



Supporting Information

Synthesis and Structural Characterization of a Non-Heme Iron Hyponitrite Complex

*M. O. Lengel, H. T. Dong, N. Lehnert**

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Experimental Section

General Considerations

Reactions were generally performed using inert gas (Schlenk) techniques or an MBraun glovebox, equipped with a circulating purifier (O₂, H₂O <0.1 ppm). All solvents and chemicals were purchased from Fisher Scientific unless stated otherwise. All chemicals were used as received unless otherwise noted. Calcium hydride (90-95%) and Iron(II) trifluoromethanesulfonate (Fe(OTf)₂) (98%) were purchased from Strem. Di(2-picolyl)amine was purchased either from Sigma-Aldrich (97%), TCI (98%), or AmBeed (>97%). Pyridine-2-carbaldehyde (97%) was purchased from Oakwood Chemical. Potassium methoxide (95%) was purchased from Sigma-Aldrich. Lithium bis(trimethylsilyl)amide was purchased from Sigma-Aldrich. Tetrahydrofuran and diethyl ether were dried by distillation from Na/benzophenone, freeze pump thawed, and stored over 4 Å molecular sieves in the glovebox. Dichloromethane, hexanes, 1,2-dichloroethane, and pentanes were dried by distillation from CaH₂, freeze pump thawed and stored over 4 Å molecular sieves in the glovebox. Methanol and acetonitrile were dried by distillation from CaH₂,

freeze pump thawed and stored over 3 Å molecular sieves in the glovebox. Sodium *trans*-hyponitrite x-hydrate was purchased from Sigma-Aldrich and either used directly as the hydrate or dried over P₂O₅ at room temperature under vacuum and again over P₂O₅ at 120 °C under vacuum to obtain the anhydrous salt. ¹⁵N-sodium *trans*-hyponitrite¹ was prepared as previously described. Tris(2-pyridylmethyl)amine (TPA)² was prepared as previously described but was purified by recrystallization from diethyl ether instead of by column chromatography.

Infrared spectra of solid samples were obtained using PerkinElmer BX spectrometer. Gas IR spectra were obtained using a Pike Technologies short-path HT gas cell with 100 mm path length, equipped with CaF₂ windows, on the same instrument.

UV-Vis absorption spectra were measured using an Analytic Jena Specord S600 UV-Vis spectrometer.

¹H-NMR spectra were recorded on a Varian Inova 400 MHz or a Varian Inova 600 MHz instrument and referenced against residual solvent signals or tetramethylsilane (TMS).

Elemental analysis: Elemental analyses were conducted by Atlantic Microlabs (Norcross, GA).

IR Gas Headspace Analysis for N₂O Detection: N₂O quantification was carried out by gas headspace analysis using infrared spectroscopy. The general protocol has been described previously by our group.^{3,4} The calibration curve used for quantitative analysis has been recently described for our gas IR cell.⁴

Syntheses.

2-((Bis(pyridin-2-ylmethyl)amino)methyl)phenol (BMPA-PhOH) was synthesized by a modified literature procedure.⁵ Under a nitrogen atmosphere, 2.511 grams (12.60 mmol) of di(2-picolyl)amine were dissolved in 50 mL of 1,2-dichloroethane (DCE) and added to a round bottom flask. Salicylaldehyde (1.6224 grams, 13.29 mmol) was dissolved in 50 mL of DCE and added to the round bottom flask. After stirring for 2.5 hours, sodium triacetoxyborohydride (4.0762 grams, 19.23 mmol) was added. The reaction was allowed to stir overnight under an N₂ atmosphere. The reaction mixture was then transferred to an Erlenmeyer flask and saturated sodium bicarbonate was added. The biphasic mixture was vigorously stirred for 1 hour. The biphasic mixture was then transferred to a separation funnel and the organic layer was collected. The aqueous layer was extracted three times with 100 mL portions of dichloromethane. The organic layers were combined, dried over sodium sulfate, and then concentrated by rotary evaporation to yield a

yellow-orange oil. Crude yield: 96%. Upon further drying on the Schlenk line under vacuum at 100°C overnight and then letting the oil sit for several hours at room temperature, a solid can be obtained. The solid can then be ground into a yellow powder. Alternatively, after further drying, the oil can be rapidly solidified by placing it in a dry ice/acetone bath to flash freeze the oil, crushing up the frozen oil, and rapidly transferring it to another vessel. Yield: 58.5%. The ^1H -NMR spectrum (400 MHz, Chloroform-*d*) of the ligand is shown in Figure S1. The ATR-IR spectrum of the ligand is shown in Figure S6. Elemental analysis calculated for $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}$: C, 74.73; H, 6.27; N, 13.76; found (%): C, 74.60; H, 6.37; N, 13.75.

Lithium 2-((bis(pyridin-2-ylmethyl)amino)methyl)phenolate (Li[BMPA-PhO]) was synthesized by deprotonation of BMPA-PhOH with lithium bis(trimethylsilyl)amide (LiHMDS). In an N_2 atmosphere in the glovebox, 0.5020 grams (1.64 mmol) BMPA-PhOH were dissolved in 2 mL of THF. A solution of 0.2760 grams (1.65 mmol) LiHMDS dissolved in 2 mL of THF was then added dropwise to the BMPA-PhOH solution. The salt of the deprotonated ligand then precipitated from solution. The product was collected and filtered on a fine frit and washed with diethyl ether to afford a fine white powder. Yield: 77.1% (^1H -NMR spectrum (400 MHz, Chloroform-*d*) of the ligand is shown in Figure S2. The ATR IR spectrum of the ligand is shown in Figure S7. Elemental analysis calculated for $\text{C}_{19}\text{H}_{18}\text{LiN}_3\text{O}$: C, 73.31; H, 5.83; N, 13.50; found (%): C, 72.82; H, 5.79; N, 13.32.

$[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2](\text{OTf})_2$: Under an inert atmosphere, $[\text{Fe}(\text{TPA})(\text{CH}_3\text{CN})_2](\text{OTf})_2$ was dissolved in a minimal amount of methanol in a 20 ml scintillation vial charged with a stir bar. An excess amount of $\text{Na}_2\text{N}_2\text{O}_2 \cdot x\text{-hydrate}$ was then added to the solution. An immediate color change of the solution to red-orange was observed (UV-Vis, 321 nm (shoulder) and 444 nm, obtained in MeOH from diluting the reaction mixture, see Figure S11). The reaction was allowed to stir overnight and the product was then collected through recrystallization with diethyl ether. Single crystals suitable for X-ray diffraction were obtained via slow diffusion of diethyl ether into an acetonitrile solution of the complex at 25°C. Despite several attempts, we were unable to obtain elementally pure material of the bulk sample. We hypothesize that at least two products are actually formed during this reaction, $[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2](\text{OTf})_2$ and $[\text{Fe}_2(\text{TPA})_2(\text{OH})_2](\text{OTf})_2$ (and potentially a mixed-ligand complex), based on the decomposition of $\text{Na}_2\text{N}_2\text{O}_2 \cdot x\text{-hydrate}$ to form sodium methoxide and sodium hydroxide. We hypothesize that triflate may further compete for binding to the iron centers, leading to a mixture of starting material and products.

A direct synthesis of $[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2]\text{X}_2$ (with PF_6^- instead of OTf^-) was achieved by reacting 104.5 mg (0.15 mmol) $[\text{Fe}(\text{TPA})(\text{CH}_3\text{CN})_2](\text{PF}_6)_2$ with 11.7 mg (0.17 mmol) KOMe directly in methanol. Methanol was then removed under reduced pressure and the resulting crude solid was redissolved in CH_2Cl_2 . The mixture was then filtered through celite to remove KPF_6 . The solvent was removed under reduced pressure and the product was dried at 70 °C overnight under vacuum. Yield: 58.4 mg (76.8%). Elemental anal. calcd. for $\text{C}_{40}\text{H}_{42}\text{F}_6\text{Fe}_2\text{N}_8\text{O}_8\text{S}_2$: C, 43.70; H, 4.05; N, 10.73; found (%): C, 42.98; H, 3.89; N, 10.55. UV-Vis (MeOH) 321 nm (shoulder) and 444 nm, Figure S13.

$[\text{Fe}_2(\text{TPA})_2(\text{NO})_2](\text{OTf})_2$: under an inert atmosphere, $[\text{Fe}(\text{TPA})(\text{CH}_3\text{CN})_2](\text{OTf})_2$ was dissolved in CH_3CN in a 20 ml scintillation vial charged with a stir bar. $\text{Na}_2\text{N}_2\text{O}_2$ (anhydrous) was then added to the solution. The reaction was allowed to stir for 3 weeks. The resulting solid was collected and characterized by IR spectroscopy. IR: 1350 (1325 cm^{-1} upon ^{15}N labelling in the mixed isotope experiment, Figure S9). The observed N-O stretching frequency is in agreement with a previous report for the same compound, $[\text{Fe}_2(\text{TPA})_2(\text{NO})_2](\text{OTf})_2$.⁶ Note that significant amounts of starting material are present in the product, based on UV-Vis spectroscopic data. Attempts at elemental analysis for the bulk material were unsuccessful, indicating that although this reaction occurs, it does not go to completion, likely due to the heterogeneous nature of this reaction.

$[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$ (2): Route A: under an inert atmosphere, 566 mg (1.85 mmol) BMPA-PhOH and 129 mg (1.84 mmol) potassium methoxide were combined in 5 mL MeOH. The resulting suspension was stirred for several minutes, and 599 mg (1.69 mmol) $[\text{Fe}(\text{OTf})_2 \cdot 2\text{MeCN}]$ was then added. The reaction mixture was stirred for 45 min, then filtered. Diethyl ether was added to the filtrate, causing a yellow solid to precipitate. The product was allowed to precipitate at -33 °C overnight. The yellow solid was isolated by vacuum filtration and recrystallized from CH_2Cl_2 /hexanes. Yield: 593 mg, 63%. Elemental analysis: Expected: C: 47.17, H: 3.56, N: 8.25; Found: C: 47.03, H: 3.75, N: 8.13. **Route B:** under an inert atmosphere, 304.5 mg (0.98 mmol) $\text{Li}[\text{BMPA-PhO}]$ and 426.3 mg (0.98 mmol) $[\text{Fe}(\text{OTf})_2 \cdot 2\text{MeCN}]$ were suspended together in 6 mL of THF and stirred for two hours. The product precipitated out of solution as a bright yellow solid. The product was isolated on a frit and washed with diethyl ether and copious amounts of THF to wash away any residual LiOTf . Yield: 398.2 mg, 80%. Elemental analysis: Expected: C: 47.17, H:

3.56, N: 8.25; Found: C: 47.01, H: 3.46, N: 8.13 Experimental data for this complex matches the previously reported data.⁵

[{Fe₂(BMPA-PhO)₂}₂(μ-N₂O₂)](OTf)₂ (3-OTf): Under an inert atmosphere, 2.701 grams (2.65 mmol) [Fe₂(BMPA-PhO)₂(OTf)₂] were dissolved in CH₃CN in a 20 ml scintillation vial charged with a stir bar. This solution was then added to a vial containing 0.5206 grams (2.65 mmol, assuming MW = 196.09) Na₂N₂O₂ • x-hydrate, and the reaction was allowed to stir overnight. The solution was then filtered through celite and the solvent was removed under vacuum. The product was re-suspended in CH₂Cl₂ and filtered through celite to remove NaOTf. The filtrate was dried under vacuum to yield a red-orange solid. The product can be recrystallized from acetonitrile and diethyl ether by slow diffusion of diethyl ether into an acetonitrile solution of the compound at -33 °C, to obtain single crystals that are suitable for X-ray diffraction. Yield: 74% Elemental analysis: Expected: C: 52.08, H: 4.03, N: 10.90; Found: C: 51.62, 4.16, 10.57 IR 1070 cm⁻¹ (1062 cm⁻¹, ¹⁵N-labelled), UV-Vis (CH₃CN) 451 nm. ¹H-NMR (Figure S3)

[{Fe₂(BMPA-PhO)₂}₂(μ-N₂O₂)](BArF)₂ (3-BArF): Under an inert atmosphere, 97.1 mg (0.095 mmol) of [Fe₂(BMPA-PhO)₂(OTf)₂] were suspended in diethyl ether. A solution containing 168.6 mg (0.19 mmol) of NaBArF in diethyl ether was then added. The solution was stirred for 1 hour and then filtered through a 0.22 μm syringe filter. The solvent was removed under vacuum. The resulting solid was redissolved in MeCN, and 23.7 mg (0.22 mmol) Na₂N₂O₂ (anhydrous) were added. The reaction was stirred for 2 days. The solution was then filtered and the solvent was removed under vacuum. Single crystals of the product were grown by a slow diffusion of pentanes into a solution of the material in benzene at room temperature. No other characterization was obtained as the structure is the same as that of **3-OTf** (with different counter ions). All physical characterization was obtained for **3-OTf**.

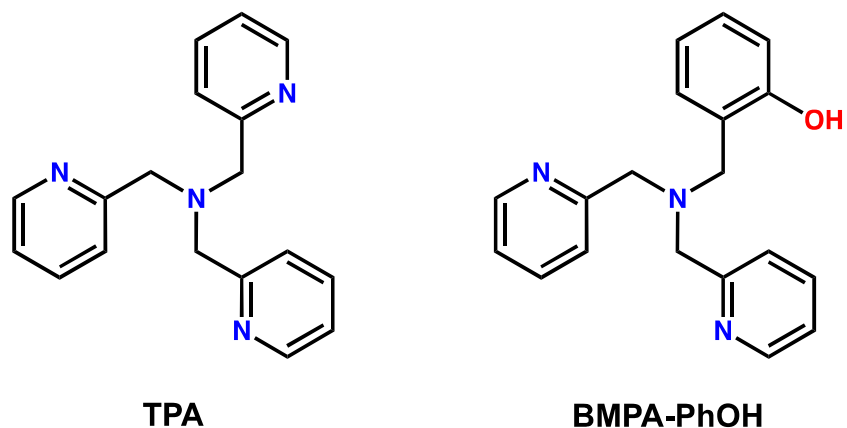


Figure S1. ChemDraw representation of the TPA ligand (left) and the BPPA-PhOH ligand (right) used in this study.

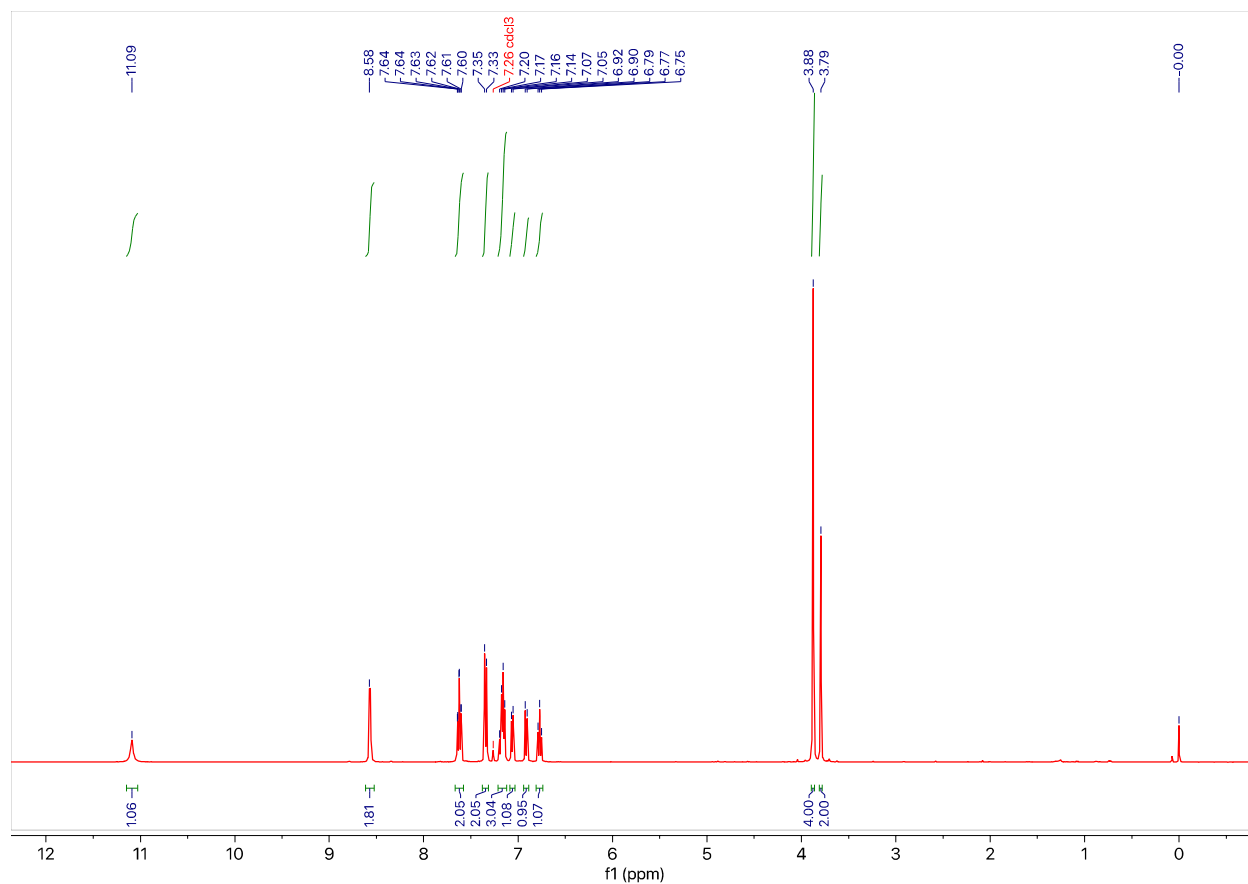


Figure S2. ^1H -NMR spectrum of 2-((bis(pyridin-2-ylmethyl)amino)methyl)phenol (BPPA-PhOH) measured at room temperature. ^1H NMR (401 MHz, Chloroform- d) δ 11.09 (s, 1H), 8.58 (s, 2H), 7.62 (td, J = 7.7, 1.6 Hz, 2H), 7.34 (d, J = 7.8 Hz, 2H), 7.17 (q, J = 8.3, 7.0 Hz, 3H), 7.06 (d, J = 7.1 Hz, 1H), 6.91 (d, J = 8.1 Hz, 1H), 6.77 (t, J = 7.3 Hz, 1H), 3.88 (s, 4H), 3.79 (s, 2H).

