C(140)-C(141)-C(167)  121.3(7)
C(142)-C(141)-C(167)  121.7(7)
C(141)-C(142)-C(143)  122.6(8)
C(141)-C(142)-H(14B)  118.7
C(143)-C(142)-H(14B)  118.7
C(144)-C(143)-C(142)  118.4(7)
C(144)-C(143)-C(171)  121.8(8)
C(142)-C(143)-C(171)  119.8(8)
C(143)-C(144)-C(139)  120.2(7)
C(143)-C(144)-H(14C)  119.9
C(139)-C(144)-H(14C)  119.9
C(146)-C(145)-C(150)  118.9(7)
C(146)-C(145)-P(4)    116.5(6)
C(150)-C(145)-P(4)    124.5(6)
C(147)-C(146)-C(145)  122.4(7)
C(147)-C(146)-H(14D)  118.8
C(145)-C(146)-H(14D)  118.8
C(146)-C(147)-C(148)  117.4(7)
C(146)-C(147)-C(175)  118.5(7)
C(148)-C(147)-C(175)  124.0(7)
C(147)-C(148)-C(149)  123.5(7)
C(147)-C(148)-H(14E)  118.3
C(149)-C(148)-H(14E)  118.3
C(150)-C(149)-C(148)  116.8(7)
C(150)-C(149)-C(179)  119.5(7)
C(148)-C(149)-C(179)  123.7(7)
C(149)-C(150)-C(145)  121.1(7)
C(149)-C(150)-H(15A)  119.5
C(145)-C(150)-H(15A)  119.5
C(154)-C(151)-C(153)  110.7(7)
C(154)-C(151)-C(152)  108.3(7)
C(153)-C(151)-C(152)  108.8(8)
C(154)-C(151)-C(129)  108.2(7)
C(153)-C(151)-C(129)  108.5(7)
C(152)-C(151)-C(129)  112.3(7)
C(151)-C(152)-H(15B)  109.5
C(151)-C(152)-H(15C)  109.5
H(15B)-C(152)-H(15C)  109.5
C(151)-C(152)-H(15D)  109.5
H(15B)-C(152)-H(15D)  109.5
H(15C)-C(152)-H(15D)  109.5
C(151)-C(153)-H(15E)  109.5
C(151)-C(153)-H(15F)  109.5
H(15E)-C(153)-H(15F)  109.5
C(151)-C(153)-H(15G)  109.5
H(15E)-C(153)-H(15G)  109.5
H(15F)-C(153)-H(15G)  109.5
C(151)-C(154)-H(15H)  109.5
C(151)-C(154)-H(15I)  109.5
H(15H)-C(154)-H(15I)  109.5
C(151)-C(154)-H(15J)  109.5
H(15I)-C(154)-H(15J)  109.5
H(15J)-C(154)-H(15K)  109.5
C(156)-C(155)-C(56")  128.6(11)
C(156)-C(155)-C(131)  115.3(9)
C(56")-C(155)-C(131)  116.0(9)
C(156)-C(155)-C(158)  109.7(12)
C(56")-C(155)-C(158)  54.5(10)
C(131)-C(155)-C(158)  108.0(9)
C(156)-C(155)-C(58")  50.7(10)
C(56")-C(155)-C(58")  110.3(13)
C(131)-C(155)-C(58")  107.6(9)
C(158)-C(155)-C(58")  144.3(11)
C(156)-C(155)-C(157)  109.8(12)
C(56")-C(155)-C(157)  52.6(10)
C(131)-C(155)-C(157)  106.9(9)
C(158)-C(155)-C(157)  106.9(11)
C(58")-C(155)-C(157)  64.6(10)
C(156)-C(155)-C(57")  57.6(10)
C(56")-C(155)-C(57")  104.8(12)
C(131)-C(155)-C(57")  110.1(9)
C(158)-C(155)-C(57")  56.7(10)
C(58")-C(155)-C(57")  107.6(12)
C(157)-C(155)-C(57")  142.7(10)
C(155)-C(156)-H(15K)  109.5
C(155)-C(156)-H(15L)  109.5
C(155)-C(156)-H(15M) 109.5
C(155)-C(157)-H(15N) 109.5
C(155)-C(157)-H(15O) 109.5
C(155)-C(157)-H(15P) 109.5
C(155)-C(158)-H(15Q) 109.5
C(155)-C(158)-H(15R) 109.5
C(155)-C(158)-H(15S) 109.5
C(155)-C(56")-H(56D) 109.5
C(155)-C(56")-H(56E) 109.5
C(155)-C(56")-H(56F) 109.5
C(155)-C(57")-H(57D) 109.5
C(155)-C(57")-H(57E) 109.5
C(155)-C(57")-H(57F) 109.5
C(155)-C(58")-H(58D) 109.5
C(155)-C(58")-H(58E) 109.5
C(155)-C(58")-H(58F) 109.5
C(161)-C(159)-C(162) 109.3(7)
C(161)-C(159)-C(160) 107.1(6)
C(162)-C(159)-C(160) 108.3(7)
C(161)-C(159)-C(135) 112.8(7)
C(162)-C(159)-C(135) 110.1(6)
C(160)-C(159)-C(135) 109.1(6)
C(159)-C(160)-H(16A) 109.5
C(159)-C(160)-H(16B) 109.5
H(16A)-C(160)-H(16B) 109.5
C(159)-C(160)-H(16C) 109.5
H(16A)-C(160)-H(16C) 109.5
H(16B)-C(160)-H(16C) 109.5
C(159)-C(161)-H(16D) 109.5
C(159)-C(161)-H(16E) 109.5
H(16D)-C(161)-H(16E) 109.5
C(159)-C(161)-H(16F) 109.5
H(16D)-C(161)-H(16F) 109.5
H(16E)-C(161)-H(16F) 109.5
C(159)-C(162)-H(16G) 109.5
C(159)-C(162)-H(16H) 109.5
H(16G)-C(162)-H(16H) 109.5
C(159)-C(162)-H(16I) 109.5
H(16G)-C(162)-H(16I) 109.5
H(16H)-C(162)-H(16I) 109.5
C(66")-C(163)-C(64") 116(3)
C(166)-C(163)-C(164) 107.9(9)
C(66")-C(163)-C(137) 109(2)
C(64")-C(163)-C(137) 117(2)
C(166)-C(163)-C(137) 109.5(7)
C(164)-C(163)-C(137) 111.4(7)
C(166)-C(163)-C(165) 110.8(8)
C(164)-C(163)-C(165) 108.2(9)
C(137)-C(163)-C(165) 109.1(7)
C(66")-C(163)-C(65") 102(3)
C(64")-C(163)-C(65") 108(3)
C(137)-C(163)-C(65") 102.9(16)
C(163)-C(164)-H(16J) 109.5
C(163)-C(164)-H(16K) 109.5
C(163)-C(164)-H(16L) 109.5
C(163)-C(165)-H(16M) 109.5
C(163)-C(165)-H(16N) 109.5
C(163)-C(165)-H(16O) 109.5
C(163)-C(166)-H(16P) 109.5
C(163)-C(166)-H(16Q) 109.5
C(163)-C(166)-H(16R) 109.5
C(163)-C(64")-H(64D) 109.5
C(163)-C(64")-H(64E) 109.5
C(163)-C(64")-H(64F) 109.5
C(163)-C(65")-H(65D) 109.5
C(163)-C(65")-H(65E) 109.5
C(163)-C(65")-H(65F) 109.5
C(163)-C(66")-H(66D) 109.5
C(163)-C(66")-H(66E) 109.5
C(163)-C(66")-H(66F) 109.5
C(170)-C(167)-C(168) 108.0(7)
C(170)-C(167)-C(141) 112.5(7)
C(168)-C(167)-C(141) 107.4(7)
C(170)-C(167)-C(169) 109.0(7)
C(168)-C(167)-C(169) 110.4(7)
C(141)-C(167)-C(169) 109.5(7)
C(167)-C(168)-H(16S) 109.5
C(167)-C(168)-H(16T) 109.5
H(16S)-C(168)-H(16T) 109.5
C(167)-C(168)-H(16U) 109.5
H(16S)-C(168)-H(16U) 109.5
H(16T)-C(168)-H(16U) 109.5
C(167)-C(169)-H(16V) 109.5
C(167)-C(169)-H(16W) 109.5
H(16V)-C(169)-H(16W) 109.5
C(167)-C(169)-H(16X) 109.5
H(16V)-C(169)-H(16X) 109.5
H(16W)-C(169)-H(16X) 109.5
C(167)-C(170)-H(17A) 109.5
C(167)-C(170)-H(17B) 109.5
H(17A)-C(170)-H(17B) 109.5
C(167)-C(170)-H(17C) 109.5
H(17A)-C(170)-H(17C) 109.5
H(17B)-C(170)-H(17C) 109.5
C(172)-C(171)-C(143) 113.8(7)
C(172)-C(171)-C(174) 108.1(7)
C(143)-C(171)-C(174) 112.6(7)
C(172)-C(171)-C(173) 106.2(8)
C(143)-C(171)-C(173) 107.6(7)
C(174)-C(171)-C(173) 108.2(7)
C(171)-C(172)-H(17D) 109.5
C(171)-C(172)-H(17E) 109.5
H(17D)-C(172)-H(17E) 109.5
C(171)-C(172)-H(17F) 109.5
H(17D)-C(172)-H(17F) 109.5
H(17E)-C(172)-H(17F) 109.5
C(171)-C(173)-H(17G) 109.5
C(171)-C(173)-H(17H) 109.5
H(17G)-C(173)-H(17H) 109.5
C(171)-C(173)-H(17I) 109.5
H(17G)-C(173)-H(17I) 109.5
H(17H)-C(173)-H(17I) 109.5
C(171)-C(174)-H(17J) 109.5
C(171)-C(174)-H(17K) 109.5
H(17J)-C(174)-H(17K) 109.5
C(171)-C(174)-H(17L) 109.5
H(17J)-C(174)-H(17L) 109.5
H(17K)-C(174)-H(17L) 109.5
C(176)-C(175)-C(178) 108.0(6)
C(176)-C(175)-C(147) 111.8(6)
C(178)-C(175)-C(147) 109.8(6)
C(176)-C(175)-C(177) 108.7(6)
C(178)-C(175)-C(177) 108.4(6)
C(147)-C(175)-C(177) 110.0(6)
C(175)-C(176)-H(17M) 109.5
C(175)-C(176)-H(17N) 109.5
H(17M)-C(176)-H(17N) 109.5
C(175)-C(176)-H(17O) 109.5
H(17M)-C(176)-H(17O) 109.5
H(17N)-C(176)-H(17O) 109.5
C(175)-C(177)-H(17P) 109.5
C(175)-C(177)-H(17Q) 109.5
H(17P)-C(177)-H(17Q) 109.5
C(175)-C(177)-H(17R) 109.5
H(17P)-C(177)-H(17R) 109.5
H(17Q)-C(177)-H(17R) 109.5
C(175)-C(178)-H(17S) 109.5
C(175)-C(178)-H(17T) 109.5
H(17S)-C(178)-H(17T) 109.5
C(175)-C(178)-H(17U) 109.5
H(17S)-C(178)-H(17U) 109.5
H(17T)-C(178)-H(17U) 109.5
C(149)-C(179)-C(180) 112.6(6)
C(149)-C(179)-C(181) 110.3(6)
C(180)-C(179)-C(181)  108.9(6)
C(149)-C(179)-C(182)  108.5(6)
C(180)-C(179)-C(182)  108.6(6)
C(181)-C(179)-C(182)  107.6(6)
C(179)-C(180)-H(18A)  109.5
C(179)-C(180)-H(18B)  109.5
H(18A)-C(180)-H(18B)  109.5
C(179)-C(180)-H(18C)  109.5
H(18A)-C(180)-H(18C)  109.5
H(18B)-C(180)-H(18C)  109.5
C(179)-C(181)-H(18D)  109.5
C(179)-C(181)-H(18E)  109.5
H(18D)-C(181)-H(18E)  109.5
C(179)-C(181)-H(18F)  109.5
H(18D)-C(181)-H(18F)  109.5
H(18E)-C(181)-H(18F)  109.5
C(179)-C(182)-H(18G)  109.5
C(179)-C(182)-H(18H)  109.5
H(18G)-C(182)-H(18H)  109.5
C(179)-C(182)-H(18I)  109.5
H(18G)-C(182)-H(18I)  109.5
H(18H)-C(182)-H(18I)  109.5
C(201)-O(1)-H(1)  109.5
O(1)-C(201)-C(202)  107.3(17)
O(1)-C(201)-C(203)  107.3(17)
C(202)-C(201)-C(203)  98.8(18)
O(1)-C(201)-H(201)  114.0
C(202)-C(201)-H(201)  114.0
C(203)-C(201)-H(201)  114.0
C(201)-C(202)-H(20A)  109.5
C(201)-C(202)-H(20B)  109.5
H(20A)-C(202)-H(20B)  109.5
C(201)-C(202)-H(20C)  109.5
H(20A)-C(202)-H(20C)  109.5
3.2 Fe(Ph)Br(SciOPP) (5-Br)