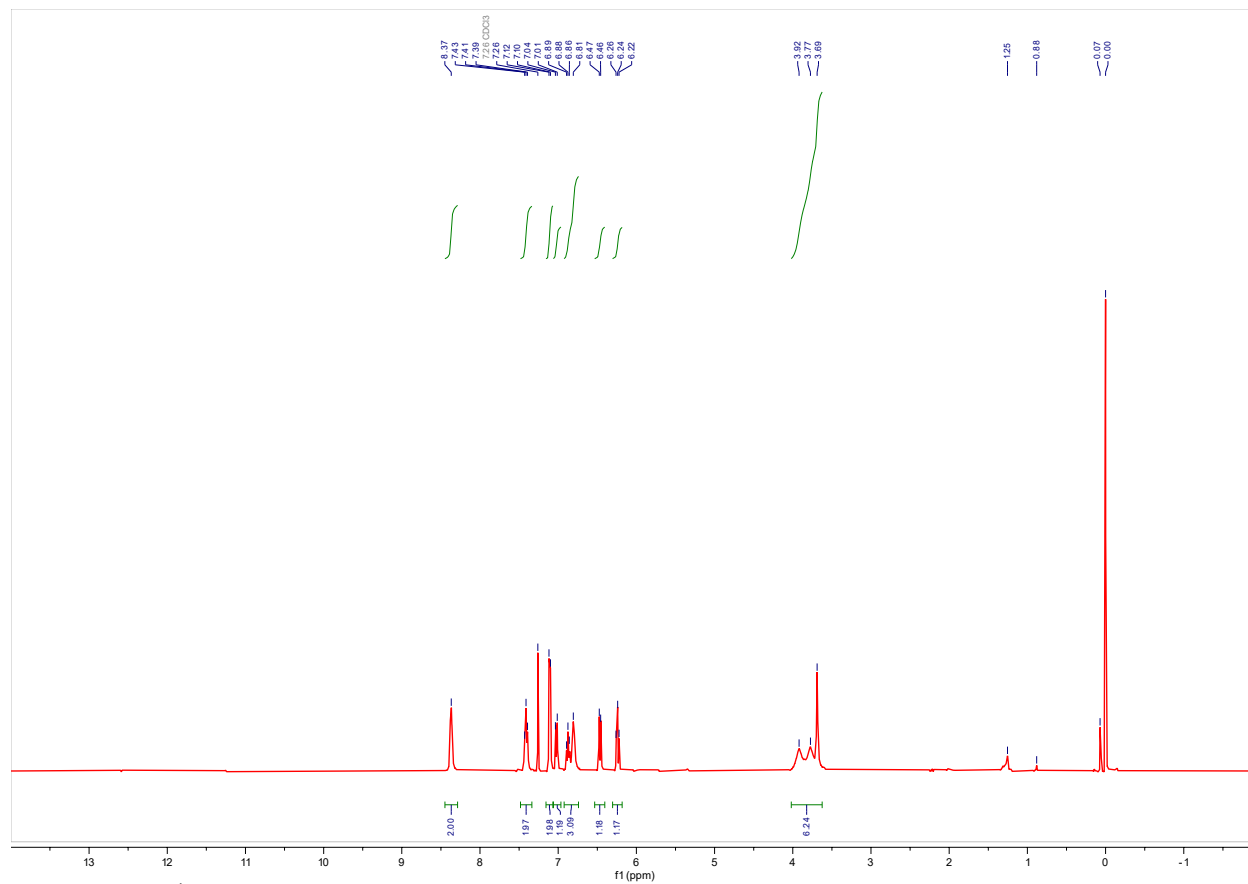


Figure S3. ^1H -NMR spectrum of lithium 2-((bis(pyridin-2-ylmethyl)amino)methyl)phenolate (Li[BMPA-PhO]) at room temperature. ^1H NMR (400 MHz, Chloroform- d) δ 8.37 (s, 2H), 7.41 (t, J = 7.2 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 7.02 (d, J = 9.1 Hz, 1H), 6.92 – 6.74 (m, 3H), 6.47 (d, J = 7.1 Hz, 1H), 6.24 (t, J = 7.8 Hz, 1H), 4.02 – 3.62 (m, 6H).

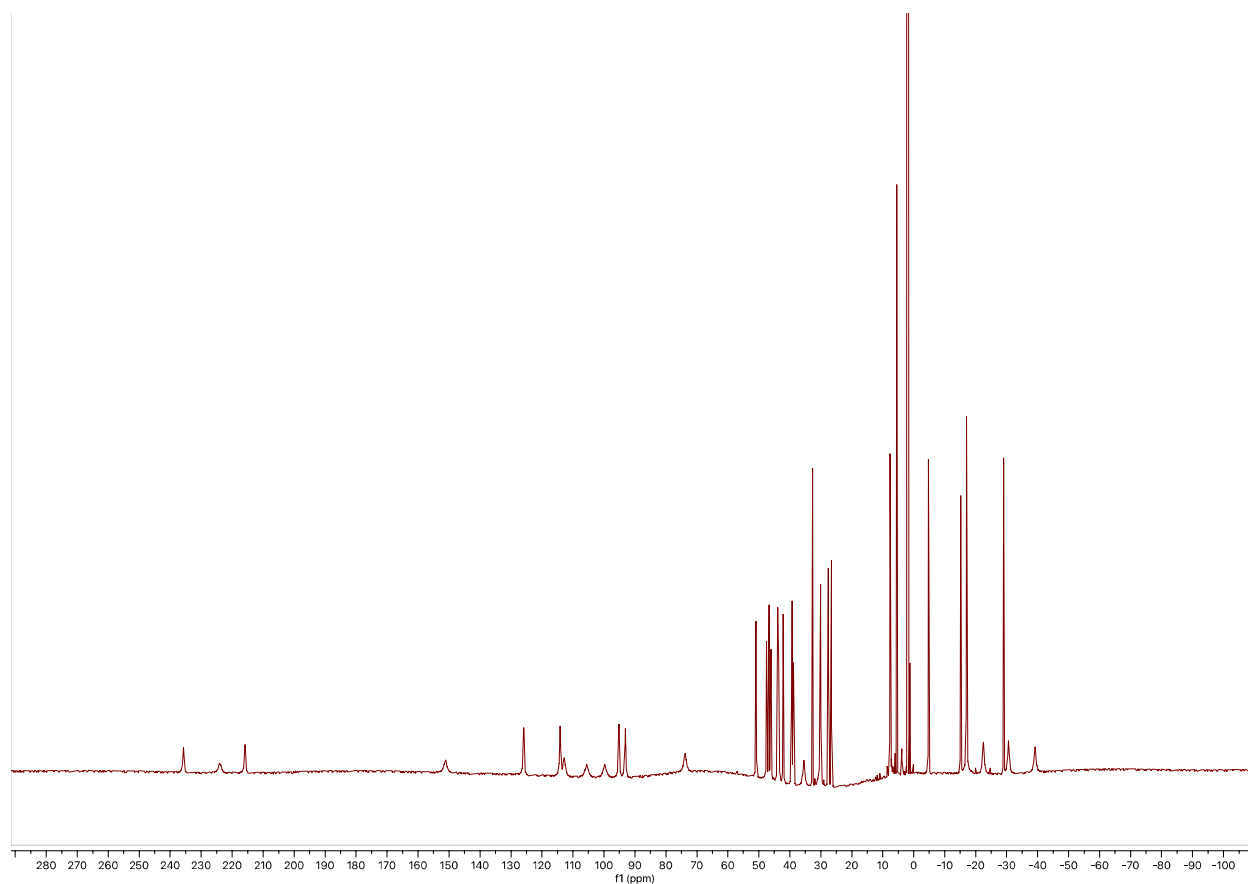


Figure S4. ^1H -NMR spectrum of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$ at room temperature in CD_3CN .

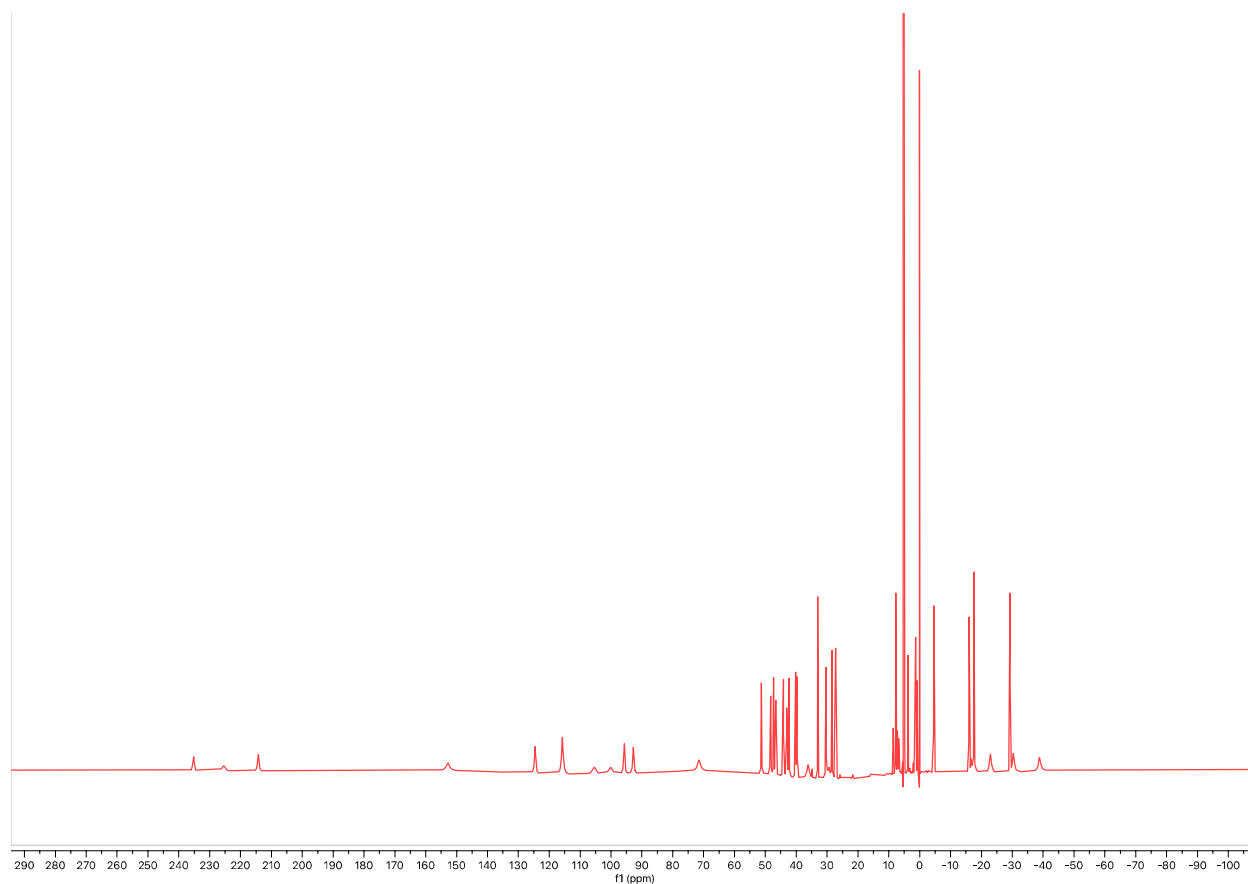


Figure S5. ^1H -NMR spectrum of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$ at room temperature in CD_2Cl_2 .

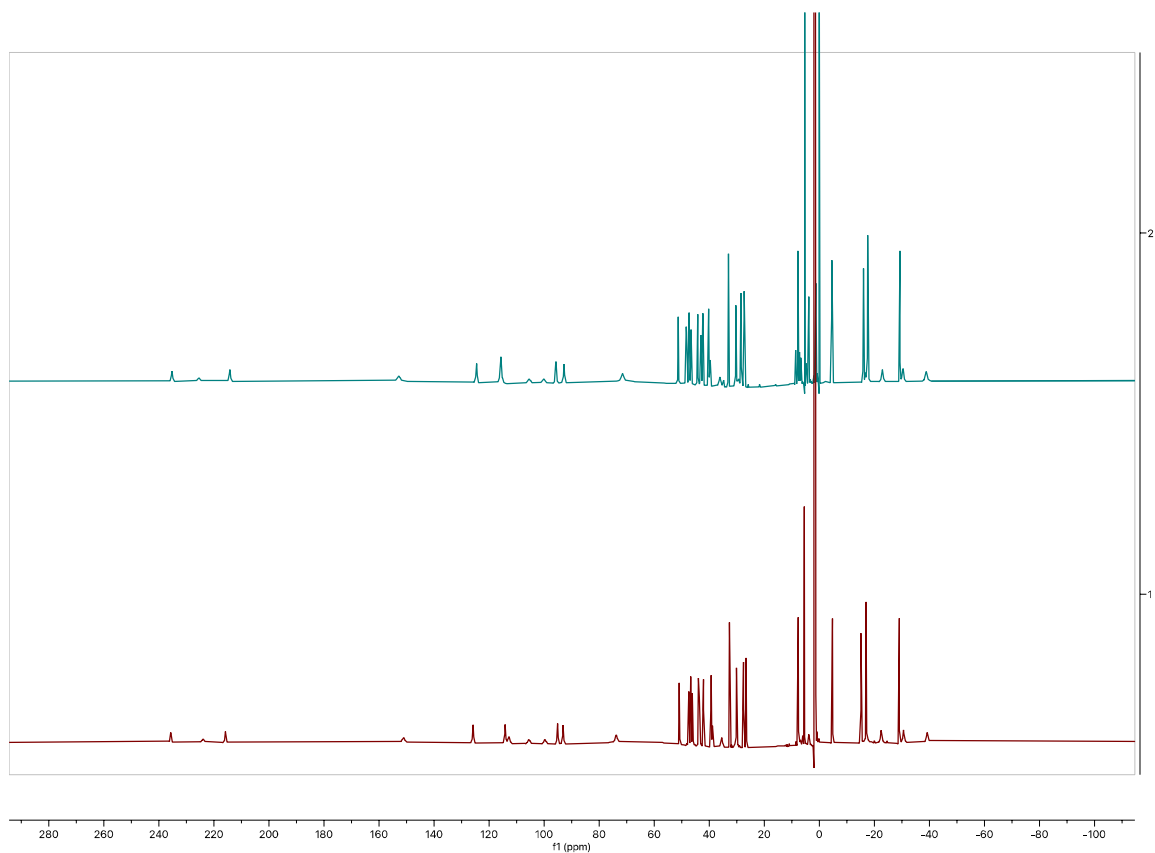


Figure S6. Stacked ¹H-NMR spectra of [$\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)\](OTf)₂ at room temperature in CD₂Cl₂ (top) and CD₃CN (bottom), indicating that [$\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)\](OTf)₂ remains a tetranuclear structure, even in the presence of coordinating solvents.$$

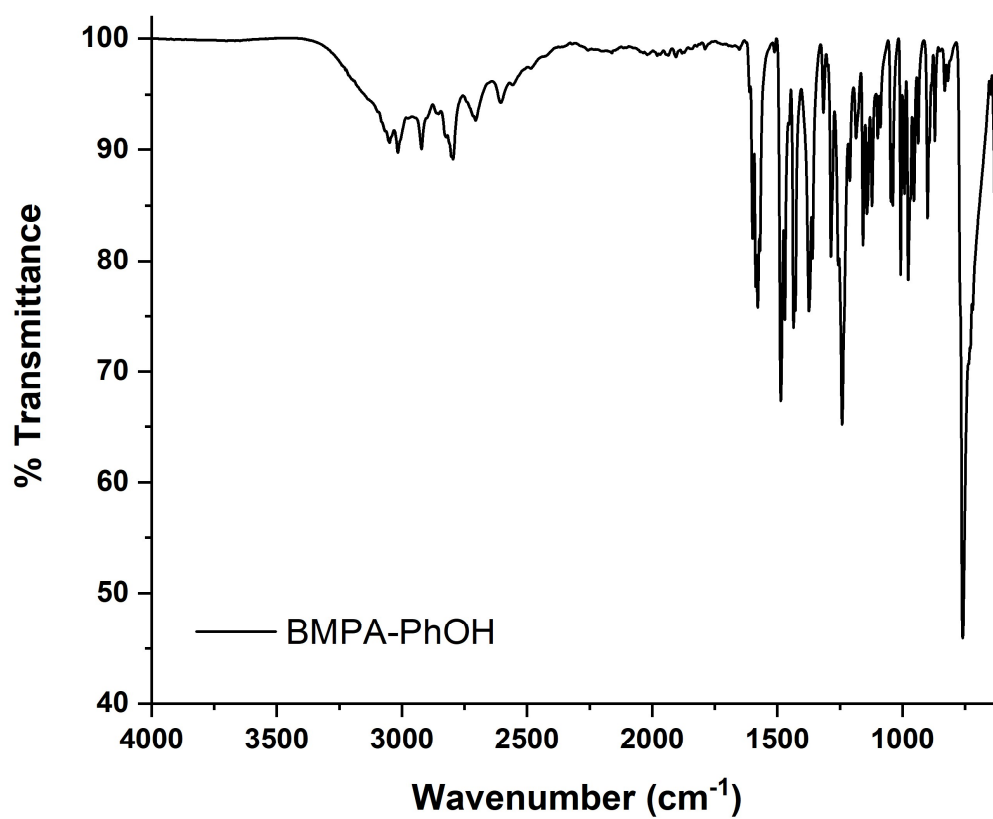


Figure S7. ATR-IR spectrum of 2-((bis(pyridin-2-ylmethyl)amino)methyl)phenol (BMPA-PhOH) at room temperature.

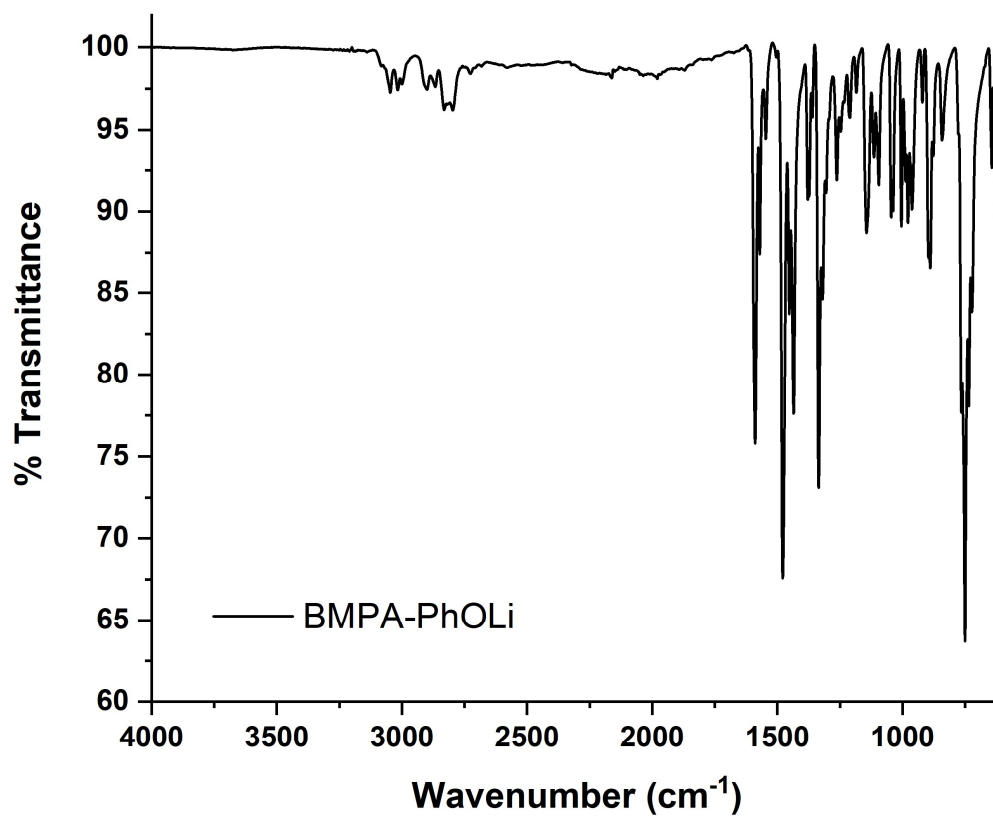


Figure S8. ATR-IR spectrum of lithium 2-((bis(pyridin-2-ylmethyl)amino)methyl)phenolate (Li[BMPA-PhO]) at room temperature.