CRYSTAL STRUCTURE REPORT

\[ \text{C}_{72} \text{H}_{103} \text{Br Fe O P}_2 \]

or

\[(\text{SciOPP})\text{Fe(Br)(Ph) \cdot Et}_2\text{O}\]

Report prepared for:

J. Kneebone, Prof. M. Neidig

April 04, 2015

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Data collection
A crystal (0.36 x 0.14 x 0.10 mm$^3$) was placed onto the tip of a thin glass optical fiber and mounted on a Bruker SMART APEX II CCD platform diffractometer for a data collection at 100.0(5) K. A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoK$_\alpha$ radiation (graphite monochromator) with a frame time of 90 seconds and a detector distance of 4.02 cm. A randomly oriented region of reciprocal space was surveyed: three major sections of frames were collected with $0.50^\circ$ steps in $\omega$ at three different $\phi$ settings and a detector position of -38$^\circ$ in 2$\theta$. The intensity data were corrected for absorption. Final cell constants were calculated from the xyz centroids of 4057 strong reflections from the actual data collection after integration. See Table 1 for additional crystal and refinement information.

Structure solution and refinement
The structure was solved using SIR2011$^4$ and refined using SHELXL-2014/7.$^5$ The space group $Pna2_1$ was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R_1 = 0.0624$ ($F^2, I > 2\sigma(I)$) and $wR_2 = 0.1258$ ($F^2$, all data).

Structure description
The structure is the one suggested. The asymmetric unit contains one iron complex and one cocrystallized diethyl ether solvent molecule, both in general positions. The phenyl ligand and tert-butyl groups C35-C38 and C55-C58 are modeled as disordered over two positions each (0.70:0.30, 0.78:0.22, and 0.72:0.28, respectively).

Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50% probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B51 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.
Some equations of interest:

\[ R_{\text{int}} = \frac{\sum |F_o^2 - \langle F_o^2 >|}{\sum |F_o^2|} \]
\[ R1 = \frac{\sum |F_o||F_c|}{\sum |F_o|} \]
\[ wR^2 = \left[ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum w(F_o^2)^2} \right]^{1/2} \]
\[ \text{where } w = \frac{1}{\sigma^2 (F_o^2) + (aP)^2 + bP} \text{ and } \]
\[ P = \frac{1}{3} \text{ max } (0, F_o^2) + \frac{2}{3} F_c^2 \]
\[ \text{GOF} = S = \left[ \frac{\sum [w(F_o^2 - F_c^2)^2]}{(m-n)} \right]^{1/2} \]

where \( m \) = number of reflections and \( n \) = number of parameters
Table S13. Crystal data and structure refinement for Fe(Ph)Br(SciOPP).

| Property                                      | Value                          |
|-----------------------------------------------|-------------------------------|
| Identification code                           | neijk42                       |
| Empirical formula                             | C72 H103 Br Fe O P2           |
| Formula weight                                | 1182.24                       |
| Temperature                                   | 100.0(5) K                    |
| Wavelength                                    | 0.71073 Å                     |
| Crystal system                                | orthorhombic                  |
| Space group                                   | Pna2_1                        |
| Unit cell dimensions                          | \( a = 31.239(7) \) Å, \( \alpha = 90^\circ \) |
|                                              | \( b = 14.820(4) \) Å, \( \beta = 90^\circ \) |
|                                              | \( c = 15.184(4) \) Å, \( \gamma = 90^\circ \) |
| Volume                                        | 7030(3) Å³                    |
| Z                                             | 4                             |
| Density (calculated)                          | 1.117 Mg/m³                   |
| Absorption coefficient                        | 0.867 mm\(^{-1}\)            |
| \( F(000) \)                                  | 2536                          |
| Crystal color, morphology                     | pale yellow, needle           |
| Crystal size                                  | 0.36 x 0.14 x 0.10 mm³       |
| Theta range for data collection               | 1.870 to 25.099°              |
| Index ranges                                  | -28 ≤ h ≤ 37, -17 ≤ k ≤ 17, -18 ≤ l ≤ 17 |
| Reflections collected                         | 47332                         |
| Independent reflections                       | 12010 \([R(int) = 0.1546]\)    |
| Observed reflections                          | 7665                          |
| Completeness to theta = 25.028°               | 99.8%                         |
| Absorption correction                         | Multi-scan                    |
| Max. and min. transmission                    | 0.7452 and 0.6336             |
| Refinement method                             | Full-matrix least-squares on \( F^2 \) |
| Data / restraints / parameters                | 12010 / 165 / 770             |
| Goodness-of-fit on \( F^2 \)                  | 1.007                         |
| Final \( R \) indices [\( I > 2 \sigma(I) \)] | \( R1 = 0.0624, wR2 = 0.1059 \) |
| \( R \) indices (all data)                   | \( R1 = 0.1208, wR2 = 0.1258 \) |
| Absolute structure parameter                  | 0.037(8)                      |
| Largest diff. peak and hole                   | 0.411 and -0.520 e.Å\(^{-3}\) |
Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3). \( U_{eq} \) is defined as one third of the trace of the orthogonalized \( U_{ij} \) tensor.

|    | x      | y      | z      | \( U_{eq} \) |
|----|--------|--------|--------|--------------|
| Fe1| 771(1) | 4990(1)| 5315(1)| 21(1)        |
| Br1| 787(1) | 4223(1)| 3940(1)| 38(1)        |
| P1 | 193(1) | 4507(1)| 6260(1)| 16(1)        |
| P2 | 1186(1)| 4299(1)| 6497(1)| 17(1)        |
| C1 | 416(2) | 4500(5)| 7376(5)| 14(2)        |
| C2 | 151(3) | 4555(5)| 8109(5)| 19(2)        |
| C3 | 322(2) | 4534(4)| 8956(6)| 21(2)        |
| C4 | 766(3) | 4496(5)| 9070(6)| 25(2)        |
| C5 | 1030(3)| 4470(5)| 8330(5)| 18(2)        |
| C6 | 868(3) | 4462(5)| 7487(5)| 17(2)        |
| C7 | -315(2)| 5109(5)| 6350(5)| 14(2)        |
| C8 | -309(3)| 6042(5)| 6251(5)| 19(2)        |
| C9 | -690(2)| 6541(5)| 6302(5)| 17(2)        |
| C10| -1063(3)| 6081(5)| 6455(5)| 21(2)        |
| C11| -1086(3)| 5147(5)| 6561(5)| 19(2)        |
| C12| -704(3)| 4669(5)| 6510(5)| 21(2)        |
| C13| 25(2)  | 3348(5)| 6069(5)| 15(2)        |
| C14| 81(2)  | 2659(5)| 6685(6)| 20(2)        |
| C15| -69(3) | 1795(5)| 6506(5)| 20(2)        |
| C16| -280(3)| 1644(5)| 5709(5)| 20(2)        |
| C17| -335(2)| 2330(5)| 5082(5)| 16(2)        |
| C18| -172(2)| 3178(5)| 5265(6)| 20(2)        |
| C19| 1272(2)| 3081(5)| 6454(5)| 16(2)        |
| C20| 1398(3)| 2576(5)| 7191(6)| 22(2)        |
| C21| 1485(3)| 1669(5)| 7119(6)| 22(2)        |
| C22| 1458(3)| 1284(5)| 6286(6)| 26(2)        |
| C23| 1333(3)| 1743(6)| 5544(6)| 25(2)        |
| C24| 1247(3)| 2660(5)| 5645(6)| 22(2)        |
| C25| 1709(3)| 4764(5)| 6765(5)| 18(2)        |
| C26| 2080(3)| 4301(5)| 6543(6)| 24(2)        |
| C27| 2479(3)| 4680(5)| 6635(6)| 25(2)        |
|  |  |  |  |  |
|---|---|---|---|---|
| C28 | 2500(3) | 5544(5) | 6994(6) | 30(2) |
| C29 | 2140(3) | 6047(5) | 7221(6) | 21(2) |
| C30 | 1743(3) | 5630(5) | 7095(6) | 23(2) |
| C31 | -663(3) | 7570(5) | 6199(6) | 26(2) |
| C32 | -1112(3) | 8015(5) | 6214(7) | 39(3) |
| C33 | -464(3) | 7803(5) | 5298(7) | 36(2) |
| C34 | -386(3) | 7946(5) | 6947(6) | 35(3) |
| C35 | -1510(3) | 4645(7) | 6674(7) | 26(2) |
| C36 | -1626(4) | 4164(10) | 5804(7) | 41(4) |
| C37 | -1875(4) | 5296(8) | 6934(11) | 49(4) |
| C38 | -1470(4) | 3933(9) | 7415(8) | 36(3) |
| C35' | -1502(7) | 4649(18) | 6790(20) | 26(2) |
| C36' | -1736(13) | 5120(30) | 7570(20) | 41(4) |
| C37' | -1445(15) | 3640(20) | 7030(30) | 49(4) |
| C38' | -1790(14) | 4710(30) | 5960(20) | 36(3) |
| C39 | -13(3) | 1012(5) | 7150(5) | 24(2) |
| C40 | 204(3) | 1307(5) | 8008(6) | 32(2) |
| C41 | -452(3) | 588(5) | 7374(6) | 33(2) |
| C42 | 269(3) | 292(5) | 6704(6) | 31(2) |
| C43 | -580(3) | 2113(5) | 4240(6) | 28(2) |
| C44 | -584(3) | 2914(6) | 3602(6) | 32(2) |
| C45 | -384(3) | 1305(5) | 3768(6) | 33(2) |
| C46 | -1047(3) | 1894(6) | 4484(6) | 36(3) |
| C47 | 1643(3) | 1103(6) | 7903(6) | 29(2) |
| C48 | 1373(3) | 242(6) | 7989(7) | 44(3) |
| C49 | 1616(3) | 1609(6) | 8778(6) | 43(3) |
| C50 | 2105(3) | 831(7) | 7751(7) | 42(3) |
| C51 | 1289(3) | 1308(6) | 4634(6) | 35(2) |
| C52 | 1503(3) | 1893(6) | 3929(7) | 48(3) |
| C53 | 810(3) | 1222(6) | 4420(6) | 40(3) |
| C54 | 1495(4) | 368(7) | 4584(8) | 61(3) |
| C55 | 2882(3) | 4151(8) | 6345(8) | 40(3) |
| C56 | 2869(5) | 4076(12) | 5344(9) | 67(5) |
| C57 | 2883(5) | 3211(9) | 6745(13) | 77(6) |
| C58 | 3298(4) | 4615(10) | 6608(12) | 56(5) |
| C55' | 2895(6) | 4201(16) | 6346(18) | 40(3) |
|     | 3212(12) | 4150(30) | 7110(20) | 67(5)  |
|-----|----------|----------|----------|--------|
| C56' |          |          |          |        |
| C57' | 3086(13) | 4780(20) | 5620(30) | 77(6)  |
| C58' | 2825(11) | 3253(19) | 5990(30) | 56(5)  |
| C59  | 2178(3)  | 6996(6)  | 7614(6)  | 30(2)  |
| C60  | 2203(4)  | 6877(7)  | 8629(7)  | 67(4)  |
| C61  | 2572(3)  | 7496(6)  | 7275(8)  | 50(3)  |
| C62  | 1786(3)  | 7571(6)  | 7375(8)  | 52(3)  |
| C63  | 801(7)   | 6391(6)  | 5334(15) | 27(3)  |
| C64  | 803(6)   | 6870(10) | 6071(14) | 31(3)  |
| C65  | 795(5)   | 7827(9)  | 6112(15) | 41(4)  |
| C66  | 786(5)   | 8301(9)  | 5320(15) | 44(4)  |
| C67  | 781(6)   | 7833(11) | 4542(13) | 43(4)  |
| C68  | 781(8)   | 6875(11) | 4548(15) | 36(3)  |
| C69  | 2982(4)  | 1171(8)  | 9688(8)  | 61(4)  |
| C70  | 3047(4)  | 2166(9)  | 9620(8)  | 62(4)  |
| O1   | 2654(2)  | 2605(5)  | 9445(5)  | 57(2)  |
| C71  | 2685(5)  | 3548(8)  | 9444(9)  | 79(4)  |
| C72  | 2260(5)  | 3969(8)  | 9149(9)  | 85(5)  |

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S72
Table S15. Bond lengths [Å] and angles [°].