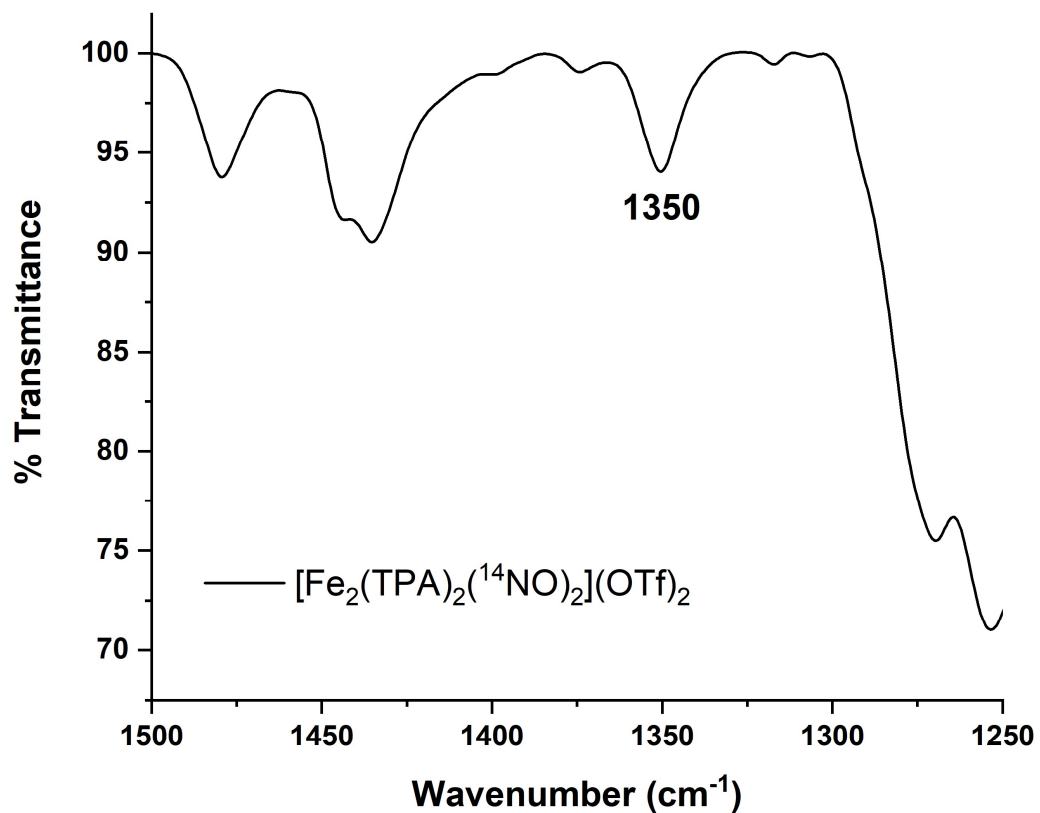


Figure S9. IR spectrum of $[\text{Fe}_2(\text{TPA})_2(^{14}\text{NO})_2](\text{OTf})_2$, formed from reacting sodium trans-hyponitrite (anhydrous) and $[\text{Fe}(\text{TPA})\cdot 2\text{MeCN}](\text{OTf})_2$, at room temperature, with the characteristic N-O stretching frequency of $[\text{Fe}_2(\text{TPA})_2(^{14}\text{NO})_2]^{2+}$ at 1350 cm^{-1} .

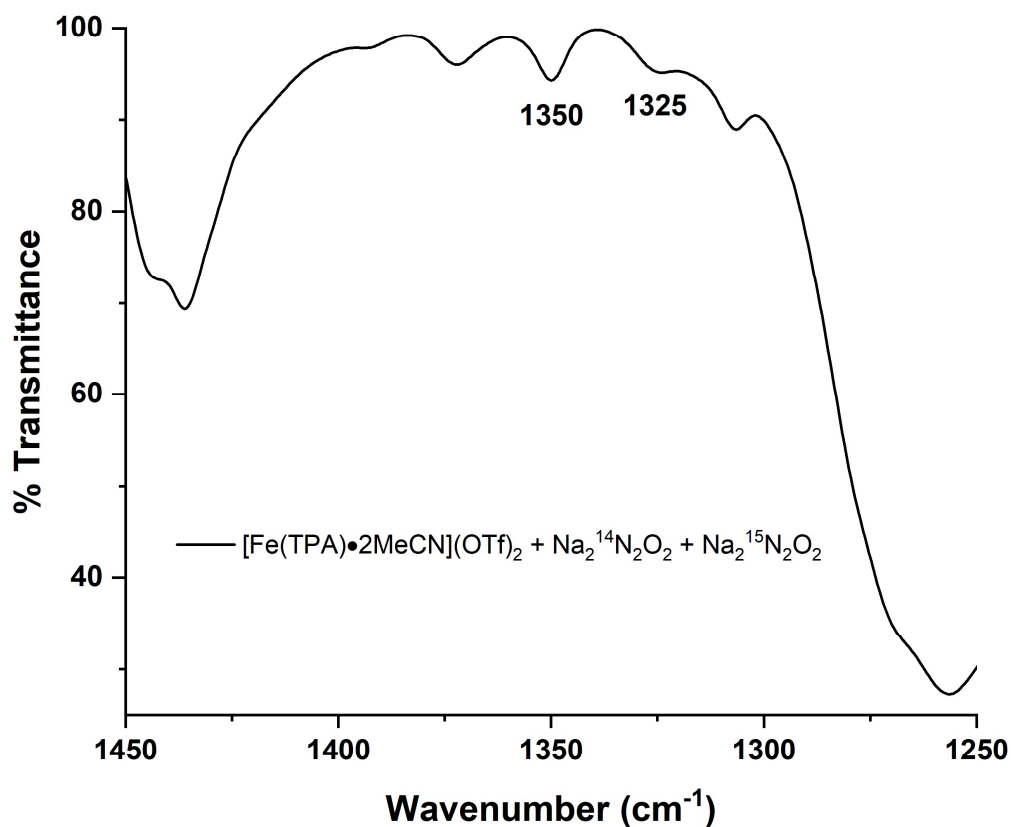


Figure S10: IR spectrum of the reaction product of the isotopic scrambling experiment where a ~1:1 mixture of ^{14/15}N-sodium *trans*-hyponitrite (anhydrous) is reacted with $[\text{Fe}(\text{TPA})\cdot 2\text{MeCN}](\text{OTf})_2$. Characteristic peaks at 1350 cm⁻¹ and 1325 cm⁻¹, corresponding to $[\text{Fe}_2(\text{TPA})_2(^{14}\text{NO})_2](\text{OTf})_2$ and $[\text{Fe}_2(\text{TPA})_2(^{15}\text{NO})_2](\text{OTf})_2$, respectively, are observed. The spectrum shows no evidence for the formation of the mixed isomer species, $[\text{Fe}_2(\text{TPA})_2(^{14}\text{NO})(^{15}\text{NO})](\text{OTf})_2$. The spectrum was obtained at room temperature.

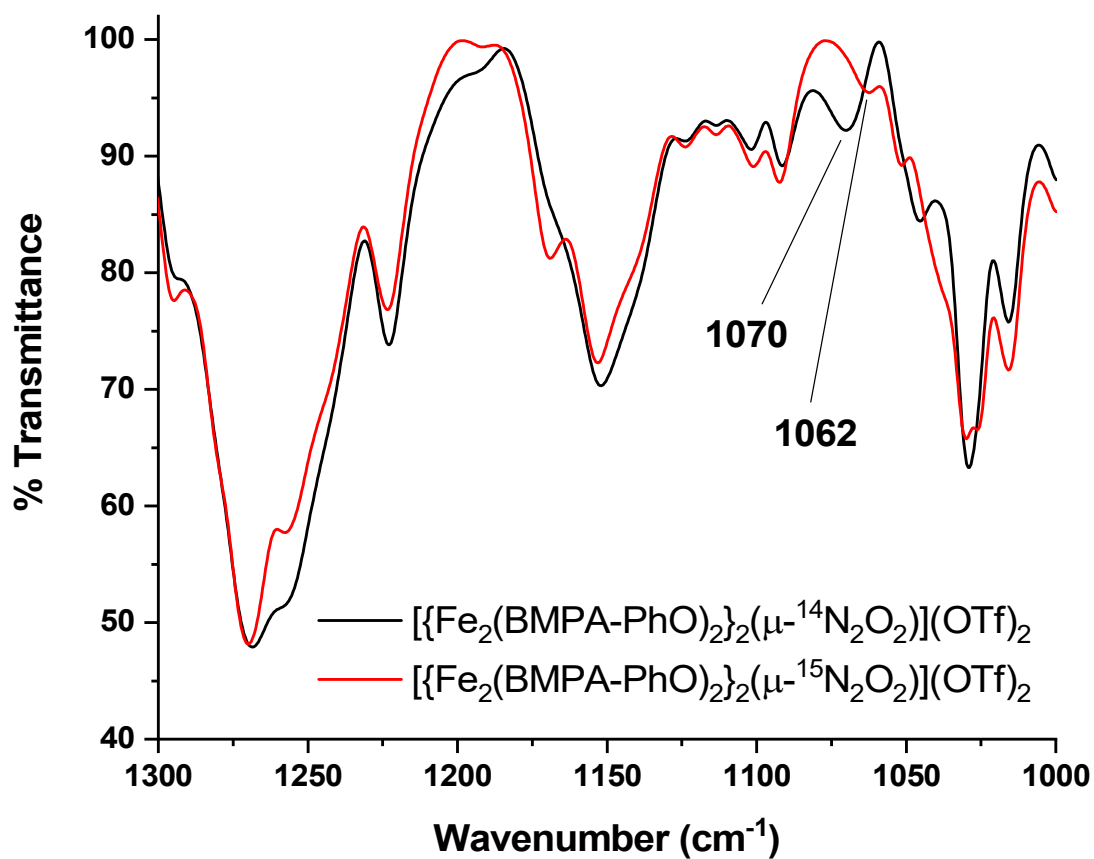


Figure S11. Overlay of the FT-IR spectra of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-}^{14}\text{N}_2\text{O}_2)](\text{OTf})_2$ (black) and $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-}^{15}\text{N}_2\text{O}_2)](\text{OTf})_2$ (red), obtained at room temperature.

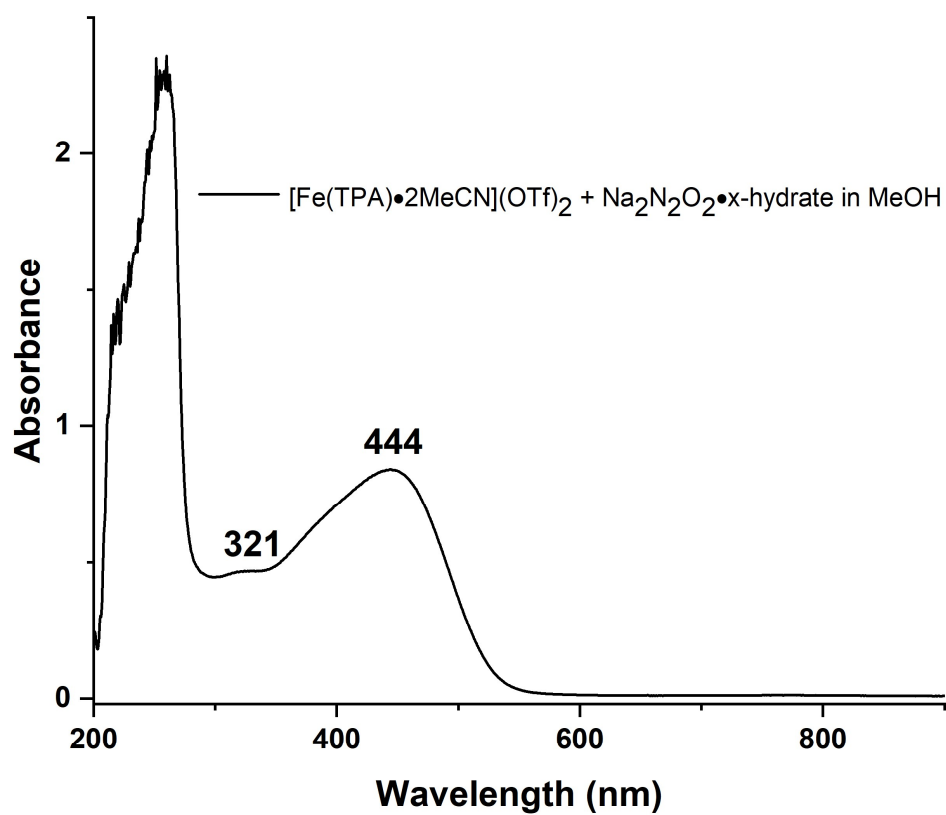


Figure S12. UV-Vis spectrum recorded at room temperature of the diluted reaction mixture of $[\text{Fe}(\text{TPA})\cdot 2\text{MeCN}](\text{OTf})_2 + \text{Na}_2\text{N}_2\text{O}_2\cdot x\text{-hydrate}$ in MeOH after 2 hours of stirring.

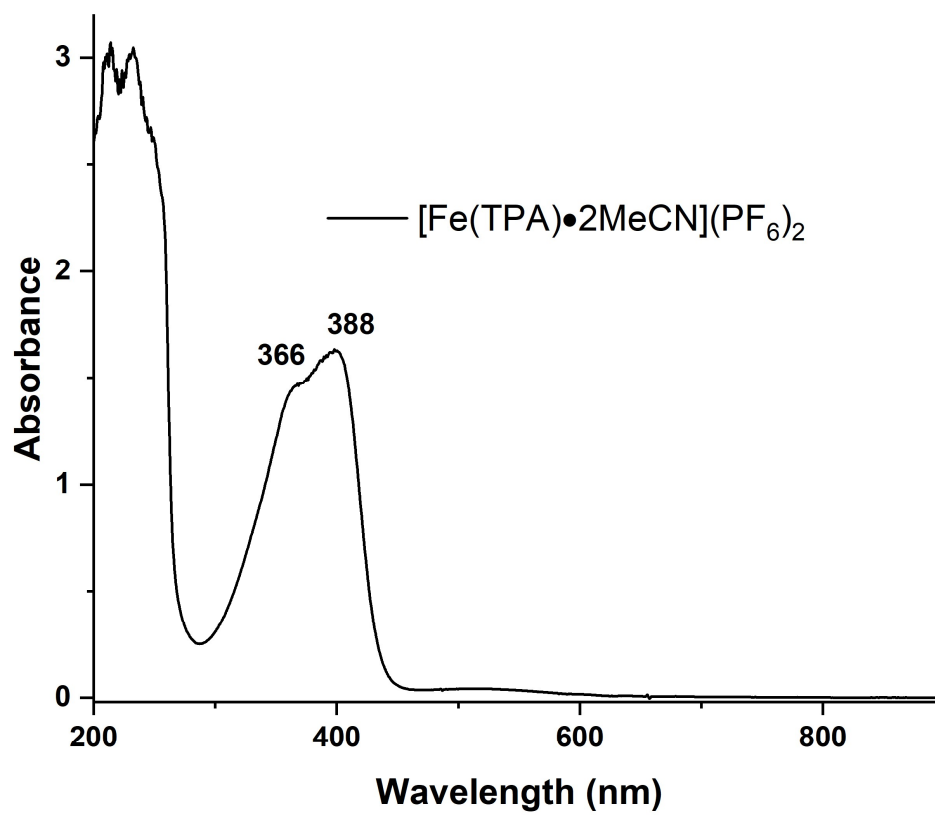


Figure S13. UV-Vis spectrum recorded at room temperature of $[\text{Fe}(\text{TPA})\cdot 2\text{MeCN}](\text{PF}_6)_2$ in MeCN.

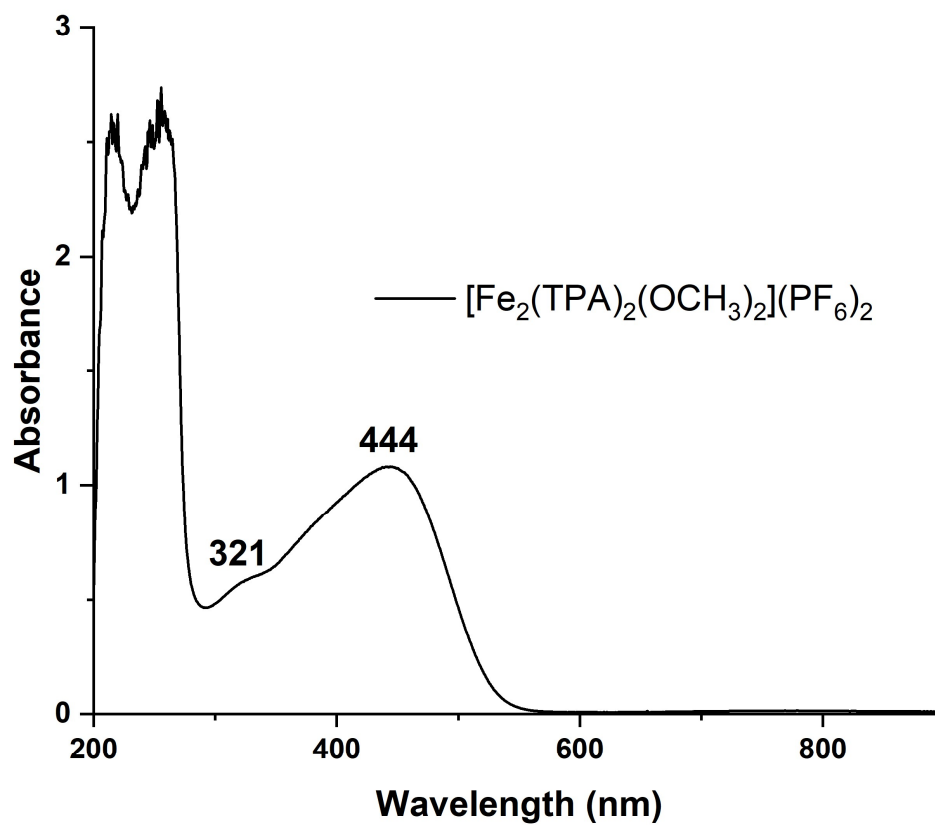


Figure S14. UV-Vis spectrum recorded at room temperature of $[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2](\text{PF}_6)_2$ in MeOH, prepared directly from $[\text{Fe}(\text{TPA})\cdot 2\text{MeCN}](\text{PF}_6)_2$ and KOMe.

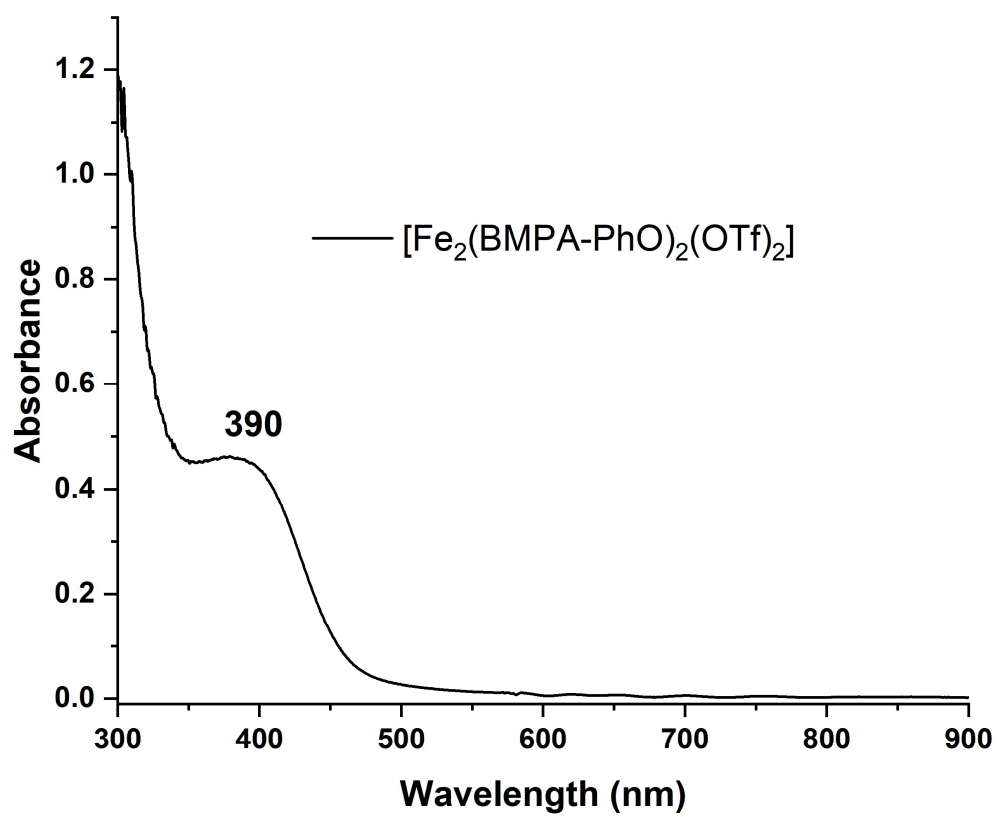


Figure S15. UV-Vis spectrum recorded at room temperature of $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$ in MeCN.