| Bond                        | Length [Å]   |
|-----------------------------|--------------|
| Fe(1)-C(63')                | 2.067(13)    |
| Fe(1)-C(63)                 | 2.079(9)     |
| Fe(1)-Br(1)                 | 2.3777(15)   |
| Fe(1)-P(1)                  | 2.415(3)     |
| Fe(1)-P(2)                  | 2.438(2)     |
| P(1)-C(13)                  | 1.819(7)     |
| P(1)-C(7)                   | 1.825(7)     |
| P(1)-C(1)                   | 1.832(8)     |
| P(2)-C(6)                   | 1.817(8)     |
| P(2)-C(25)                  | 1.820(8)     |
| P(2)-C(19)                  | 1.826(7)     |
| C(1)-C(2)                   | 1.390(10)    |
| C(1)-C(6)                   | 1.425(10)    |
| C(2)-C(3)                   | 1.394(11)    |
| C(2)-H(2)                   | 0.9500       |
| C(3)-C(4)                   | 1.398(11)    |
| C(3)-H(3)                   | 0.9500       |
| C(4)-C(5)                   | 1.394(11)    |
| C(4)-H(4)                   | 0.9500       |
| C(5)-C(6)                   | 1.376(11)    |
| C(5)-H(5)                   | 0.9500       |
| C(7)-C(8)                   | 1.390(10)    |
| C(7)-C(12)                  | 1.401(10)    |
| C(8)-C(9)                   | 1.403(10)    |
| C(8)-H(8)                   | 0.9500       |
| C(9)-C(10)                  | 1.371(11)    |
| C(9)-C(31)                  | 1.535(10)    |
| C(10)-C(11)                 | 1.396(10)    |
| C(10)-H(10)                 | 0.9500       |
| C(11)-C(12)                 | 1.390(10)    |
| C(11)-C(35)                 | 1.529(11)    |
| C(11)-C(35')                | 1.534(15)    |
| C(12)-H(12)                 | 0.9500       |
| C(13)-C(18)                 | 1.390(11)    |
| Bond                  | Distance (Å) |
|----------------------|--------------|
| C(13)-C(14)          | 1.397(10)    |
| C(14)-C(15)          | 1.390(10)    |
| C(14)-H(14)          | 0.9500       |
| C(15)-C(16)          | 1.395(11)    |
| C(15)-C(39)          | 1.528(11)    |
| C(16)-C(17)          | 1.404(11)    |
| C(16)-H(16)          | 0.9500       |
| C(17)-C(18)          | 1.384(10)    |
| C(17)-C(43)          | 1.524(11)    |
| C(18)-H(18)          | 0.9500       |
| C(19)-C(24)          | 1.379(11)    |
| C(19)-C(20)          | 1.403(11)    |
| C(20)-C(21)          | 1.376(11)    |
| C(20)-H(20)          | 0.9500       |
| C(21)-C(22)          | 1.391(12)    |
| C(21)-C(47)          | 1.539(12)    |
| C(22)-C(23)          | 1.372(11)    |
| C(22)-H(22)          | 0.9500       |
| C(23)-C(24)          | 1.395(11)    |
| C(23)-C(51)          | 1.530(12)    |
| C(24)-H(24)          | 0.9500       |
| C(25)-C(30)          | 1.381(11)    |
| C(25)-C(26)          | 1.388(11)    |
| C(26)-C(27)          | 1.377(11)    |
| C(26)-H(26)          | 0.9500       |
| C(27)-C(28)          | 1.393(11)    |
| C(27)-C(55)          | 1.544(16)    |
| C(27)-C(55')         | 1.546(12)    |
| C(28)-C(29)          | 1.392(11)    |
| C(28)-H(28)          | 0.9500       |
| C(29)-C(30)          | 1.400(11)    |
| C(29)-C(59)          | 1.533(11)    |
| C(30)-H(30)          | 0.9500       |
| C(31)-C(34)          | 1.532(12)    |
| C(31)-C(33)          | 1.543(12)    |
| C(31)-C(32)          | 1.549(11)    |
C(32)-H(32A) 0.9800
C(32)-H(32B) 0.9800
C(32)-H(32C) 0.9800
C(33)-H(33A) 0.9800
C(33)-H(33B) 0.9800
C(33)-H(33C) 0.9800
C(34)-H(34A) 0.9800
C(34)-H(34B) 0.9800
C(34)-H(34C) 0.9800
C(35)-C(36) 1.544(10)
C(35)-C(37) 1.544(10)
C(35)-C(38) 1.547(10)
C(36)-H(36A) 0.9800
C(36)-H(36B) 0.9800
C(36)-H(36C) 0.9800
C(37)-H(37A) 0.9800
C(37)-H(37B) 0.9800
C(37)-H(37C) 0.9800
C(38)-H(38A) 0.9800
C(38)-H(38B) 0.9800
C(38)-H(38C) 0.9800
C(39)-C(40) 1.531(11)
C(39)-C(42) 1.541(11)
C(39)-C(41) 1.546(12)
C(40)-H(40A) 0.9800
C(40)-H(40B) 0.9800
C(40)-H(40C) 0.9800
C(41)-H(41A) 0.9800
C(41)-H(41B) 0.9800
C(41)-H(41C) 0.9800
C(42)-H(42A) 0.9800
C(42)-H(42B) 0.9800
C(42)-H(42C) 0.9800
C(43)-C(45) 1.525(11)
C(43)-C(44) 1.532(11)
C(43)-C(46) 1.538(12)
C(44)-H(44A) 0.9800
C(44)-H(44B) 0.9800
C(44)-H(44C) 0.9800
C(45)-H(45A) 0.9800
C(45)-H(45B) 0.9800
C(45)-H(45C) 0.9800
C(46)-H(46A) 0.9800
C(46)-H(46B) 0.9800
C(46)-H(46C) 0.9800
C(47)-C(50) 1.517(12)
C(47)-C(49) 1.527(13)
C(47)-C(48) 1.537(11)
C(48)-H(48A) 0.9800
C(48)-H(48B) 0.9800
C(48)-H(48C) 0.9800
C(49)-H(49A) 0.9800
C(49)-H(49B) 0.9800
C(49)-H(49C) 0.9800
C(50)-H(50A) 0.9800
C(50)-H(50B) 0.9800
C(50)-H(50C) 0.9800
C(51)-C(52) 1.531(13)
C(51)-C(54) 1.538(13)
C(51)-C(53) 1.537(12)
C(52)-H(52A)  0.9800
C(52)-H(52B)  0.9800
C(52)-H(52C)  0.9800
C(53)-H(53A)  0.9800
C(53)-H(53B)  0.9800
C(53)-H(53C)  0.9800
C(54)-H(54A)  0.9800
C(54)-H(54B)  0.9800
C(54)-H(54C)  0.9800
C(55)-C(57)   1.519(11)
C(55)-C(56)   1.524(11)
C(55)-C(58)   1.525(11)
C(56)-H(56A)  0.9800
C(56)-H(56B)  0.9800
C(56)-H(56C)  0.9800
C(57)-H(57A)  0.9800
C(57)-H(57B)  0.9800
C(57)-H(57C)  0.9800
C(58)-H(58A)  0.9800
C(58)-H(58B)  0.9800
C(58)-H(58C)  0.9800
C(55')-C(58') 1.521(12)
C(55')-C(56') 1.521(13)
C(55')-C(57') 1.523(13)
C(56')-H(56D) 0.9800
C(56')-H(56E) 0.9800
C(56')-H(56F) 0.9800
C(57')-H(57D) 0.9800
C(57')-H(57E) 0.9800
C(57')-H(57F) 0.9800
C(58')-H(58D) 0.9800
C(58')-H(58E) 0.9800
C(58')-H(58F) 0.9800
C(59)-C(61)   1.528(12)
C(59)-C(62)   1.534(12)
C(59)-C(60)   1.553(13)
| Bond                  | Distance (Å) |
|-----------------------|--------------|
| C(60)-H(60A)          | 0.9800       |
| C(60)-H(60B)          | 0.9800       |
| C(60)-H(60C)          | 0.9800       |
| C(61)-H(61A)          | 0.9800       |
| C(61)-H(61B)          | 0.9800       |
| C(61)-H(61C)          | 0.9800       |
| C(62)-H(62A)          | 0.9800       |
| C(62)-H(62B)          | 0.9800       |
| C(62)-H(62C)          | 0.9800       |
| C(63)-C(64)           | 1.325(14)    |
| C(63)-C(68)           | 1.393(13)    |
| C(64)-C(65)           | 1.420(14)    |
| C(64)-H(64)           | 0.9500       |
| C(65)-C(66)           | 1.394(15)    |
| C(65)-H(65)           | 0.9500       |
| C(66)-C(67)           | 1.370(16)    |
| C(66)-H(66)           | 0.9500       |
| C(67)-C(68)           | 1.419(15)    |
| C(67)-H(67)           | 0.9500       |
| C(68)-H(68)           | 0.9500       |
| C(69)-C(70)           | 1.493(15)    |
| C(69)-H(69A)          | 0.9800       |
| C(69)-H(69B)          | 0.9800       |
| C(69)-H(69C)          | 0.9800       |
| C(70)-O(1)            | 1.415(12)    |
C(70)-H(70A) 0.9900
C(70)-H(70B) 0.9900
O(1)-C(71) 1.401(13)
C(71)-C(72) 1.536(16)
C(71)-H(71A) 0.9900
C(71)-H(71B) 0.9900
C(72)-H(72A) 0.9800
C(72)-H(72B) 0.9800
C(72)-H(72C) 0.9800
C(63')-Fe(1)-Br(1) 114.2(14)
C(63)-Fe(1)-Br(1) 119.3(7)
C(63')-Fe(1)-P(1) 112.1(15)
C(63)-Fe(1)-P(1) 108.7(6)
Br(1)-Fe(1)-P(1) 113.29(8)
C(63')-Fe(1)-P(2) 116.5(14)
C(63)-Fe(1)-P(2) 112.7(6)
Br(1)-Fe(1)-P(2) 115.74(7)
P(1)-Fe(1)-P(2) 80.51(8)
C(13)-P(1)-C(7) 102.9(4)
C(13)-P(1)-C(1) 104.6(4)
C(7)-P(1)-C(1) 105.2(3)
C(13)-P(1)-Fe(1) 113.6(3)
C(7)-P(1)-Fe(1) 123.3(3)
C(1)-P(1)-Fe(1) 105.5(3)
C(6)-P(2)-C(25) 104.8(4)
C(6)-P(2)-C(19) 104.0(3)
C(25)-P(2)-C(19) 104.4(3)
C(6)-P(2)-Fe(1) 105.3(3)
C(25)-P(2)-Fe(1) 118.8(3)
C(19)-P(2)-Fe(1) 117.8(3)
C(2)-C(1)-C(6) 119.9(7)
C(2)-C(1)-P(1) 121.0(6)
C(6)-C(1)-P(1) 119.1(6)
C(1)-C(2)-C(3) 120.6(8)
C(1)-C(2)-H(2) 119.7
C(3)-C(2)-H(2) 119.7
| Bond                  | Angle (°) |
|----------------------|-----------|
| C(2)-C(3)-C(4)       | 119.7(8)  |
| C(2)-C(3)-H(3)       | 120.1     |
| C(4)-C(3)-H(3)       | 120.1     |
| C(5)-C(4)-C(3)       | 119.3(8)  |
| C(5)-C(4)-H(4)       | 120.4     |
| C(3)-C(4)-H(4)       | 120.4     |
| C(6)-C(5)-C(4)       | 122.1(8)  |
| C(6)-C(5)-H(5)       | 118.9     |
| C(4)-C(5)-H(5)       | 118.9     |
| C(5)-C(6)-C(1)       | 118.3(7)  |
| C(5)-C(6)-P(2)       | 124.7(6)  |
| C(1)-C(6)-P(2)       | 116.7(6)  |
| C(8)-C(7)-C(12)      | 119.5(7)  |
| C(8)-C(7)-P(1)       | 117.8(6)  |
| C(12)-C(7)-P(1)      | 122.6(6)  |
| C(7)-C(8)-C(9)       | 120.5(7)  |
| C(7)-C(8)-H(8)       | 119.8     |
| C(9)-C(8)-H(8)       | 119.8     |
| C(10)-C(9)-C(8)      | 118.0(7)  |
| C(10)-C(9)-C(31)     | 123.9(7)  |
| C(8)-C(9)-C(31)      | 118.1(7)  |
| C(9)-C(10)-C(11)     | 123.8(8)  |
| C(9)-C(10)-H(10)     | 118.1     |
| C(11)-C(10)-H(10)    | 118.1     |
| C(12)-C(11)-C(10)    | 117.1(8)  |
| C(12)-C(11)-C(35)    | 120.2(7)  |
| C(10)-C(11)-C(35)    | 122.6(8)  |
| C(12)-C(11)-C(35')   | 119.7(13) |
| C(10)-C(11)-C(35')   | 123.1(13) |
| C(11)-C(12)-C(7)     | 121.2(7)  |
| C(11)-C(12)-H(12)    | 119.4     |
| C(7)-C(12)-H(12)     | 119.4     |
| C(18)-C(13)-C(14)    | 120.7(7)  |
| C(18)-C(13)-P(1)     | 116.1(6)  |
| C(14)-C(13)-P(1)     | 123.2(6)  |
| C(15)-C(14)-C(13)    | 120.0(7)  |
| Bond                  | Angle (°) |
|----------------------|-----------|
| C(15)-C(14)-H(14)   | 120.0     |
| C(13)-C(14)-H(14)   | 120.0     |
| C(14)-C(15)-C(16)   | 118.5(7)  |
| C(14)-C(15)-C(39)   | 122.3(7)  |
| C(16)-C(15)-C(39)   | 119.2(7)  |
| C(15)-C(16)-C(17)   | 122.0(7)  |
| C(15)-C(16)-H(16)   | 119.0     |
| C(17)-C(16)-H(16)   | 119.0     |
| C(18)-C(17)-C(16)   | 118.4(7)  |
| C(18)-C(17)-C(43)   | 123.0(7)  |
| C(16)-C(17)-C(43)   | 118.6(7)  |
| C(17)-C(18)-C(13)   | 120.3(7)  |