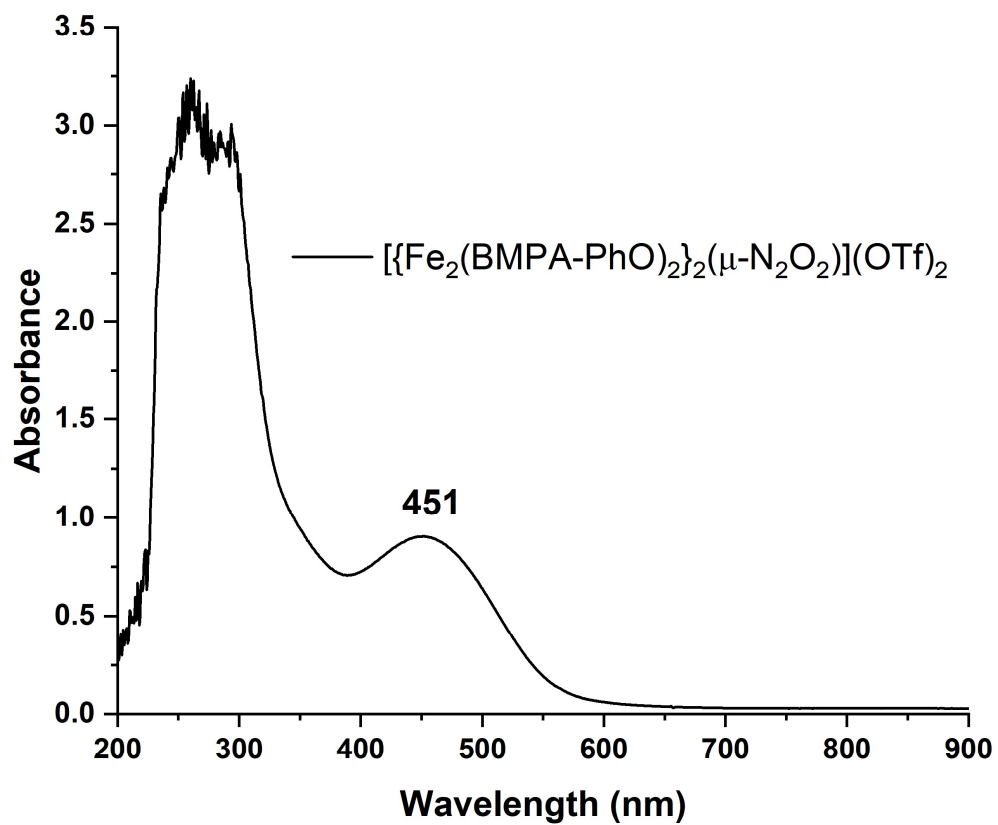


Figure S16. UV-Vis spectrum recorded at room temperature of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$ in MeCN.

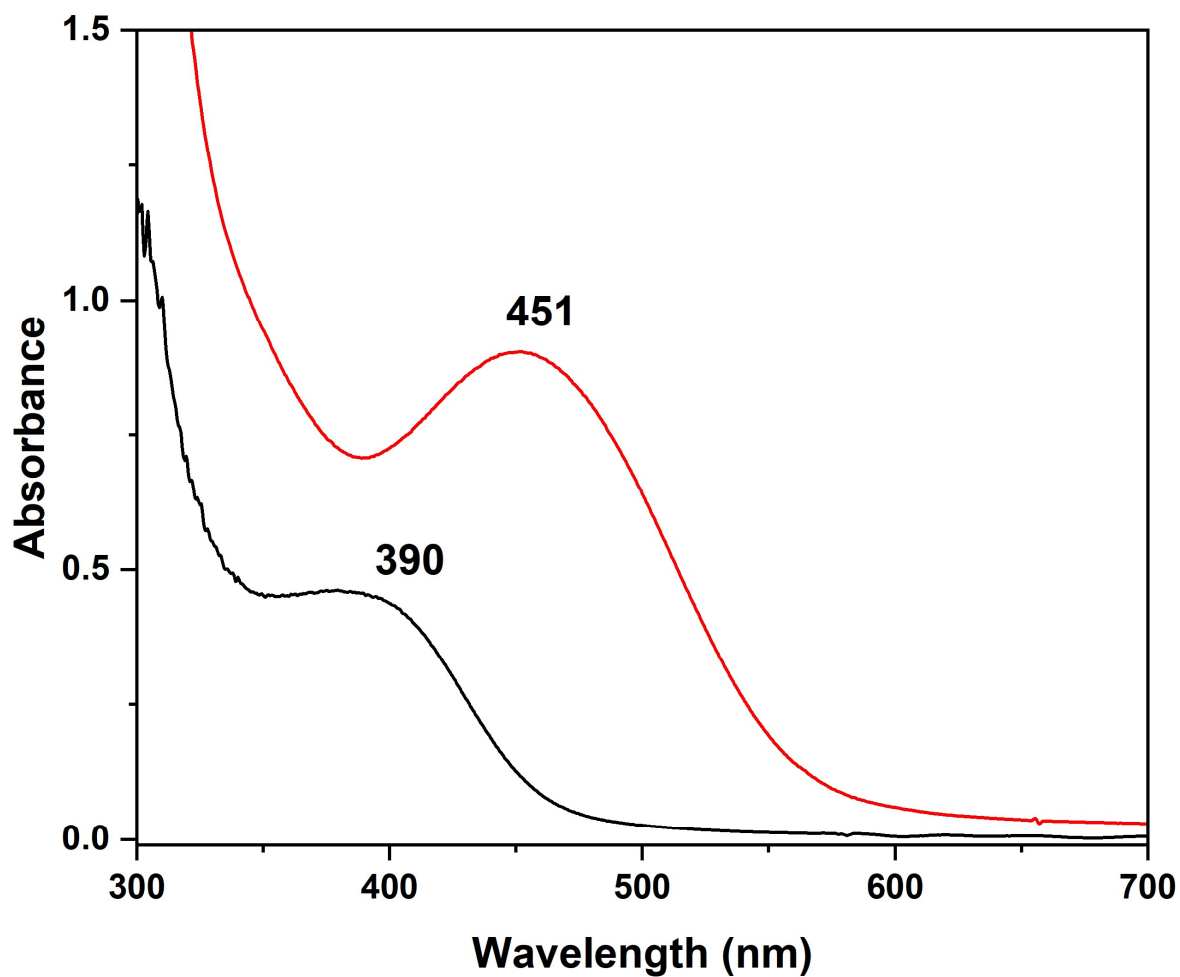


Figure S17. Overlay of the UV-Vis spectra of $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$ (black) and $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$ (red) taken in MeCN at room temperature.

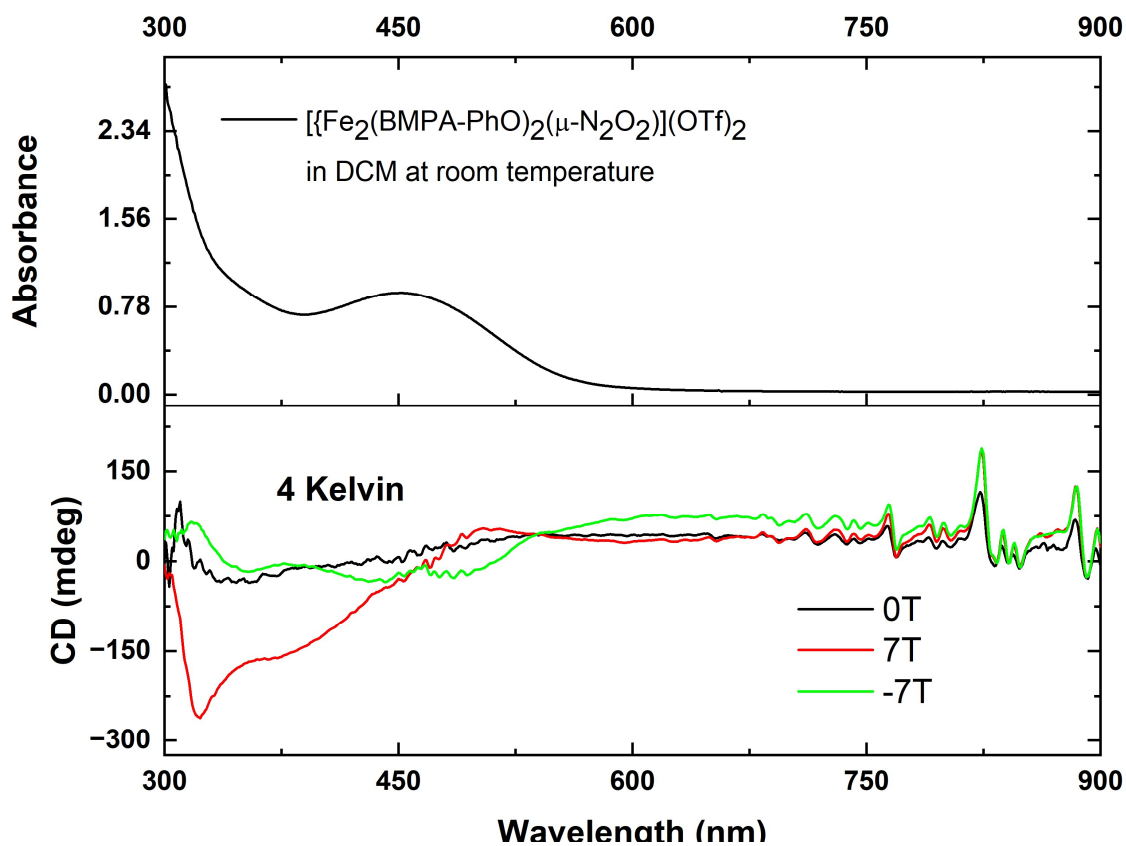


Figure S18. UV-Vis (top, recorded at room temperature in dichloromethane) and Magnetic Circular Dichroism (MCD) (bottom, recorded at 4 K) spectra of **3-OTf**, indicating a diamagnetic ground state evident from the lack of an MCD signal for the absorption band of the compound at 451 nm at 4 K.

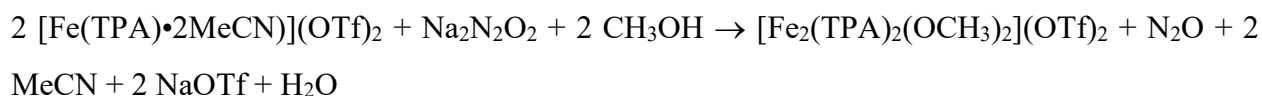
N₂O Yields

Table S1. N₂O yields of [Fe(TPA)•2MeCN](OTf)₂ + Na₂N₂O₂ (anhydrous) in MeOH, and of Na₂N₂O₂ (anhydrous) dissolved in MeOH, after 3 hours.

Reaction Mixture	% N ₂ O yield observed (based on hyponitrite used)
[Fe(TPA)•2MeCN](OTf) ₂ + Na ₂ N ₂ O ₂ (anhydrous) + MeOH	83% ± 1.4%
Na ₂ N ₂ O ₂ (anhydrous) + MeOH	67% ± 11%

* Each experiment was taken in duplicate. Note that standard deviation is high for these experiments due to the difficulty of accurately weighing 1.5 mg of sodium *trans*-hyponitrite for these experiments.

Scheme S1. Proposed Reactivity of Na₂N₂O₂ with methanol in the presence of [Fe(TPA)•2MeCN](OTf)₂.



Scheme S2. Proposed Reactivity of Na₂N₂O₂ with methanol only.

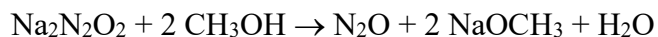


Table S2. N₂O yields of **3-OTf** after 2 hours of stirring with different equiv.s of HBArF in dichloromethane. Average and standard deviation obtained from triplicate experiments.

Equivalents of HBArF	% N ₂ O Yield Averaged
1	5.9% ± 1.7%
2	19.9% ± 4.3%
3	31.1% ± 3.6%
4	60.2% ± 2.1%
5	93% ± 5.3%

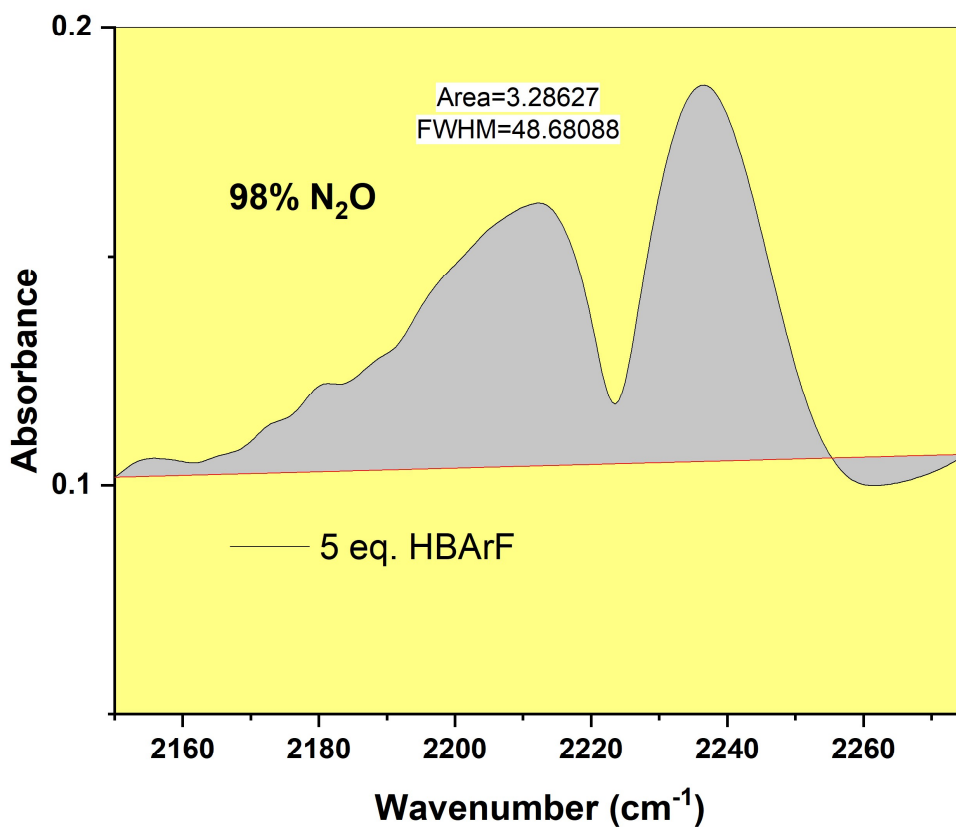


Figure S19. Representative gas-phase IR spectrum for N₂O yield determination, obtained from the reaction of 5 equiv.s of HBArF and **3-OTf** after 2 hours.

Table S3. N₂O yields of **3-OTf** at different time points using 5 equiv.s of HBArF in dichloromethane. Average and standard deviation obtained from triplicate experiments.

Reaction Time	% N ₂ O Yield Averaged
15 minutes	55.4% ± 7.8%
30 minutes	99% ± 2.5%
60 minutes	100.9% ± 7.5%
120 minutes	93% ± 5.3%

Table S4. N₂O yields of **3-OTf** from the reaction with 1 and 2 equiv.s of ferrocenium hexafluorophosphate (FcPF₆) as a chemical oxidant in dichloromethane after 2 hours of stirring. Average and standard deviation obtained from triplicate experiments.

Equivalents of FcPF ₆	% N ₂ O Yield Averaged
1	22.7% ± 1.5%
2	109% ± 2%

Table S5. Predicted vibrational N-O stretching frequencies of the ¹⁴N-¹⁴N, ¹⁴N-¹⁵N, and ¹⁵N-¹⁵N isotope labelled [Fe₂(TPA)₂(NO)₂]²⁺ diamond core complex using BP86/TZVP.

Isotope structure	Predicted IR Vibrational Frequencies
[Fe ₂ (TPA) ₂ (¹⁴ NO)(¹⁴ NO)] ²⁺	1345 cm ⁻¹
[Fe ₂ (TPA) ₂ (¹⁴ NO)(¹⁵ NO)] ²⁺	1339 cm ⁻¹
[Fe ₂ (TPA) ₂ (¹⁵ NO)(¹⁵ NO)] ²⁺	1333 cm ⁻¹

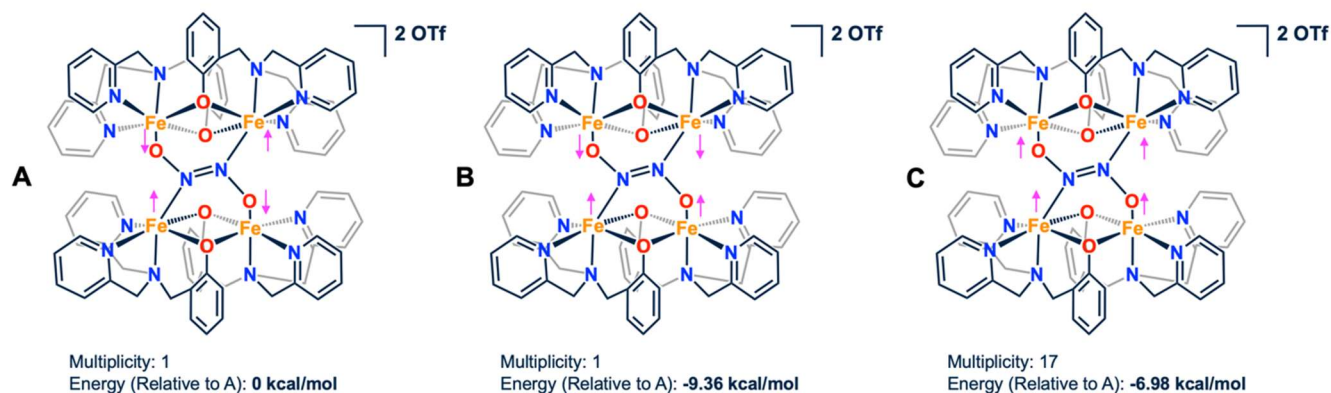


Figure S20. The electronic coupling states of **3** investigated by DFT using BP86/TZVP, with the listed energies given relative to the antiferromagnetically coupled state A.

Table S6. Comparison of key bond distance parameters for **3-OTf**, **3-BArF**, and free sodium *trans*-hyponitrite.

Bonds	Bond Distances for 3-BArF (Å)	Bond Distances for 3-OTf (Å)	Bond Distances for sodium <i>trans</i> -hyponitrite ⁷
Fe1-N7	2.214(5)	2.279(18)	N/A
Fe2-O4	1.981(3)	2.028(10)	N/A
Fe3-O3	2.026(3)	2.011(10)	N/A
Fe4-N8	2.211(5)	2.253(17)	N/A
O(A)-N(A)	1.358(6)	1.37(2)	1.3622(11)
O(B)-N(B)	1.358(6)	1.32(2)	N/A
N-N	1.257(8)	1.24(4)	1.256(2)
Na---O	N/A	N/A	2.5178(8)

Crystal Structure determination of $[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2](\text{OTf})_2$

Red blocks of $[\text{Fe}_2(\text{TPA})_2(\text{OCH}_3)_2](\text{OTf})_2$ were grown from an acetonitrile/diethyl ether solution of the compound at 25 °C. A crystal of dimensions 0.10 x 0.08 x 0.06 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and a Micromax-007HF Cu-target micro-focus rotating anode ($\lambda = 1.54187$ Å), operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85(1) K with the detector placed at a distance of 42.00 mm from the crystal. A total of 2028 images were collected with an oscillation width of 1.0° in ω . The exposure times were 1 sec. for the low angle images, 5 sec. for high angle. Rigaku d*trek images were exported to CrysAlisPro for processing and corrected for absorption. The integration of the data yielded a total of 32,060 reflections to a maximum 2θ value of 139.60° of which 4008 were independent and 3579 were greater than $2\sigma(I)$. The final cell constants (Table S7) were based on the xyz centroids of 10,100 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection. The structure was solved and refined with the Bruker SHELXTL (version 2016/6) software package, using the space group P2(1)/n with $Z = 2$ for the formula $\text{C}_{40}\text{H}_{42}\text{N}_8\text{O}_8\text{F}_6\text{S}_2\text{Fe}_2$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0598$ and $wR2 = 0.1635$ [based on $I > 2\sigma(I)$], $R1 = 0.0662$ and $wR2 = 0.1760$ for all data. Additional details are presented in Tables S7-12 and are given as Supporting Information in a CIF file. Acknowledgement is made for funding from NSF grant CHE-0840456 for X-ray instrumentation.