| C(17)-C(18)-H(18)   | 119.9     |
| C(13)-C(18)-H(18)   | 119.9     |
| C(24)-C(19)-C(20)   | 119.0(7)  |
| C(24)-C(19)-P(2)    | 118.1(6)  |
| C(20)-C(19)-P(2)    | 122.7(6)  |
| C(21)-C(20)-C(19)   | 120.8(8)  |
| C(21)-C(20)-H(20)   | 119.6     |
| C(19)-C(20)-H(20)   | 119.6     |
| C(20)-C(21)-C(22)   | 117.5(8)  |
| C(20)-C(21)-C(47)   | 122.3(8)  |
| C(22)-C(21)-C(47)   | 120.0(7)  |
| C(23)-C(22)-C(21)   | 124.1(7)  |
| C(23)-C(22)-H(22)   | 118.0     |
| C(21)-C(22)-H(22)   | 118.0     |
| C(22)-C(23)-C(24)   | 116.6(8)  |
| C(22)-C(23)-C(51)   | 123.9(8)  |
| C(24)-C(23)-C(51)   | 119.5(8)  |
| C(19)-C(24)-C(23)   | 121.9(8)  |
| C(19)-C(24)-H(24)   | 119.1     |
| C(23)-C(24)-H(24)   | 119.1     |
| C(30)-C(25)-C(26)   | 119.0(8)  |
| C(30)-C(25)-P(2)    | 120.1(6)  |
| C(26)-C(25)-P(2)    | 120.5(6)  |
| C(27)-C(26)-C(25)   | 122.0(8)  |
| Bond                  | Angle (°) |
|-----------------------|-----------|
| C(27)-C(26)-H(26)    | 119.0     |
| C(25)-C(26)-H(26)    | 119.0     |
| C(26)-C(27)-C(28)    | 117.2(8)  |
| C(26)-C(27)-C(55')   | 123.1(12) |
| C(28)-C(27)-C(55')   | 119.7(12) |
| C(26)-C(27)-C(55)    | 120.1(8)  |
| C(28)-C(27)-C(55)    | 122.7(9)  |
| C(29)-C(28)-C(27)    | 123.5(8)  |
| C(29)-C(28)-H(28)    | 118.3     |
| C(27)-C(28)-H(28)    | 118.3     |
| C(28)-C(29)-C(30)    | 116.5(7)  |
| C(28)-C(29)-C(59)    | 121.7(8)  |
| C(30)-C(29)-C(59)    | 121.7(8)  |
| C(25)-C(30)-C(29)    | 121.8(8)  |
| C(25)-C(30)-H(30)    | 119.1     |
| C(29)-C(30)-H(30)    | 119.1     |
| C(34)-C(31)-C(9)     | 108.5(7)  |
| C(34)-C(31)-C(33)    | 110.3(7)  |
| C(9)-C(31)-C(33)     | 109.6(7)  |
| C(34)-C(31)-C(32)    | 110.2(7)  |
| C(9)-C(31)-C(32)     | 111.9(7)  |
| C(33)-C(31)-C(32)    | 106.4(7)  |
| C(31)-C(32)-H(32A)   | 109.5     |
| C(31)-C(32)-H(32B)   | 109.5     |
| H(32A)-C(32)-H(32B)  | 109.5     |
| C(31)-C(32)-H(32C)   | 109.5     |
| H(32A)-C(32)-H(32C)  | 109.5     |
| H(32B)-C(32)-H(32C)  | 109.5     |
| C(31)-C(33)-H(33A)   | 109.5     |
| C(31)-C(33)-H(33B)   | 109.5     |
| H(33A)-C(33)-H(33B)  | 109.5     |
| C(31)-C(33)-H(33C)   | 109.5     |
| H(33A)-C(33)-H(33C)  | 109.5     |
| H(33B)-C(33)-H(33C)  | 109.5     |
| C(31)-C(34)-H(34A)   | 109.5     |
| C(31)-C(34)-H(34B)   | 109.5     |
H(34A)-C(34)-H(34B) 109.5
C(31)-C(34)-H(34C) 109.5
H(34A)-C(34)-H(34C) 109.5
H(34B)-C(34)-H(34C) 109.5
C(11)-C(35)-C(36) 109.4(8)
C(11)-C(35)-C(37) 111.4(8)
C(36)-C(35)-C(37) 109.5(9)
C(11)-C(35)-C(38) 110.0(9)
C(36)-C(35)-C(38) 109.0(8)
C(37)-C(35)-C(38) 107.5(8)
C(35)-C(36)-H(36A) 109.5
C(35)-C(36)-H(36B) 109.5
H(36A)-C(36)-H(36B) 109.5
C(35)-C(36)-H(36C) 109.5
H(36A)-C(36)-H(36C) 109.5
H(36B)-C(36)-H(36C) 109.5
C(35)-C(37)-H(37A) 109.5
C(35)-C(37)-H(37B) 109.5
H(37A)-C(37)-H(37B) 109.5
C(35)-C(37)-H(37C) 109.5
H(37A)-C(37)-H(37C) 109.5
H(37B)-C(37)-H(37C) 109.5
C(35)-C(38)-H(38A) 109.5
C(35)-C(38)-H(38B) 109.5
H(38A)-C(38)-H(38B) 109.5
C(35)-C(38)-H(38C) 109.5
H(38A)-C(38)-H(38C) 109.5
H(38B)-C(38)-H(38C) 109.5
C(11)-C(35')-C(38') 106(2)
C(11)-C(35')-C(36') 111(2)
C(38')-C(35')-C(36') 108.5(14)
C(11)-C(35')-C(37') 115(3)
C(38')-C(35')-C(37') 108.1(14)
C(36')-C(35')-C(37') 107.9(14)
C(35')-C(36')-H(36D) 109.5
C(35')-C(36')-H(36E) 109.5
H(36D)-C(36')-H(36E)  109.5
C(35')-C(36')-H(36F)  109.5
H(36D)-C(36')-H(36F)  109.5
H(36E)-C(36')-H(36F)  109.5
C(35')-C(37')-H(37D)  108.4
C(35')-C(37')-H(37E)  109.0
H(37D)-C(37')-H(37E)  109.6
C(35')-C(37')-H(37F)  108.6
H(37D)-C(37')-H(37F)  109.6
H(37E)-C(37')-H(37F)  111.4
C(35')-C(38')-H(38D)  109.5
C(35')-C(38')-H(38E)  109.5
H(38D)-C(38')-H(38E)  109.5
C(35')-C(38')-H(38F)  109.5
H(38D)-C(38')-H(38F)  109.5
H(38E)-C(38')-H(38F)  109.5
C(15)-C(39)-C(40)    112.3(7)
C(15)-C(39)-C(42)    108.1(7)
C(40)-C(39)-C(42)    108.5(7)
C(15)-C(39)-C(41)    110.4(7)
C(40)-C(39)-C(41)    108.7(7)
C(42)-C(39)-C(41)    108.8(7)
C(39)-C(40)-H(40A)   109.5
C(39)-C(40)-H(40B)   109.5
H(40A)-C(40)-H(40B)  109.5
C(39)-C(40)-H(40C)   109.5
H(40A)-C(40)-H(40C)  109.5
H(40B)-C(40)-H(40C)  109.5
C(39)-C(41)-H(41A)   109.5
C(39)-C(41)-H(41B)   109.5
H(41A)-C(41)-H(41B)  109.5
C(39)-C(41)-H(41C)   109.5
H(41A)-C(41)-H(41C)  109.5
H(41B)-C(41)-H(41C)  109.5
C(39)-C(42)-H(42A)   109.5
C(39)-C(42)-H(42B)   109.5
H(42A)-C(42)-H(42B)  109.5
C(39)-C(42)-H(42C)  109.5
H(42A)-C(42)-H(42C)  109.5
H(42B)-C(42)-H(42C)  109.5
C(17)-C(43)-C(45)  111.0(7)
C(17)-C(43)-C(44)  111.7(6)
C(45)-C(43)-C(44)  108.3(8)
C(17)-C(43)-C(46)  108.6(7)
C(45)-C(43)-C(46)  109.2(7)
C(44)-C(43)-C(46)  108.0(7)
C(43)-C(44)-H(44A)  109.5
C(43)-C(44)-H(44B)  109.5