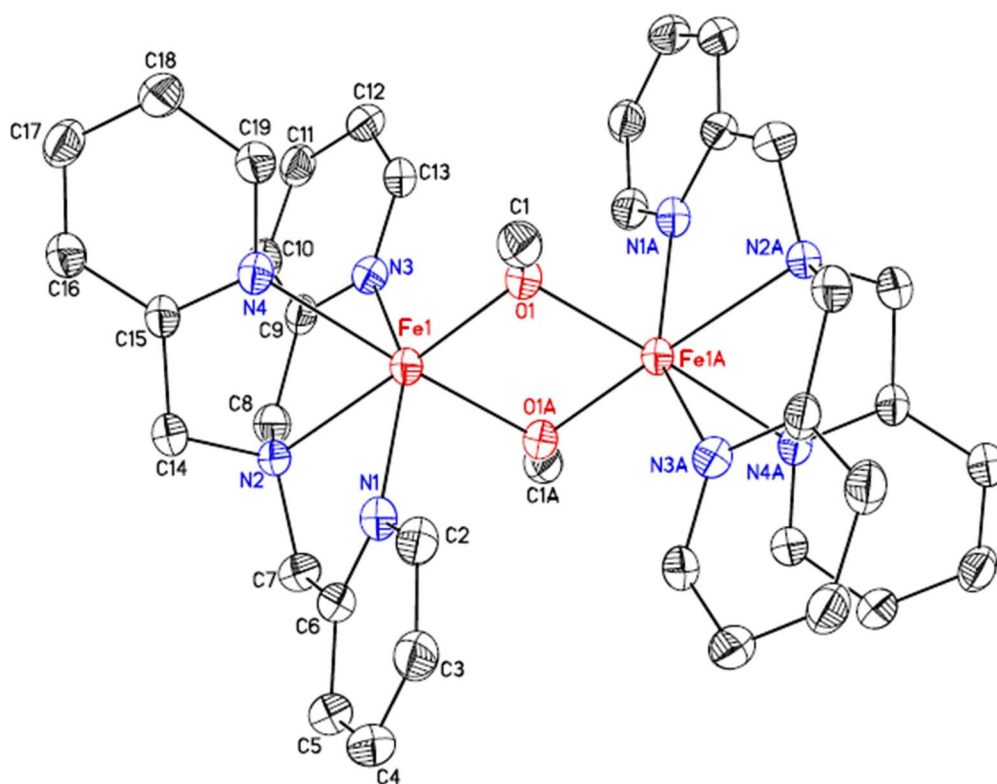


Figure S21. Crystal structure of $[\text{Fe}_2(\text{TPA})_2(\text{OMe})_2](\text{OTf})_2$ (CCDC # 2084197) with ellipsoid drawn at 50% probability. The triflate counter anions, solvent molecules, and hydrogens atoms were omitted for clarity.

Table S7. Crystal data and structure refinement for [Fe₂(TPA)₂(OMe)₂](OTf)₂.

Identification code	hd1204
CCDC Deposit Number	2084197
Empirical formula	C ₄₀ H ₄₂ F ₆ Fe ₂ N ₈ O ₈ S ₂
Formula weight	1052.63
Temperature	85(2) K
Wavelength	1.54184 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 8.0357(2) Å alpha = 90 deg. b = 15.7752(5) Å beta = 101.313(3) deg. c = 17.3269(5) Å gamma = 90 deg.
Volume	2153.76(11) Å ³
Z, Calculated density	2, 1.623 Mg/m ³
Absorption coefficient	7.092 mm ⁻¹
F(000)	1080
Crystal size	0.100 x 0.080 x 0.060 mm
Theta range for data collection	3.824 to 69.802 deg.
Limiting indices	-9<=h<=9, -19<=k<=18, -20<=l<=20
Reflections collected / unique	32060 / 4008 [R(int) = 0.0869]
Completeness to theta = 67.684	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.69947
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4008 / 0 / 299
Goodness-of-fit on F ²	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1635
R indices (all data)	R1 = 0.0662, wR2 = 0.1760
Extinction coefficient	n/a
Largest diff. peak and hole	0.888 and -0.871 e.Å ⁻³

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{TPA})_2(\text{OMe})_2](\text{OTf})_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
S(1)	8014(1)	6680(1)	6126(1)	44(1)
Fe(1)	4554(1)	5193(1)	9106(1)	24(1)
O(1)	6157(3)	4450(2)	9818(1)	26(1)
O(2)	9687(5)	6986(2)	6408(2)	66(1)
O(3)	7133(6)	6458(3)	6748(2)	72(1)
O(4)	7062(5)	7129(2)	5463(2)	58(1)
F(1)	6922(4)	5254(2)	5426(2)	62(1)
F(2)	9341(4)	5150(2)	6217(2)	48(1)
F(3)	9121(4)	5762(2)	5087(2)	62(1)
N(1)	5905(4)	6415(2)	9078(2)	27(1)
N(2)	2828(4)	6026(2)	8249(2)	25(1)
N(3)	2346(4)	4401(2)	8728(2)	27(1)
N(4)	4950(4)	4713(2)	7948(2)	26(1)
C(1)	7822(5)	4322(2)	9718(2)	31(1)
C(2)	7559(5)	6556(2)	9352(2)	30(1)
C(3)	8251(5)	7358(2)	9455(2)	33(1)
C(4)	7178(5)	8049(2)	9265(2)	34(1)
C(5)	5481(5)	7912(2)	8965(2)	32(1)
C(6)	4877(5)	7086(2)	8880(2)	28(1)
C(7)	3031(5)	6896(2)	8573(2)	30(1)
C(8)	1068(4)	5710(2)	8159(2)	28(1)
C(9)	1018(4)	4754(2)	8241(2)	25(1)
C(10)	-346(5)	4276(2)	7861(2)	31(1)
C(11)	-342(5)	3404(2)	7997(2)	31(1)
C(12)	1024(5)	3040(2)	8492(2)	31(1)
C(13)	2361(5)	3555(2)	8835(2)	28(1)
C(14)	3446(5)	5996(2)	7493(2)	29(1)
C(15)	4047(5)	5122(2)	7326(2)	26(1)
C(16)	3690(5)	4768(2)	6577(2)	31(1)
C(17)	4281(5)	3961(2)	6466(2)	33(1)
C(18)	5175(5)	3529(2)	7110(2)	30(1)
C(19)	5480(4)	3918(2)	7837(2)	27(1)
C(20)	8382(6)	5662(3)	5700(2)	40(1)

Table S9. Bond lengths [Å] and angles [deg] for [Fe₂(TPA)₂(OMe)₂](OTf)₂.

S(1)-O(2)	1.422(4)
S(1)-O(4)	1.435(3)
S(1)-O(3)	1.444(4)
S(1)-C(20)	1.816(4)
Fe(1)-O(1)	1.982(2)
Fe(1)-O(1)#1	2.130(2)
Fe(1)-N(3)	2.163(3)
Fe(1)-N(1)	2.218(3)
Fe(1)-N(4)	2.226(3)
Fe(1)-N(2)	2.247(3)
O(1)-C(1)	1.397(4)
F(1)-C(20)	1.341(5)
F(2)-C(20)	1.333(5)
F(3)-C(20)	1.324(5)
N(1)-C(2)	1.339(5)
N(1)-C(6)	1.344(5)
N(2)-C(8)	1.478(4)
N(2)-C(7)	1.479(4)
N(2)-C(14)	1.489(4)
N(3)-C(9)	1.345(5)
N(3)-C(13)	1.347(5)
N(4)-C(15)	1.340(5)
N(4)-C(19)	1.350(5)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.380(5)
C(2)-H(2)	0.9500
C(3)-C(4)	1.389(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.377(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.505(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.516(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.386(5)
C(10)-C(11)	1.397(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.379(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.385(5)
C(12)-H(12)	0.9500

C(13)-H(13)	0.9500
C(14)-C(15)	1.508(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.390(5)
C(16)-C(17)	1.386(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.382(6)
C(17)-H(17)	0.9500
C(18)-C(19)	1.379(5)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
O(2)-S(1)-O(4)	115.3(2)
O(2)-S(1)-O(3)	113.3(3)
O(4)-S(1)-O(3)	117.0(2)
O(2)-S(1)-C(20)	102.8(2)
O(4)-S(1)-C(20)	102.4(2)
O(3)-S(1)-C(20)	103.4(2)
O(1)-Fe(1)-O(1)#1	82.24(10)
O(1)-Fe(1)-N(3)	103.96(11)
O(1)#1-Fe(1)-N(3)	94.21(10)
O(1)-Fe(1)-N(1)	105.46(11)
O(1)#1-Fe(1)-N(1)	90.29(10)
N(3)-Fe(1)-N(1)	150.57(11)
O(1)-Fe(1)-N(4)	99.77(10)
O(1)#1-Fe(1)-N(4)	171.75(10)
N(3)-Fe(1)-N(4)	77.55(11)
N(1)-Fe(1)-N(4)	96.83(11)
O(1)-Fe(1)-N(2)	176.82(10)
O(1)#1-Fe(1)-N(2)	100.76(10)
N(3)-Fe(1)-N(2)	76.97(11)
N(1)-Fe(1)-N(2)	73.62(11)
N(4)-Fe(1)-N(2)	77.40(11)
C(1)-O(1)-Fe(1)	121.9(2)
C(1)-O(1)-Fe(1)#1	125.0(2)
Fe(1)-O(1)-Fe(1)#1	97.76(10)
C(2)-N(1)-C(6)	118.5(3)
C(2)-N(1)-Fe(1)	126.3(2)
C(6)-N(1)-Fe(1)	114.3(2)
C(8)-N(2)-C(7)	112.6(3)
C(8)-N(2)-C(14)	111.9(3)
C(7)-N(2)-C(14)	109.4(3)
C(8)-N(2)-Fe(1)	109.0(2)
C(7)-N(2)-Fe(1)	106.5(2)
C(14)-N(2)-Fe(1)	107.0(2)
C(9)-N(3)-C(13)	118.8(3)
C(9)-N(3)-Fe(1)	117.0(2)
C(13)-N(3)-Fe(1)	123.0(2)
C(15)-N(4)-C(19)	118.0(3)
C(15)-N(4)-Fe(1)	114.2(2)

C(19)-N(4)-Fe(1)	123.3(2)
O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	123.0(3)
N(1)-C(2)-H(2)	118.5
C(3)-C(2)-H(2)	118.5
C(2)-C(3)-C(4)	118.2(4)
C(2)-C(3)-H(3)	120.9
C(4)-C(3)-H(3)	120.9
C(5)-C(4)-C(3)	119.3(3)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	119.1(4)
C(4)-C(5)-H(5)	120.4
C(6)-C(5)-H(5)	120.4
N(1)-C(6)-C(5)	121.8(3)
N(1)-C(6)-C(7)	116.6(3)
C(5)-C(6)-C(7)	121.6(3)
N(2)-C(7)-C(6)	110.3(3)
N(2)-C(7)-H(7A)	109.6
C(6)-C(7)-H(7A)	109.6
N(2)-C(7)-H(7B)	109.6
C(6)-C(7)-H(7B)	109.6
H(7A)-C(7)-H(7B)	108.1
N(2)-C(8)-C(9)	111.6(3)
N(2)-C(8)-H(8A)	109.3
C(9)-C(8)-H(8A)	109.3
N(2)-C(8)-H(8B)	109.3
C(9)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0
N(3)-C(9)-C(10)	121.9(3)
N(3)-C(9)-C(8)	116.0(3)
C(10)-C(9)-C(8)	122.0(3)
C(9)-C(10)-C(11)	118.8(3)
C(9)-C(10)-H(10)	120.6
C(11)-C(10)-H(10)	120.6
C(12)-C(11)-C(10)	119.4(3)
C(12)-C(11)-H(11)	120.3
C(10)-C(11)-H(11)	120.3
C(11)-C(12)-C(13)	118.6(3)
C(11)-C(12)-H(12)	120.7
C(13)-C(12)-H(12)	120.7
N(3)-C(13)-C(12)	122.5(3)
N(3)-C(13)-H(13)	118.8
C(12)-C(13)-H(13)	118.8
N(2)-C(14)-C(15)	111.9(3)
N(2)-C(14)-H(14A)	109.2

C(15)-C(14)-H(14A)	109.2
N(2)-C(14)-H(14B)	109.2
C(15)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
N(4)-C(15)-C(16)	122.5(3)
N(4)-C(15)-C(14)	115.4(3)
C(16)-C(15)-C(14)	122.1(3)
C(17)-C(16)-C(15)	119.0(3)
C(17)-C(16)-H(16)	120.5
C(15)-C(16)-H(16)	120.5
C(18)-C(17)-C(16)	118.6(3)
C(18)-C(17)-H(17)	120.7
C(16)-C(17)-H(17)	120.7
C(19)-C(18)-C(17)	119.3(3)
C(19)-C(18)-H(18)	120.4
C(17)-C(18)-H(18)	120.4
N(4)-C(19)-C(18)	122.6(3)
N(4)-C(19)-H(19)	118.7
C(18)-C(19)-H(19)	118.7
F(3)-C(20)-F(2)	108.7(4)
F(3)-C(20)-F(1)	105.8(4)
F(2)-C(20)-F(1)	107.3(3)
F(3)-C(20)-S(1)	110.8(3)
F(2)-C(20)-S(1)	112.4(3)
F(1)-C(20)-S(1)	111.5(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{TPA})_2(\text{OMe})_2](\text{OTf})_2$. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U11 + \dots + 2 h k a^* b^* U12]$$

	U11	U22	U33	U23	U13	U12
S(1)	55(1)	31(1)	39(1)	-4(1)	-4(1)	8(1)
Fe(1)	30(1)	22(1)	17(1)	1(1)	-1(1)	0(1)
O(1)	32(1)	26(1)	19(1)	0(1)	2(1)	1(1)
O(2)	73(2)	42(2)	68(2)	-1(2)	-26(2)	-12(2)
O(3)	89(3)	76(3)	56(2)	4(2)	30(2)	28(2)
O(4)	66(2)	40(2)	59(2)	2(2)	-14(2)	15(2)
F(1)	77(2)	43(2)	56(2)	-2(1)	-15(2)	-18(1)
F(2)	72(2)	35(1)	34(1)	3(1)	2(1)	12(1)
F(3)	96(2)	58(2)	36(1)	6(1)	27(1)	12(2)
N(1)	33(2)	27(2)	20(1)	1(1)	2(1)	1(1)
N(2)	34(2)	21(1)	18(1)	1(1)	1(1)	2(1)
N(3)	34(2)	24(2)	22(1)	-1(1)	4(1)	-1(1)
N(4)	32(2)	27(2)	18(1)	0(1)	3(1)	-1(1)
C(1)	32(2)	31(2)	28(2)	1(2)	3(1)	5(1)
C(2)	36(2)	31(2)	23(2)	0(2)	5(1)	-2(2)
C(3)	38(2)	32(2)	26(2)	0(2)	2(2)	-6(2)
C(4)	47(2)	25(2)	31(2)	-3(2)	6(2)	-7(2)
C(5)	42(2)	25(2)	27(2)	-2(1)	5(2)	0(2)
C(6)	38(2)	23(2)	21(2)	-1(1)	6(1)	1(1)
C(7)	37(2)	25(2)	28(2)	-3(2)	4(2)	1(1)
C(8)	28(2)	30(2)	24(2)	1(1)	-1(1)	1(1)
C(9)	28(2)	30(2)	18(2)	-1(1)	2(1)	-1(1)
C(10)	34(2)	37(2)	21(2)	1(2)	3(1)	-3(2)
C(11)	36(2)	34(2)	23(2)	-4(2)	2(1)	-7(2)
C(12)	42(2)	26(2)	26(2)	-3(1)	8(2)	-2(2)
C(13)	38(2)	27(2)	18(2)	2(1)	4(1)	2(1)
C(14)	37(2)	27(2)	21(2)	3(1)	3(1)	2(1)
C(15)	31(2)	27(2)	18(2)	2(1)	2(1)	0(1)
C(16)	36(2)	30(2)	24(2)	2(1)	1(2)	1(1)
C(17)	37(2)	37(2)	23(2)	-6(2)	3(2)	0(2)
C(18)	34(2)	28(2)	28(2)	-4(2)	2(2)	-2(1)
C(19)	30(2)	25(2)	24(2)	1(1)	3(1)	0(1)
C(20)	56(2)	37(2)	25(2)	5(2)	-1(2)	2(2)

Table S11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{TPA})_2(\text{OMe})_2](\text{OTf})_2$.

	x	y	z	U(eq)
H(1A)	7950	4547	9206	46
H(1B)	8077	3714	9741	46
H(1C)	8607	4616	10137	46
H(2)	8289	6082	9480	36
H(3)	9431	7436	9652	39
H(4)	7609	8610	9341	41
H(5)	4734	8376	8818	38
H(7A)	2392	6953	9004	36
H(7B)	2562	7308	8156	36
H(8A)	416	5877	7635	34
H(8B)	522	5976	8564	34
H(10)	-1267	4538	7515	37
H(11)	-1271	3064	7749	38
H(12)	1047	2448	8596	37
H(13)	3325	3303	9159	34
H(14A)	4392	6403	7516	34
H(14B)	2518	6170	7058	34
H(16)	3050	5075	6148	37
H(17)	4076	3709	5958	39
H(18)	5575	2970	7052	36
H(19)	6088	3615	8277	32

Table S12. Torsion angles [deg] for [Fe₂(TPA)₂(OMe)₂](OTf)₂.

C(6)-N(1)-C(2)-C(3)	1.4(5)
Fe(1)-N(1)-C(2)-C(3)	-167.0(3)
N(1)-C(2)-C(3)-C(4)	-0.1(6)
C(2)-C(3)-C(4)-C(5)	-1.4(5)
C(3)-C(4)-C(5)-C(6)	1.7(5)
C(2)-N(1)-C(6)-C(5)	-1.1(5)
Fe(1)-N(1)-C(6)-C(5)	168.6(3)
C(2)-N(1)-C(6)-C(7)	179.8(3)
Fe(1)-N(1)-C(6)-C(7)	-10.5(4)
C(4)-C(5)-C(6)-N(1)	-0.4(5)
C(4)-C(5)-C(6)-C(7)	178.7(3)
C(8)-N(2)-C(7)-C(6)	162.8(3)
C(14)-N(2)-C(7)-C(6)	-72.0(3)
Fe(1)-N(2)-C(7)-C(6)	43.3(3)
N(1)-C(6)-C(7)-N(2)	-23.1(4)
C(5)-C(6)-C(7)-N(2)	157.8(3)
C(7)-N(2)-C(8)-C(9)	-150.7(3)
C(14)-N(2)-C(8)-C(9)	85.5(3)
Fe(1)-N(2)-C(8)-C(9)	-32.7(3)
C(13)-N(3)-C(9)-C(10)	1.3(5)
Fe(1)-N(3)-C(9)-C(10)	169.4(3)
C(13)-N(3)-C(9)-C(8)	178.9(3)
Fe(1)-N(3)-C(9)-C(8)	-13.1(4)
N(2)-C(8)-C(9)-N(3)	31.4(4)
N(2)-C(8)-C(9)-C(10)	-151.0(3)
N(3)-C(9)-C(10)-C(11)	0.7(5)
C(8)-C(9)-C(10)-C(11)	-176.8(3)
C(9)-C(10)-C(11)-C(12)	-1.0(5)
C(10)-C(11)-C(12)-C(13)	-0.6(5)
C(9)-N(3)-C(13)-C(12)	-3.1(5)
Fe(1)-N(3)-C(13)-C(12)	-170.3(3)
C(11)-C(12)-C(13)-N(3)	2.7(5)
C(8)-N(2)-C(14)-C(15)	-81.2(4)
C(7)-N(2)-C(14)-C(15)	153.3(3)
Fe(1)-N(2)-C(14)-C(15)	38.2(3)
C(19)-N(4)-C(15)-C(16)	-2.0(5)
Fe(1)-N(4)-C(15)-C(16)	-159.0(3)
C(19)-N(4)-C(15)-C(14)	178.2(3)
Fe(1)-N(4)-C(15)-C(14)	21.1(4)
N(2)-C(14)-C(15)-N(4)	-41.3(4)
N(2)-C(14)-C(15)-C(16)	138.9(4)
N(4)-C(15)-C(16)-C(17)	0.2(6)
C(14)-C(15)-C(16)-C(17)	-179.9(3)
C(15)-C(16)-C(17)-C(18)	1.4(6)
C(16)-C(17)-C(18)-C(19)	-1.3(6)
C(15)-N(4)-C(19)-C(18)	2.1(5)
Fe(1)-N(4)-C(19)-C(18)	156.9(3)
C(17)-C(18)-C(19)-N(4)	-0.5(5)

O(2)-S(1)-C(20)-F(3)	-64.9(4)
O(4)-S(1)-C(20)-F(3)	55.0(4)
O(3)-S(1)-C(20)-F(3)	177.0(3)
O(2)-S(1)-C(20)-F(2)	56.9(4)
O(4)-S(1)-C(20)-F(2)	176.8(3)
O(3)-S(1)-C(20)-F(2)	-61.2(4)
O(2)-S(1)-C(20)-F(1)	177.5(3)
O(4)-S(1)-C(20)-F(1)	-62.6(3)
O(3)-S(1)-C(20)-F(1)	59.4(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2

Crystal Structure Determination of $[Fe_2(BMPA-PhO)_2](OTf)_2$

Yellow needles of $[Fe_2(BMPA-PhO)_2](OTf)_2$ were grown from an acetonitrile/diethyl ether solution of the compound at 25 °C. A crystal of dimensions 0.16 x 0.11 x 0.09 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and a Micromax-007HF Cu-target micro-focus rotating anode ($\lambda = 1.54187$ Å), operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85(1) K with the detector placed at a distance of 42.00 mm from the crystal. A total of 2028 images were collected with an oscillation width of 1.0° in ω . The exposure times were 1 sec. for the low angle images, 5 sec. for high angle. Rigaku d*trek images were exported to CrysAlisPro for processing and corrected for absorption. The integration of the data yielded a total of 63,339 reflections to a maximum 2θ value of 139.11° of which 7873 were independent and 7043 were greater than $2\sigma(I)$. The final cell constants (Table S13) were based on the xyz centroids of 22,120 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection. The structure was solved and refined with the Bruker SHELXTL (version 2016/6) software package, using the space group $P2(1)/n$ with $Z = 4$ for the formula $C_{40}H_{36}N_6O_8F_6S_2Fe_2$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0658$ and $wR2 = 0.1701$ [based on $I > 2\sigma(I)$], $R1 = 0.0713$ and $wR2 = 0.1825$ for all data. Additional details are presented in Tables S13-18 and are given as Supporting Information in a CIF file. Acknowledgement is made for funding from NSF grant CHE-0840456 for X-ray instrumentation.

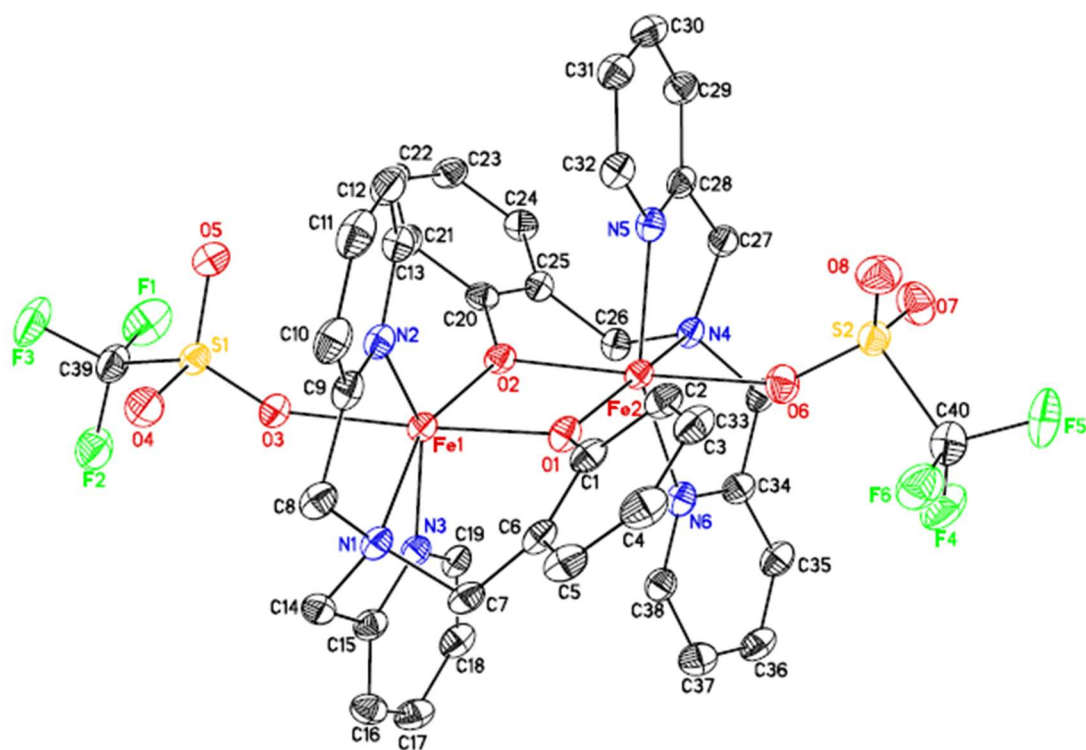


Figure S22. Crystal structure of $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$ (CCDC # 2084198) with ellipsoid at 50% probability. Solvent molecules and hydrogens atoms were omitted for clarity.

Table S13. Crystal data and structure refinement for [Fe₂(BMPA-PhO)₂(OTf)₂].

Identification code	hd1208
CCDC Deposit Number	2084198
Empirical formula	C ₄₀ H ₃₆ F ₆ Fe ₂ N ₆ O ₈ S ₂
Formula weight	1018.57
Temperature	85(2) K
Wavelength	1.54184 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 16.7692(3) Å alpha = 90 deg. b = 15.0560(3) Å beta = 100.613(2) deg. c = 17.0467(3) Å gamma = 90 deg.
Volume	4230.28(14) Å ³
Z, Calculated density	4, 1.599 Mg/m ³
Absorption coefficient	7.188 mm ⁻¹
F(000)	2080
Crystal size	0.160 x 0.110 x 0.090 mm
Theta range for data collection	3.397 to 69.549 deg.
Limiting indices	-20<=h<=19, -17<=k<=18, -20<=l<=20
Reflections collected / unique	63339 / 7873 [R(int) = 0.1536]
Completeness to theta = 67.684	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.37376
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7873 / 0 / 577
Goodness-of-fit on F ²	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0658, wR2 = 0.1701
R indices (all data)	R1 = 0.0713, wR2 = 0.1825
Extinction coefficient	n/a
Largest diff. peak and hole	0.993 and -1.243 e.Å ⁻³

Table S14. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Fe(1)	3489(1)	3385(1)	7462(1)	17(1)
Fe(2)	5113(1)	2562(1)	6938(1)	17(1)
S(1)	1508(1)	3897(1)	6929(1)	20(1)
S(2)	7104(1)	2984(1)	6674(1)	23(1)
O(1)	4772(1)	3609(2)	7533(1)	21(1)
O(2)	3821(1)	2386(2)	6783(1)	20(1)
O(3)	2122(1)	3268(2)	7318(1)	21(1)
O(4)	1417(1)	4667(2)	7402(1)	30(1)
O(5)	1515(1)	4052(2)	6100(1)	26(1)
O(6)	6401(1)	2857(2)	7047(1)	26(1)
O(7)	7334(2)	2196(2)	6293(2)	34(1)
O(8)	7117(2)	3801(2)	6246(2)	34(1)
F(1)	542(1)	2555(2)	6467(2)	43(1)
F(2)	473(1)	3047(2)	7640(1)	40(1)
F(3)	-67(1)	3794(2)	6597(2)	45(1)
F(4)	7914(1)	2428(2)	8046(2)	42(1)
F(5)	8627(1)	3186(2)	7351(2)	46(1)
F(6)	7779(1)	3847(2)	7955(1)	39(1)
N(1)	3546(2)	4359(2)	8480(2)	20(1)
N(2)	3295(1)	4655(2)	6866(2)	20(1)
N(3)	3457(2)	2547(2)	8482(2)	20(1)
N(4)	5278(2)	1221(2)	6434(2)	20(1)
N(5)	4997(2)	2832(2)	5674(2)	21(1)
N(6)	5578(2)	1756(2)	7968(2)	21(1)
C(1)	5149(2)	4380(2)	7759(2)	20(1)
C(2)	5723(2)	4741(2)	7348(2)	24(1)
C(3)	6119(2)	5527(2)	7594(2)	26(1)
C(4)	5936(2)	5986(2)	8245(2)	29(1)
C(5)	5370(2)	5638(2)	8653(2)	25(1)
C(6)	4974(2)	4835(2)	8430(2)	21(1)
C(7)	4404(2)	4445(2)	8911(2)	22(1)
C(8)	3221(2)	5233(2)	8182(2)	23(1)
C(9)	3310(2)	5381(2)	7324(2)	21(1)
C(10)	3348(2)	6236(2)	7020(2)	27(1)
C(11)	3383(2)	6334(3)	6224(2)	30(1)
C(12)	3351(2)	5589(3)	5743(2)	28(1)
C(13)	3307(2)	4764(2)	6084(2)	23(1)
C(14)	3061(2)	3934(2)	9018(2)	23(1)
C(15)	3293(2)	2969(2)	9134(2)	22(1)
C(16)	3329(2)	2541(2)	9861(2)	25(1)
C(17)	3541(2)	1648(2)	9918(2)	29(1)
C(18)	3707(2)	1214(2)	9252(2)	26(1)
C(19)	3648(2)	1678(2)	8543(2)	22(1)

C(20)	3429(2)	1888(2)	6173(2)	20(1)
C(21)	2699(2)	2174(2)	5702(2)	22(1)
C(22)	2310(2)	1668(2)	5066(2)	27(1)
C(23)	2634(2)	871(2)	4879(2)	27(1)
C(24)	3358(2)	577(2)	5341(2)	24(1)
C(25)	3761(2)	1077(2)	5984(2)	19(1)
C(26)	4524(2)	714(2)	6489(2)	21(1)
C(27)	5419(2)	1295(2)	5610(2)	22(1)
C(28)	5074(2)	2140(2)	5202(2)	20(1)
C(29)	4911(2)	2209(2)	4373(2)	25(1)
C(30)	4675(2)	3018(2)	4026(2)	26(1)
C(31)	4601(2)	3742(2)	4516(2)	24(1)
C(32)	4764(2)	3615(2)	5330(2)	23(1)
C(33)	5977(2)	797(2)	6965(2)	23(1)
C(34)	5972(2)	1015(2)	7828(2)	23(1)
C(35)	6390(2)	489(2)	8445(2)	26(1)
C(36)	6396(2)	741(2)	9226(2)	28(1)
C(37)	5978(2)	1506(2)	9369(2)	28(1)
C(38)	5585(2)	1988(2)	8730(2)	22(1)
C(39)	563(2)	3285(3)	6910(2)	30(1)
C(40)	7894(2)	3116(3)	7557(2)	32(1)

Table S15. Bond lengths [Å] and angles [deg] for [Fe₂(BMPA-PhO)₂(OTf)₂].

Fe(1)-O(2)	2.037(2)
Fe(1)-N(3)	2.157(3)
Fe(1)-O(1)	2.159(2)
Fe(1)-N(2)	2.162(3)
Fe(1)-N(1)	2.261(3)
Fe(1)-O(3)	2.267(2)
Fe(2)-O(1)	2.014(2)
Fe(2)-O(2)	2.150(2)
Fe(2)-N(6)	2.159(3)
Fe(2)-N(5)	2.166(3)
Fe(2)-O(6)	2.179(2)
Fe(2)-N(4)	2.231(3)
S(1)-O(5)	1.436(2)
S(1)-O(4)	1.436(3)
S(1)-O(3)	1.463(2)
S(1)-C(39)	1.827(4)
S(2)-O(8)	1.432(3)
S(2)-O(7)	1.439(3)
S(2)-O(6)	1.452(2)
S(2)-C(40)	1.825(4)
O(1)-C(1)	1.343(4)
O(2)-C(20)	1.350(4)
F(1)-C(39)	1.331(5)
F(2)-C(39)	1.331(4)
F(3)-C(39)	1.335(4)
F(4)-C(40)	1.327(5)
F(5)-C(40)	1.343(4)
F(6)-C(40)	1.326(5)
N(1)-C(14)	1.479(4)
N(1)-C(8)	1.479(4)
N(1)-C(7)	1.495(4)
N(2)-C(9)	1.341(4)
N(2)-C(13)	1.346(4)
N(3)-C(19)	1.346(4)
N(3)-C(15)	1.351(4)
N(4)-C(27)	1.470(4)
N(4)-C(33)	1.487(4)
N(4)-C(26)	1.496(4)
N(5)-C(28)	1.337(4)
N(5)-C(32)	1.342(4)
N(6)-C(34)	1.340(4)
N(6)-C(38)	1.342(4)
C(1)-C(2)	1.401(5)
C(1)-C(6)	1.410(5)
C(2)-C(3)	1.384(5)
C(2)-H(2)	0.9500

C(3)-C(4)	1.388(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.381(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.398(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.490(5)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.515(5)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.394(5)
C(10)-C(11)	1.377(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.385(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.379(5)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(15)	1.508(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.389(5)
C(16)-C(17)	1.389(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.382(5)
C(17)-H(17)	0.9500
C(18)-C(19)	1.384(5)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.402(4)
C(20)-C(25)	1.404(5)
C(21)-C(22)	1.387(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.378(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.393(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.397(4)
C(24)-H(24)	0.9500
C(25)-C(26)	1.506(4)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.513(5)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.393(5)
C(29)-C(30)	1.380(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.393(5)

C(30)-H(30)	0.9500
C(31)-C(32)	1.377(5)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(34)	1.509(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.397(5)
C(35)-C(36)	1.382(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.393(5)
C(36)-H(36)	0.9500
C(37)-C(38)	1.373(5)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
O(2)-Fe(1)-N(3)	94.38(10)
O(2)-Fe(1)-O(1)	76.91(9)
N(3)-Fe(1)-O(1)	102.68(9)
O(2)-Fe(1)-N(2)	114.77(10)
N(3)-Fe(1)-N(2)	150.74(10)
O(1)-Fe(1)-N(2)	87.14(9)
O(2)-Fe(1)-N(1)	159.70(9)
N(3)-Fe(1)-N(1)	76.37(10)
O(1)-Fe(1)-N(1)	87.41(9)
N(2)-Fe(1)-N(1)	76.63(10)
O(2)-Fe(1)-O(3)	104.94(9)
N(3)-Fe(1)-O(3)	82.37(9)
O(1)-Fe(1)-O(3)	174.56(9)
N(2)-Fe(1)-O(3)	87.45(9)
N(1)-Fe(1)-O(3)	91.87(9)
O(1)-Fe(2)-O(2)	77.60(9)
O(1)-Fe(2)-N(6)	97.15(10)
O(2)-Fe(2)-N(6)	103.65(9)
O(1)-Fe(2)-N(5)	111.83(10)
O(2)-Fe(2)-N(5)	89.80(9)
N(6)-Fe(2)-N(5)	150.17(10)
O(1)-Fe(2)-O(6)	99.55(9)
O(2)-Fe(2)-O(6)	174.85(9)
N(6)-Fe(2)-O(6)	80.87(10)
N(5)-Fe(2)-O(6)	87.29(9)
O(1)-Fe(2)-N(4)	165.80(10)
O(2)-Fe(2)-N(4)	92.00(9)
N(6)-Fe(2)-N(4)	75.71(10)
N(5)-Fe(2)-N(4)	77.35(10)
O(6)-Fe(2)-N(4)	91.51(9)
O(5)-S(1)-O(4)	116.22(15)
O(5)-S(1)-O(3)	114.68(14)
O(4)-S(1)-O(3)	114.06(14)
O(5)-S(1)-C(39)	103.19(15)
O(4)-S(1)-C(39)	103.62(16)

O(3)-S(1)-C(39)	102.61(15)
O(8)-S(2)-O(7)	116.65(17)
O(8)-S(2)-O(6)	115.25(15)
O(7)-S(2)-O(6)	113.30(15)
O(8)-S(2)-C(40)	104.44(17)
O(7)-S(2)-C(40)	104.35(17)
O(6)-S(2)-C(40)	100.20(16)
C(1)-O(1)-Fe(2)	131.2(2)
C(1)-O(1)-Fe(1)	124.19(19)
Fe(2)-O(1)-Fe(1)	102.81(9)
C(20)-O(2)-Fe(1)	134.61(19)
C(20)-O(2)-Fe(2)	119.99(19)
Fe(1)-O(2)-Fe(2)	102.34(9)
S(1)-O(3)-Fe(1)	127.78(13)
S(2)-O(6)-Fe(2)	149.47(16)
C(14)-N(1)-C(8)	112.8(3)
C(14)-N(1)-C(7)	108.8(2)
C(8)-N(1)-C(7)	110.6(2)
C(14)-N(1)-Fe(1)	104.17(19)
C(8)-N(1)-Fe(1)	110.65(18)
C(7)-N(1)-Fe(1)	109.55(19)
C(9)-N(2)-C(13)	118.3(3)
C(9)-N(2)-Fe(1)	117.6(2)
C(13)-N(2)-Fe(1)	123.0(2)
C(19)-N(3)-C(15)	118.3(3)
C(19)-N(3)-Fe(1)	126.2(2)
C(15)-N(3)-Fe(1)	115.3(2)
C(27)-N(4)-C(33)	111.5(2)
C(27)-N(4)-C(26)	112.7(2)
C(33)-N(4)-C(26)	108.9(3)
C(27)-N(4)-Fe(2)	110.6(2)
C(33)-N(4)-Fe(2)	107.08(19)
C(26)-N(4)-Fe(2)	105.72(18)
C(28)-N(5)-C(32)	118.3(3)
C(28)-N(5)-Fe(2)	116.9(2)
C(32)-N(5)-Fe(2)	124.4(2)
C(34)-N(6)-C(38)	118.3(3)
C(34)-N(6)-Fe(2)	116.0(2)
C(38)-N(6)-Fe(2)	125.2(2)
O(1)-C(1)-C(2)	121.4(3)
O(1)-C(1)-C(6)	119.7(3)
C(2)-C(1)-C(6)	118.9(3)
C(3)-C(2)-C(1)	121.0(3)
C(3)-C(2)-H(2)	119.5
C(1)-C(2)-H(2)	119.5
C(2)-C(3)-C(4)	120.3(3)
C(2)-C(3)-H(3)	119.8
C(4)-C(3)-H(3)	119.8
C(5)-C(4)-C(3)	119.1(3)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4

C(4)-C(5)-C(6)	121.8(3)
C(4)-C(5)-H(5)	119.1
C(6)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	118.8(3)
C(5)-C(6)-C(7)	120.7(3)
C(1)-C(6)-C(7)	120.4(3)
C(6)-C(7)-N(1)	114.9(2)
C(6)-C(7)-H(7A)	108.5
N(1)-C(7)-H(7A)	108.5
C(6)-C(7)-H(7B)	108.5
N(1)-C(7)-H(7B)	108.5
H(7A)-C(7)-H(7B)	107.5
N(1)-C(8)-C(9)	111.5(3)
N(1)-C(8)-H(8A)	109.3
C(9)-C(8)-H(8A)	109.3
N(1)-C(8)-H(8B)	109.3
C(9)-C(8)-H(8B)	109.3
H(8A)-C(8)-H(8B)	108.0
N(2)-C(9)-C(10)	122.3(3)
N(2)-C(9)-C(8)	116.6(3)
C(10)-C(9)-C(8)	120.9(3)
C(11)-C(10)-C(9)	118.5(3)
C(11)-C(10)-H(10)	120.7
C(9)-C(10)-H(10)	120.7
C(10)-C(11)-C(12)	119.6(3)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	118.6(3)
C(13)-C(12)-H(12)	120.7
C(11)-C(12)-H(12)	120.7
N(2)-C(13)-C(12)	122.7(3)
N(2)-C(13)-H(13)	118.7
C(12)-C(13)-H(13)	118.7
N(1)-C(14)-C(15)	109.9(3)
N(1)-C(14)-H(14A)	109.7
C(15)-C(14)-H(14A)	109.7
N(1)-C(14)-H(14B)	109.7
C(15)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
N(3)-C(15)-C(16)	122.3(3)
N(3)-C(15)-C(14)	115.6(3)
C(16)-C(15)-C(14)	122.1(3)
C(17)-C(16)-C(15)	118.7(3)
C(17)-C(16)-H(16)	120.7
C(15)-C(16)-H(16)	120.7
C(18)-C(17)-C(16)	119.2(3)
C(18)-C(17)-H(17)	120.4
C(16)-C(17)-H(17)	120.4
C(17)-C(18)-C(19)	119.0(3)
C(17)-C(18)-H(18)	120.5
C(19)-C(18)-H(18)	120.5