H(44A)-C(44)-H(44B)  109.5
C(43)-C(44)-H(44C)  109.5
H(44A)-C(44)-H(44C)  109.5
H(44B)-C(44)-H(44C)  109.5
C(43)-C(45)-H(45A)  109.5
C(43)-C(45)-H(45B)  109.5
H(45A)-C(45)-H(45B)  109.5
C(43)-C(45)-H(45C)  109.5
H(45A)-C(45)-H(45C)  109.5
H(45B)-C(45)-H(45C)  109.5
C(43)-C(46)-H(46A)  109.5
C(43)-C(46)-H(46B)  109.5
H(46A)-C(46)-H(46B)  109.5
C(43)-C(46)-H(46C)  109.5
H(46A)-C(46)-H(46C)  109.5
H(46B)-C(46)-H(46C)  109.5
C(50)-C(47)-C(49)  108.5(8)
C(50)-C(47)-C(48)  108.4(7)
C(49)-C(47)-C(48)  107.6(8)
C(50)-C(47)-C(21)  109.5(7)
C(49)-C(47)-C(21)  112.8(7)
C(48)-C(47)-C(21)  110.0(7)
C(47)-C(48)-H(48A)  109.5
C(47)-C(48)-H(48B)  109.5
H(48A)-C(48)-H(48B) 109.5
C(47)-C(48)-H(48C) 109.5
H(48A)-C(48)-H(48C) 109.5
H(48B)-C(48)-H(48C) 109.5
C(47)-C(49)-H(49A) 109.5
C(47)-C(49)-H(49B) 109.5
H(49A)-C(49)-H(49B) 109.5
C(47)-C(49)-H(49C) 109.5
H(49A)-C(49)-H(49C) 109.5
H(49B)-C(49)-H(49C) 109.5
C(47)-C(50)-H(50A) 109.5
C(47)-C(50)-H(50B) 109.5
H(50A)-C(50)-H(50B) 109.5
C(47)-C(50)-H(50C) 109.5
H(50A)-C(50)-H(50C) 109.5
H(50B)-C(50)-H(50C) 109.5
C(23)-C(51)-C(52) 110.7(8)
C(23)-C(51)-C(54) 112.9(8)
C(52)-C(51)-C(54) 107.2(8)
C(23)-C(51)-C(53) 108.3(8)
C(52)-C(51)-C(53) 108.9(8)
C(54)-C(51)-C(53) 108.8(8)
C(51)-C(52)-H(52A) 109.5
C(51)-C(52)-H(52B) 109.5
H(52A)-C(52)-H(52B) 109.5
C(51)-C(52)-H(52C) 109.5
H(52A)-C(52)-H(52C) 109.5
H(52B)-C(52)-H(52C) 109.5
C(51)-C(53)-H(53A) 109.5
C(51)-C(53)-H(53B) 109.5
H(53A)-C(53)-H(53B) 109.5
C(51)-C(53)-H(53C) 109.5
H(53A)-C(53)-H(53C) 109.5
H(53B)-C(53)-H(53C) 109.5
C(51)-C(54)-H(54A) 109.5
C(51)-C(54)-H(54B) 109.5
H(54A)-C(54)-H(54B) 109.5
C(51)-C(54)-H(54C) 109.5
H(54A)-C(54)-H(54C) 109.5
H(54B)-C(54)-H(54C) 109.5
C(57)-C(55)-C(56) 109.4(10)
C(57)-C(55)-C(58) 107.8(10)
C(56)-C(55)-C(58) 108.5(10)
C(57)-C(55)-C(27) 110.7(10)
C(56)-C(55)-C(27) 107.5(9)
C(58)-C(55)-C(27) 113.0(9)
C(55)-C(56)-H(56A) 109.5
C(55)-C(56)-H(56B) 109.5
H(56A)-C(56)-H(56B) 109.5
C(55)-C(56)-H(56C) 109.5
H(56A)-C(56)-H(56C) 109.5
H(56B)-C(56)-H(56C) 109.5
C(55)-C(57)-H(57A) 109.5
C(55)-C(57)-H(57B) 109.5
H(57A)-C(57)-H(57B) 109.5
C(55)-C(57)-H(57C) 109.5
H(57A)-C(57)-H(57C) 109.5
H(57B)-C(57)-H(57C) 109.5
C(55)-C(58)-H(58A) 109.5
C(55)-C(58)-H(58B) 109.5
H(58A)-C(58)-H(58B) 109.5
C(55)-C(58)-H(58C) 109.5
H(58A)-C(58)-H(58C) 109.5
H(58B)-C(58)-H(58C) 109.5
C(58')-C(55')-C(56') 108.7(14)
C(58')-C(55')-C(57') 109.0(14)
C(56')-C(55')-C(57') 108.7(14)
C(58')-C(55')-C(27) 114(2)
C(56')-C(55')-C(27) 111(2)
C(57')-C(55')-C(27) 106(2)
C(55')-C(56')-H(56D) 109.5
C(55')-C(56')-H(56E) 109.5
H(62A)-C(62)-H(62B) 109.5
C(59)-C(62)-H(62C) 109.5
H(62A)-C(62)-H(62C) 109.5
H(62B)-C(62)-H(62C) 109.5
C(64)-C(63)-C(68) 116.6(10)
C(64)-C(63)-Fe(1) 123.1(12)
C(68)-C(63)-Fe(1) 120.0(12)
C(63)-C(64)-C(65) 124.8(12)
C(63)-C(64)-H(64) 117.6
C(65)-C(64)-H(64) 117.6
C(66)-C(65)-C(64) 117.8(13)
C(66)-C(65)-H(65) 121.1
C(64)-C(65)-H(65) 121.1
C(67)-C(66)-C(65) 119.2(13)
C(67)-C(66)-H(66) 120.4
C(65)-C(66)-H(66) 120.4
C(66)-C(67)-C(68) 120.1(13)
C(66)-C(67)-H(67) 120.0
C(68)-C(67)-H(67) 120.0
C(63)-C(68)-C(67) 121.4(13)
C(63)-C(68)-H(68) 119.3
C(67)-C(68)-H(68) 119.3
C(64')-C(63')-C(68') 122(2)
C(64')-C(63')-Fe(1) 127(3)
C(68')-C(63')-Fe(1) 111(3)
C(63')-C(64')-C(65') 122(2)
C(63')-C(64')-H(64') 118.9
C(65')-C(64')-H(64') 118.9
C(66')-C(65')-C(64') 116(2)
C(66')-C(65')-H(65') 121.9
C(64')-C(65')-H(65') 121.9
C(67')-C(66')-C(65') 122(2)
C(67')-C(66')-H(66') 119.1
C(65')-C(66')-H(66') 119.1
C(66')-C(67')-C(68') 119(2)
C(66')-C(67')-H(67') 120.3
| Bond                  | Angle  |
|----------------------|--------|
| C(68')-C(67')-H(67') | 120.3  |
| C(63')-C(68')-C(67') | 118(2) |
| C(63')-C(68')-H(68') | 120.8  |
| C(67')-C(68')-H(68') | 120.8  |
| C(70)-C(69)-H(69A)   | 109.5  |
| C(70)-C(69)-H(69B)   | 109.5  |
| H(69A)-C(69)-H(69B)  | 109.5  |
| C(70)-C(69)-H(69C)   | 109.5  |
| H(69A)-C(69)-H(69C)  | 109.5  |
| H(69B)-C(69)-H(69C)  | 109.5  |
| O(1)-C(70)-C(69)     | 110.4(10) |
| O(1)-C(70)-H(70A)    | 109.6  |
| C(69)-C(70)-H(70A)   | 109.6  |
| O(1)-C(70)-H(70B)    | 109.6  |
| C(69)-C(70)-H(70B)   | 109.6  |
| H(70A)-C(70)-H(70B)  | 108.1  |
| C(71)-O(1)-C(70)     | 113.4(9) |
| O(1)-C(71)-C(72)     | 110.2(11) |
| O(1)-C(71)-H(71A)    | 109.6  |
| C(72)-C(71)-H(71A)   | 109.6  |
| O(1)-C(71)-H(71B)    | 109.6  |
| C(72)-C(71)-H(71B)   | 109.6  |
| H(71A)-C(71)-H(71B)  | 108.1  |
| C(71)-C(72)-H(72A)   | 109.5  |
| C(71)-C(72)-H(72B)   | 109.5  |
| H(72A)-C(72)-H(72B)  | 109.5  |
| C(71)-C(72)-H(72C)   | 109.5  |
| H(72A)-C(72)-H(72C)  | 109.5  |
| H(72B)-C(72)-H(72C)  | 109.5  |