N(3)-C(19)-C(18)	122.5(3)
N(3)-C(19)-H(19)	118.8
C(18)-C(19)-H(19)	118.8
O(2)-C(20)-C(21)	121.3(3)
O(2)-C(20)-C(25)	120.2(3)
C(21)-C(20)-C(25)	118.5(3)
C(22)-C(21)-C(20)	121.0(3)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	120.7(3)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	119.0(3)
C(22)-C(23)-H(23)	120.5
C(24)-C(23)-H(23)	120.5
C(23)-C(24)-C(25)	121.2(3)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4
C(24)-C(25)-C(20)	119.6(3)
C(24)-C(25)-C(26)	119.3(3)
C(20)-C(25)-C(26)	121.0(3)
N(4)-C(26)-C(25)	114.7(3)
N(4)-C(26)-H(26A)	108.6
C(25)-C(26)-H(26A)	108.6
N(4)-C(26)-H(26B)	108.6
C(25)-C(26)-H(26B)	108.6
H(26A)-C(26)-H(26B)	107.6
N(4)-C(27)-C(28)	112.9(3)
N(4)-C(27)-H(27A)	109.0
C(28)-C(27)-H(27A)	109.0
N(4)-C(27)-H(27B)	109.0
C(28)-C(27)-H(27B)	109.0
H(27A)-C(27)-H(27B)	107.8
N(5)-C(28)-C(29)	122.0(3)
N(5)-C(28)-C(27)	116.7(3)
C(29)-C(28)-C(27)	121.1(3)
C(30)-C(29)-C(28)	119.2(3)
C(30)-C(29)-H(29)	120.4
C(28)-C(29)-H(29)	120.4
C(29)-C(30)-C(31)	119.0(3)
C(29)-C(30)-H(30)	120.5
C(31)-C(30)-H(30)	120.5
C(32)-C(31)-C(30)	118.1(3)
C(32)-C(31)-H(31)	120.9
C(30)-C(31)-H(31)	120.9
N(5)-C(32)-C(31)	123.4(3)
N(5)-C(32)-H(32)	118.3
C(31)-C(32)-H(32)	118.3
N(4)-C(33)-C(34)	110.8(3)
N(4)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33A)	109.5

N(4)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	108.1
N(6)-C(34)-C(35)	122.1(3)
N(6)-C(34)-C(33)	116.5(3)
C(35)-C(34)-C(33)	121.3(3)
C(36)-C(35)-C(34)	118.9(3)
C(36)-C(35)-H(35)	120.5
C(34)-C(35)-H(35)	120.5
C(35)-C(36)-C(37)	118.8(3)
C(35)-C(36)-H(36)	120.6
C(37)-C(36)-H(36)	120.6
C(38)-C(37)-C(36)	118.8(3)
C(38)-C(37)-H(37)	120.6
C(36)-C(37)-H(37)	120.6
N(6)-C(38)-C(37)	123.2(3)
N(6)-C(38)-H(38)	118.4
C(37)-C(38)-H(38)	118.4
F(2)-C(39)-F(1)	108.1(3)
F(2)-C(39)-F(3)	108.1(3)
F(1)-C(39)-F(3)	108.1(3)
F(2)-C(39)-S(1)	111.6(2)
F(1)-C(39)-S(1)	111.1(2)
F(3)-C(39)-S(1)	109.8(3)
F(6)-C(40)-F(4)	108.4(3)
F(6)-C(40)-F(5)	107.2(3)
F(4)-C(40)-F(5)	107.9(3)
F(6)-C(40)-S(2)	111.1(2)
F(4)-C(40)-S(2)	111.3(3)
F(5)-C(40)-S(2)	110.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Fe(1)	18(1)	15(1)	18(1)	-1(1)	1(1)	1(1)
Fe(2)	17(1)	16(1)	18(1)	0(1)	1(1)	1(1)
S(1)	18(1)	19(1)	20(1)	-1(1)	0(1)	0(1)
S(2)	20(1)	24(1)	24(1)	0(1)	3(1)	-1(1)
O(1)	19(1)	17(1)	25(1)	-3(1)	0(1)	-2(1)
O(2)	21(1)	19(1)	18(1)	-5(1)	0(1)	-1(1)
O(3)	20(1)	20(1)	24(1)	2(1)	1(1)	0(1)
O(4)	32(1)	27(1)	29(1)	-7(1)	2(1)	4(1)
O(5)	26(1)	26(1)	23(1)	1(1)	0(1)	0(1)
O(6)	22(1)	26(1)	31(1)	1(1)	5(1)	-4(1)
O(7)	35(1)	34(1)	37(1)	-9(1)	13(1)	-1(1)
O(8)	38(1)	33(2)	30(1)	9(1)	5(1)	-3(1)
F(1)	38(1)	35(1)	50(2)	0(1)	-9(1)	-16(1)
F(2)	27(1)	52(2)	44(1)	19(1)	10(1)	2(1)
F(3)	20(1)	53(2)	58(2)	23(1)	-2(1)	4(1)
F(4)	36(1)	41(1)	44(1)	16(1)	-9(1)	2(1)
F(5)	18(1)	51(2)	66(2)	-4(1)	4(1)	-4(1)
F(6)	37(1)	40(1)	37(1)	-9(1)	-2(1)	-4(1)
N(1)	17(1)	20(1)	21(1)	-1(1)	-1(1)	-1(1)
N(2)	16(1)	20(1)	23(1)	1(1)	1(1)	-1(1)
N(3)	17(1)	20(2)	20(1)	-2(1)	0(1)	-3(1)
N(4)	16(1)	20(1)	21(1)	0(1)	0(1)	2(1)
N(5)	18(1)	20(1)	24(1)	-2(1)	2(1)	0(1)
N(6)	20(1)	16(1)	26(1)	0(1)	2(1)	2(1)
C(1)	22(1)	13(2)	22(2)	4(1)	-3(1)	0(1)
C(2)	25(2)	22(2)	22(2)	1(1)	-1(1)	4(1)
C(3)	24(2)	26(2)	26(2)	4(1)	-3(1)	-4(1)
C(4)	31(2)	24(2)	29(2)	0(1)	-4(1)	-7(1)
C(5)	30(2)	21(2)	23(2)	-1(1)	-4(1)	1(1)
C(6)	18(1)	19(2)	21(2)	0(1)	-4(1)	3(1)
C(7)	22(1)	21(2)	19(2)	-2(1)	-4(1)	-1(1)
C(8)	26(2)	16(2)	25(2)	-2(1)	-2(1)	3(1)
C(9)	18(1)	18(2)	27(2)	-2(1)	-1(1)	3(1)
C(10)	22(2)	20(2)	36(2)	2(1)	-1(1)	0(1)
C(11)	21(2)	23(2)	43(2)	10(2)	0(1)	-2(1)
C(12)	20(1)	34(2)	28(2)	10(2)	1(1)	3(1)
C(13)	18(1)	27(2)	24(2)	1(1)	3(1)	2(1)
C(14)	25(2)	26(2)	18(2)	-4(1)	3(1)	3(1)
C(15)	20(1)	24(2)	21(2)	0(1)	-1(1)	-4(1)
C(16)	27(2)	28(2)	20(2)	-4(1)	4(1)	-7(1)

C(17)	32(2)	30(2)	22(2)	6(1)	-1(1)	-5(1)
C(18)	24(2)	21(2)	29(2)	4(1)	-3(1)	-5(1)
C(19)	18(1)	23(2)	24(2)	-1(1)	-1(1)	1(1)
C(20)	24(2)	20(2)	17(2)	-2(1)	4(1)	-4(1)
C(21)	22(1)	19(2)	25(2)	-1(1)	1(1)	4(1)
C(22)	26(2)	26(2)	26(2)	0(1)	-3(1)	3(1)
C(23)	30(2)	27(2)	22(2)	-4(1)	-2(1)	-1(1)
C(24)	29(2)	20(2)	23(2)	-4(1)	4(1)	-1(1)
C(25)	19(1)	17(2)	22(2)	2(1)	3(1)	-2(1)
C(26)	22(2)	16(2)	25(2)	-3(1)	4(1)	1(1)
C(27)	22(1)	23(2)	22(2)	-3(1)	3(1)	2(1)
C(28)	16(1)	21(2)	23(2)	1(1)	0(1)	-3(1)
C(29)	27(2)	25(2)	22(2)	-3(1)	1(1)	0(1)
C(30)	27(2)	29(2)	21(2)	2(1)	-2(1)	-1(1)
C(31)	25(2)	20(2)	28(2)	4(1)	2(1)	0(1)
C(32)	22(2)	20(2)	26(2)	-2(1)	1(1)	0(1)
C(33)	20(1)	20(2)	28(2)	2(1)	0(1)	3(1)
C(34)	23(1)	20(2)	23(2)	0(1)	0(1)	-3(1)
C(35)	26(2)	19(2)	30(2)	4(1)	-1(1)	2(1)
C(36)	28(2)	28(2)	26(2)	6(1)	-4(1)	1(1)
C(37)	32(2)	26(2)	25(2)	1(1)	2(1)	-3(1)
C(38)	21(1)	21(2)	24(2)	-1(1)	2(1)	0(1)
C(39)	20(2)	34(2)	33(2)	5(2)	0(1)	0(1)
C(40)	26(2)	31(2)	37(2)	1(2)	5(1)	-1(2)

Table S17. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}_2(\text{BMPA-PhO})_2(\text{OTf})_2]$.

	x	y	z	U(eq)
H(2)	5843	4441	6893	28
H(3)	6518	5753	7317	32
H(4)	6198	6533	8407	35
H(5)	5245	5953	9098	30
H(7A)	4410	4820	9389	26
H(7B)	4604	3849	9097	26
H(8A)	3513	5708	8521	28
H(8B)	2640	5269	8221	28
H(10)	3351	6741	7355	32
H(11)	3429	6908	6006	36
H(12)	3358	5644	5189	33
H(13)	3284	4252	5755	28
H(14A)	2476	3983	8785	28
H(14B)	3158	4241	9540	28
H(16)	3212	2853	10311	30
H(17)	3571	1340	10409	35
H(18)	3858	605	9281	31
H(19)	3747	1373	8083	27
H(21)	2469	2723	5821	27
H(22)	1814	1872	4756	33
H(23)	2367	528	4441	32
H(24)	3582	26	5218	29
H(26A)	4454	708	7053	25
H(26B)	4595	91	6328	25
H(27A)	5170	779	5299	27
H(27B)	6010	1277	5615	27
H(29)	4961	1705	4050	30
H(30)	4564	3080	3462	32
H(31)	4442	4308	4295	29
H(32)	4708	4106	5665	28
H(33A)	6490	1008	6820	28
H(33B)	5949	145	6889	28
H(35)	6665	-33	8331	31
H(36)	6679	399	9657	34
H(37)	5966	1691	9900	33
H(38)	5304	2512	8831	26

Table S18. Torsion angles [deg] for [Fe₂(BMPA-PhO)₂(OTf)₂].

O(5)-S(1)-O(3)-Fe(1)	60.6(2)
O(4)-S(1)-O(3)-Fe(1)	-76.9(2)
C(39)-S(1)-O(3)-Fe(1)	171.70(17)
O(8)-S(2)-O(6)-Fe(2)	73.9(3)
O(7)-S(2)-O(6)-Fe(2)	-64.1(3)
C(40)-S(2)-O(6)-Fe(2)	-174.7(3)
Fe(2)-O(1)-C(1)-C(2)	25.9(4)
Fe(1)-O(1)-C(1)-C(2)	-136.3(3)
Fe(2)-O(1)-C(1)-C(6)	-153.2(2)
Fe(1)-O(1)-C(1)-C(6)	44.7(4)
O(1)-C(1)-C(2)-C(3)	-178.7(3)
C(6)-C(1)-C(2)-C(3)	0.3(4)
C(1)-C(2)-C(3)-C(4)	-1.7(5)
C(2)-C(3)-C(4)-C(5)	1.6(5)
C(3)-C(4)-C(5)-C(6)	0.0(5)
C(4)-C(5)-C(6)-C(1)	-1.3(5)
C(4)-C(5)-C(6)-C(7)	176.1(3)
O(1)-C(1)-C(6)-C(5)	-179.7(3)
C(2)-C(1)-C(6)-C(5)	1.2(4)
O(1)-C(1)-C(6)-C(7)	2.8(4)
C(2)-C(1)-C(6)-C(7)	-176.3(3)
C(5)-C(6)-C(7)-N(1)	117.5(3)
C(1)-C(6)-C(7)-N(1)	-65.1(4)
C(14)-N(1)-C(7)-C(6)	177.8(3)
C(8)-N(1)-C(7)-C(6)	-57.7(3)
Fe(1)-N(1)-C(7)-C(6)	64.5(3)
C(14)-N(1)-C(8)-C(9)	-142.9(3)
C(7)-N(1)-C(8)-C(9)	94.9(3)
Fe(1)-N(1)-C(8)-C(9)	-26.6(3)
C(13)-N(2)-C(9)-C(10)	-0.8(4)
Fe(1)-N(2)-C(9)-C(10)	167.4(2)
C(13)-N(2)-C(9)-C(8)	174.7(3)
Fe(1)-N(2)-C(9)-C(8)	-17.0(3)
N(1)-C(8)-C(9)-N(2)	29.5(4)
N(1)-C(8)-C(9)-C(10)	-154.8(3)
N(2)-C(9)-C(10)-C(11)	-0.9(5)
C(8)-C(9)-C(10)-C(11)	-176.3(3)
C(9)-C(10)-C(11)-C(12)	2.2(5)
C(10)-C(11)-C(12)-C(13)	-1.8(5)
C(9)-N(2)-C(13)-C(12)	1.3(4)
Fe(1)-N(2)-C(13)-C(12)	-166.3(2)
C(11)-C(12)-C(13)-N(2)	0.0(5)
C(8)-N(1)-C(14)-C(15)	166.0(2)
C(7)-N(1)-C(14)-C(15)	-70.9(3)
Fe(1)-N(1)-C(14)-C(15)	45.9(3)
C(19)-N(3)-C(15)-C(16)	1.1(4)
Fe(1)-N(3)-C(15)-C(16)	-173.5(2)

C(19)-N(3)-C(15)-C(14)	-178.4(3)
Fe(1)-N(3)-C(15)-C(14)	7.0(3)
N(1)-C(14)-C(15)-N(3)	-37.7(4)
N(1)-C(14)-C(15)-C(16)	142.8(3)
N(3)-C(15)-C(16)-C(17)	-0.1(5)
C(14)-C(15)-C(16)-C(17)	179.4(3)
C(15)-C(16)-C(17)-C(18)	-0.1(5)
C(16)-C(17)-C(18)-C(19)	-0.7(5)
C(15)-N(3)-C(19)-C(18)	-2.0(4)
Fe(1)-N(3)-C(19)-C(18)	171.9(2)
C(17)-C(18)-C(19)-N(3)	1.8(5)
Fe(1)-O(2)-C(20)-C(21)	21.0(5)
Fe(2)-O(2)-C(20)-C(21)	-135.3(3)
Fe(1)-O(2)-C(20)-C(25)	-160.8(2)
Fe(2)-O(2)-C(20)-C(25)	42.8(4)
O(2)-C(20)-C(21)-C(22)	178.6(3)
C(25)-C(20)-C(21)-C(22)	0.4(5)
C(20)-C(21)-C(22)-C(23)	-0.4(5)
C(21)-C(22)-C(23)-C(24)	0.4(5)
C(22)-C(23)-C(24)-C(25)	-0.5(5)
C(23)-C(24)-C(25)-C(20)	0.6(5)
C(23)-C(24)-C(25)-C(26)	177.3(3)
O(2)-C(20)-C(25)-C(24)	-178.7(3)
C(21)-C(20)-C(25)-C(24)	-0.5(5)
O(2)-C(20)-C(25)-C(26)	4.6(5)
C(21)-C(20)-C(25)-C(26)	-177.2(3)
C(27)-N(4)-C(26)-C(25)	-56.2(3)
C(33)-N(4)-C(26)-C(25)	179.5(3)
Fe(2)-N(4)-C(26)-C(25)	64.7(3)
C(24)-C(25)-C(26)-N(4)	113.4(3)
C(20)-C(25)-C(26)-N(4)	-69.9(4)
C(33)-N(4)-C(27)-C(28)	-143.7(3)
C(26)-N(4)-C(27)-C(28)	93.5(3)
Fe(2)-N(4)-C(27)-C(28)	-24.6(3)
C(32)-N(5)-C(28)-C(29)	-0.8(4)
Fe(2)-N(5)-C(28)-C(29)	171.7(2)
C(32)-N(5)-C(28)-C(27)	174.0(3)
Fe(2)-N(5)-C(28)-C(27)	-13.5(3)
N(4)-C(27)-C(28)-N(5)	26.0(4)
N(4)-C(27)-C(28)-C(29)	-159.2(3)
N(5)-C(28)-C(29)-C(30)	1.1(5)
C(27)-C(28)-C(29)-C(30)	-173.4(3)
C(28)-C(29)-C(30)-C(31)	-0.5(5)
C(29)-C(30)-C(31)-C(32)	-0.3(5)
C(28)-N(5)-C(32)-C(31)	-0.1(4)
Fe(2)-N(5)-C(32)-C(31)	-172.0(2)
C(30)-C(31)-C(32)-N(5)	0.7(5)
C(27)-N(4)-C(33)-C(34)	159.5(3)
C(26)-N(4)-C(33)-C(34)	-75.5(3)
Fe(2)-N(4)-C(33)-C(34)	38.4(3)
C(38)-N(6)-C(34)-C(35)	-0.5(5)

Fe(2)-N(6)-C(34)-C(35)	172.0(2)
C(38)-N(6)-C(34)-C(33)	-177.7(3)
Fe(2)-N(6)-C(34)-C(33)	-5.2(4)
N(4)-C(33)-C(34)-N(6)	-23.6(4)
N(4)-C(33)-C(34)-C(35)	159.2(3)
N(6)-C(34)-C(35)-C(36)	0.1(5)
C(33)-C(34)-C(35)-C(36)	177.1(3)
C(34)-C(35)-C(36)-C(37)	0.6(5)
C(35)-C(36)-C(37)-C(38)	-0.8(5)
C(34)-N(6)-C(38)-C(37)	0.3(5)
Fe(2)-N(6)-C(38)-C(37)	-171.5(2)
C(36)-C(37)-C(38)-N(6)	0.4(5)
O(5)-S(1)-C(39)-F(2)	177.1(2)
O(4)-S(1)-C(39)-F(2)	-61.3(3)
O(3)-S(1)-C(39)-F(2)	57.7(3)
O(5)-S(1)-C(39)-F(1)	56.4(3)
O(4)-S(1)-C(39)-F(1)	178.0(2)
O(3)-S(1)-C(39)-F(1)	-63.0(3)
O(5)-S(1)-C(39)-F(3)	-63.1(3)
O(4)-S(1)-C(39)-F(3)	58.5(3)
O(3)-S(1)-C(39)-F(3)	177.5(2)
O(8)-S(2)-C(40)-F(6)	54.5(3)
O(7)-S(2)-C(40)-F(6)	177.4(2)
O(6)-S(2)-C(40)-F(6)	-65.1(3)
O(8)-S(2)-C(40)-F(4)	175.4(3)
O(7)-S(2)-C(40)-F(4)	-61.6(3)
O(6)-S(2)-C(40)-F(4)	55.8(3)
O(8)-S(2)-C(40)-F(5)	-64.6(3)
O(7)-S(2)-C(40)-F(5)	58.4(3)
O(6)-S(2)-C(40)-F(5)	175.8(3)

Crystal Structure Determination for $[\{Fe_2(BMPA-PhO)_2\}_2(\mu-N_2O_2)](OTf)_2$

Orange plates of $[\{Fe_2(BMPA-PhO)_2\}_2(\mu-N_2O_2)](OTf)_2$ were grown from a diethyl ether/acetonitrile solution of the compound at -33 °C. A crystal of dimensions 0.17 x 0.10 x 0.04 mm was mounted on a Rigaku AFC10K Saturn 944+ CCD-based X-ray diffractometer equipped with a low temperature device and a Micromax-007HF Cu-target micro-focus rotating anode ($\lambda = 1.54187 \text{ \AA}$), operated at 1.2 kW power (40 kV, 30 mA). The X-ray intensities were measured at 85(1) K with the detector placed at a distance of 42.00 mm from the crystal. A total of 2028 images were collected with an oscillation width of 1.0° in ω . The exposure times were 1 sec. for the low angle images, 10 sec. for high angle. Rigaku d*trek images were exported to CrysAlisPro for processing and corrected for absorption. The integration of the data yielded a total of 83,013 reflections to a maximum 2θ value of 138.89° of which 10,090 were independent and 8361 were greater than $2\sigma(I)$. The final cell constants (Table S19) were based on the xyz centroids of 20,341 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection. The structure was solved and refined with the Bruker SHELXTL (version 2018/3) software package, using the space group Fdd2 with $Z = 8$ for the formula $C_{78}H_{72}N_{14}O_{12}F_6S_2Fe_4$. The structure was refined as a two-component inversion twin. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at $R1 = 0.0461$ and $wR2 = 0.1277$ [based on $I > 2\sigma(I)$], $R1 = 0.0571$ and $wR2 = 0.1393$ for all data. The SQUEEZE subroutine of the PLATON program suite was used to address the disordered solvent in the large cavity present in the structure. Additional details are presented in Tables S19-24 and are given as Supporting Information in a CIF file. Acknowledgement is made for funding from NSF grant CHE-0840456 for X-ray instrumentation.

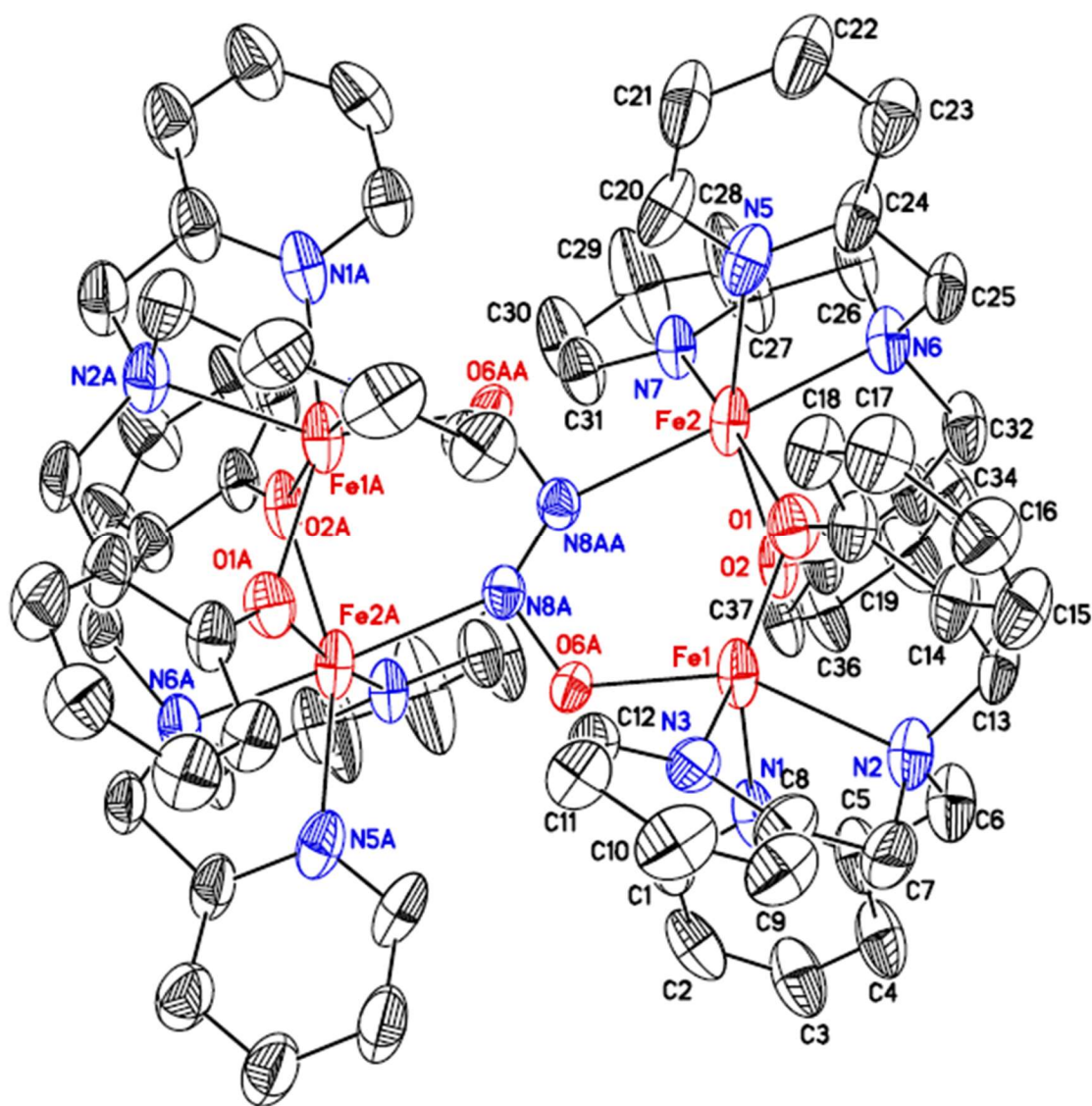


Figure S23. Crystal structure of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$ (CCDC # 2084199) with ellipsoid at 50% probability. The triflate counter anions, solvent molecules, and hydrogens atoms were omitted for clarity.

Table S19. Crystal data and structure refinement for [$\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$.

Identification code	hd1220a_b_sq
CCDC Deposit Number	2084199
Empirical formula	$\text{C}_{78} \text{H}_{72} \text{F}_6 \text{Fe}_4 \text{N}_{14} \text{O}_{12} \text{S}_2$
Formula weight	1799.01
Temperature	85(2) K
Wavelength	1.54184 Å
Crystal system, space group	Orthorhombic, Fdd2
Unit cell dimensions	a = 43.3568(6) Å alpha = 90 deg. b = 31.3029(5) Å beta = 90 deg. c = 16.0529(2) Å gamma = 90 deg.
Volume	21786.9(5) Å ³
Z, Calculated density	8, 1.097 Mg/m ³
Absorption coefficient	5.069 mm ⁻¹
F(000)	7392
Crystal size	0.170 x 0.100 x 0.040 mm
Theta range for data collection	3.258 to 69.443 deg.
Limiting indices	-51<=h<=48, -37<=k<=37, -19<=l<=19
Reflections collected / unique	83013 / 10090 [R(int) = 0.0537]
Completeness to theta = 67.684	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.62843
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10090 / 49 / 543
Goodness-of-fit on F ²	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1277
R indices (all data)	R1 = 0.0571, wR2 = 0.1393
Absolute structure parameter	0.367(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.243 and -0.472 e.Å ⁻³

Table S20. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5547(1)	4544(1)	6324(1)	59(1)
Fe(2)	5545(1)	5452(1)	5683(1)	58(1)
O(1)	5688(1)	5127(1)	6797(3)	61(1)
O(2)	5683(1)	4868(2)	5220(2)	59(1)
N(1)	5599(1)	3942(2)	5709(4)	66(1)
N(2)	5989(1)	4284(2)	6857(3)	64(1)
N(3)	5406(1)	4334(1)	7567(3)	50(1)
N(5)	5584(1)	6076(2)	6290(4)	66(1)
N(6)	5992(1)	5721(2)	5198(3)	62(1)
O(6A)	5101(2)	4471(3)	5971(5)	44(2)
O(6B)	4893(2)	4472(3)	6074(4)	40(2)
N(8A)	4923(4)	4833(7)	5933(7)	45(4)
N(8B)	5069(4)	4817(7)	6062(6)	43(4)
C(1)	5373(2)	3715(2)	5311(4)	68(2)
C(2)	5446(2)	3327(3)	4864(5)	85(2)
C(3)	5736(2)	3187(3)	4860(6)	94(3)
C(4)	5958(2)	3396(3)	5314(5)	86(2)
C(5)	5887(2)	3774(3)	5715(5)	76(2)
C(6)	6122(2)	4023(3)	6173(5)	80(2)
C(7)	5906(2)	3994(2)	7562(5)	74(2)
C(8)	5630(2)	4157(2)	8023(4)	67(2)
C(9)	5598(2)	4108(2)	8902(4)	74(2)
C(10)	5337(2)	4252(2)	9269(4)	79(2)
C(11)	5108(2)	4439(2)	8817(4)	66(2)
C(12)	5151(1)	4464(2)	7950(3)	49(1)
C(13)	6209(1)	4619(2)	7108(5)	69(2)
C(14)	6069(2)	4913(2)	7759(4)	68(2)
C(15)	6203(2)	4955(3)	8559(4)	79(2)
C(16)	6091(2)	5249(2)	9109(4)	76(2)
C(17)	5844(2)	5518(2)	8904(4)	74(2)
C(18)	5711(2)	5478(2)	8093(4)	66(2)
C(19)	5820(1)	5174(2)	7534(4)	60(2)
C(20)	5368(2)	6282(3)	6678(5)	80(2)
C(21)	5417(2)	6657(3)	7084(6)	96(3)
C(22)	5714(2)	6815(3)	7123(6)	101(3)
C(23)	5948(2)	6589(3)	6730(5)	90(2)
C(24)	5877(1)	6228(2)	6310(5)	70(2)
C(25)	6122(1)	5943(2)	5913(4)	69(2)
C(26)	5927(1)	5988(3)	4492(4)	73(2)
N(7)	5418(1)	5674(2)	4441(3)	56(1)
C(27)	5645(2)	5851(3)	3983(4)	77(2)
C(28)	5606(2)	5932(5)	3171(6)	157(6)
C(29)	5335(2)	5850(5)	2764(6)	168(6)
C(30)	5106(2)	5651(4)	3243(5)	106(3)

C(31)	5154(2)	5565(2)	4047(4)	67(2)
C(32)	6212(2)	5364(3)	4951(5)	75(2)
C(33)	6091(2)	5068(2)	4301(4)	66(2)
C(34)	6233(2)	5015(3)	3558(5)	90(3)
C(35)	6133(2)	4718(3)	2949(6)	102(3)
C(36)	5869(2)	4488(3)	3147(5)	85(2)
C(37)	5726(1)	4522(2)	3882(4)	65(2)
C(38)	5827(1)	4813(2)	4488(4)	59(2)
S(1)	5458(1)	3518(1)	1333(1)	101(1)
O(3)	5775(2)	3492(3)	1283(7)	177(4)
O(4)	5342(2)	3956(2)	1465(5)	136(2)
O(5)	5258(3)	3286(4)	784(6)	230(6)
C(39)	5369(2)	3261(3)	2333(6)	91(2)
F(1)	5554(2)	3431(2)	2882(4)	156(3)
F(2)	5462(2)	2855(2)	2293(6)	156(3)
F(3)	5102(1)	3263(2)	2589(5)	159(3)

Table S21. Bond lengths [Å] and angles [deg] for [$\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$.

Fe(1)-O(6A)	2.028(10)
Fe(1)-O(1)	2.068(4)
Fe(1)-O(2)	2.125(4)
Fe(1)-N(1)	2.141(6)
Fe(1)-N(3)	2.187(5)
Fe(1)-N(2)	2.250(5)
Fe(1)-N(8B)	2.279(18)
Fe(2)-O(6B)#1	2.011(10)
Fe(2)-O(2)	2.065(5)
Fe(2)-O(1)	2.151(4)
Fe(2)-N(7)	2.180(5)
Fe(2)-N(5)	2.189(6)
Fe(2)-N(8A)#1	2.253(17)
Fe(2)-N(6)	2.255(5)
O(1)-C(19)	1.322(7)
O(2)-C(38)	1.341(7)
N(1)-C(5)	1.354(9)
N(1)-C(1)	1.367(8)
N(2)-C(13)	1.477(9)
N(2)-C(6)	1.485(9)
N(2)-C(7)	1.495(9)
N(3)-C(12)	1.330(7)
N(3)-C(8)	1.339(8)
N(5)-C(20)	1.297(8)
N(5)-C(24)	1.356(9)
N(6)-C(26)	1.436(9)
N(6)-C(25)	1.455(8)
N(6)-C(32)	1.522(8)
O(6A)-N(8A)	1.37(2)
O(6B)-N(8B)	1.32(2)
N(8A)-N(8A)#1	1.24(4)
N(8B)-N(8B)#1	1.29(4)
C(1)-C(2)	1.446(11)
C(2)-C(3)	1.334(12)
C(3)-C(4)	1.373(11)
C(4)-C(5)	1.383(10)
C(5)-C(6)	1.479(10)
C(7)-C(8)	1.492(10)
C(8)-C(9)	1.426(10)
C(9)-C(10)	1.353(11)
C(10)-C(11)	1.363(10)
C(11)-C(12)	1.407(9)
C(13)-C(14)	1.518(9)
C(14)-C(19)	1.403(9)
C(14)-C(15)	1.414(9)
C(15)-C(16)	1.365(10)
C(16)-C(17)	1.399(10)

C(17)-C(18)	1.431(9)
C(18)-C(19)	1.391(9)
C(20)-C(21)	1.359(12)
C(21)-C(22)	1.381(12)
C(22)-C(23)	1.389(11)
C(23)-C(24)	1.351(10)
C(24)-C(25)	1.524(9)
C(26)-C(27)	1.532(9)
N(7)-C(27)	1.348(8)
N(7)-C(31)	1.353(7)
C(27)-C(28)	1.338(11)
C(28)-C(29)	1.372(12)
C(29)-C(30)	1.401(11)
C(30)-C(31)	1.335(10)
C(32)-C(33)	1.491(9)
C(33)-C(34)	1.352(10)
C(33)-C(38)	1.426(9)
C(34)-C(35)	1.416(11)
C(35)-C(36)	1.389(10)
C(36)-C(37)	1.338(10)
C(37)-C(38)	1.404(9)
S(1)-O(3)	1.379(7)
S(1)-O(5)	1.435(8)
S(1)-O(4)	1.475(6)
S(1)-C(39)	1.838(9)
C(39)-F(3)	1.230(8)
C(39)-F(1)	1.305(9)
C(39)-F(2)	1.334(10)
O(6A)-Fe(1)-O(1)	119.0(3)
O(6A)-Fe(1)-O(2)	95.0(3)
O(1)-Fe(1)-O(2)	78.70(16)
O(6A)-Fe(1)-N(1)	82.7(3)
O(1)-Fe(1)-N(1)	156.19(18)
O(2)-Fe(1)-N(1)	90.3(2)
O(6A)-Fe(1)-N(3)	87.4(3)
O(1)-Fe(1)-N(3)	90.71(17)
O(2)-Fe(1)-N(3)	168.96(18)
N(1)-Fe(1)-N(3)	100.71(19)
O(6A)-Fe(1)-N(2)	151.3(3)
O(1)-Fe(1)-N(2)	85.82(18)
O(2)-Fe(1)-N(2)	104.61(18)
N(1)-Fe(1)-N(2)	76.5(2)
N(3)-Fe(1)-N(2)	77.42(19)
O(1)-Fe(1)-N(8B)	90.4(5)
O(2)-Fe(1)-N(8B)	85.4(3)
N(1)-Fe(1)-N(8B)	109.9(5)
N(3)-Fe(1)-N(8B)	91.6(3)
N(2)-Fe(1)-N(8B)	168.3(3)
O(6B)#1-Fe(2)-O(2)	119.4(3)
O(6B)#1-Fe(2)-O(1)	93.9(2)

O(2)-Fe(2)-O(1)	78.18(15)
O(2)-Fe(2)-N(7)	91.48(18)
O(1)-Fe(2)-N(7)	169.65(19)
O(6B)#1-Fe(2)-N(5)	80.3(3)
O(2)-Fe(2)-N(5)	158.08(17)
O(1)-Fe(2)-N(5)	91.68(19)
N(7)-Fe(2)-N(5)	98.2(2)
O(2)-Fe(2)-N(8A)#1	88.6(6)
O(1)-Fe(2)-N(8A)#1	85.6(4)
N(7)-Fe(2)-N(8A)#1	93.6(4)
N(5)-Fe(2)-N(8A)#1	110.2(6)
O(6B)#1-Fe(2)-N(6)	151.1(3)
O(2)-Fe(2)-N(6)	87.45(18)
O(1)-Fe(2)-N(6)	102.40(19)
N(7)-Fe(2)-N(6)	77.39(19)
N(5)-Fe(2)-N(6)	75.7(2)
N(8A)#1-Fe(2)-N(6)	170.1(3)
C(19)-O(1)-Fe(1)	123.8(4)
C(19)-O(1)-Fe(2)	144.7(4)
Fe(1)-O(1)-Fe(2)	91.50(16)
C(38)-O(2)-Fe(2)	124.3(4)
C(38)-O(2)-Fe(1)	143.1(4)
Fe(2)-O(2)-Fe(1)	92.34(16)
C(5)-N(1)-C(1)	117.6(6)
C(5)-N(1)-Fe(1)	115.8(4)
C(1)-N(1)-Fe(1)	126.6(5)
C(13)-N(2)-C(6)	109.9(5)
C(13)-N(2)-C(7)	112.4(5)
C(6)-N(2)-C(7)	108.7(6)
C(13)-N(2)-Fe(1)	113.5(4)
C(6)-N(2)-Fe(1)	104.4(4)
C(7)-N(2)-Fe(1)	107.6(4)
C(12)-N(3)-C(8)	118.6(5)
C(12)-N(3)-Fe(1)	124.2(4)
C(8)-N(3)-Fe(1)	114.9(4)
C(20)-N(5)-C(24)	119.4(7)
C(20)-N(5)-Fe(2)	126.9(6)
C(24)-N(5)-Fe(2)	113.4(4)
C(26)-N(6)-C(25)	114.9(5)
C(26)-N(6)-C(32)	110.2(6)
C(25)-N(6)-C(32)	108.3(5)
C(26)-N(6)-Fe(2)	108.7(4)
C(25)-N(6)-Fe(2)	103.8(4)
C(32)-N(6)-Fe(2)	110.8(4)
N(8A)-O(6A)-Fe(1)	117.0(11)
N(8A)#1-N(8A)-O(6A)	113(3)
N(8A)#1-N(8A)-Fe(2)#1	145(2)
O(6A)-N(8A)-Fe(2)#1	100.7(11)
N(8B)#1-N(8B)-O(6B)	117(2)
N(8B)#1-N(8B)-Fe(1)	139(2)
O(6B)-N(8B)-Fe(1)	102.6(12)

N(1)-C(1)-C(2)	120.7(7)
C(3)-C(2)-C(1)	119.1(7)
C(2)-C(3)-C(4)	120.1(8)
C(3)-C(4)-C(5)	119.9(8)
N(1)-C(5)-C(4)	122.3(6)
N(1)-C(5)-C(6)	115.7(6)
C(4)-C(5)-C(6)	121.9(7)
C(5)-C(6)-N(2)	112.9(6)
C(8)-C(7)-N(2)	111.2(5)
N(3)-C(8)-C(9)	121.0(7)
N(3)-C(8)-C(7)	116.8(6)
C(9)-C(8)-C(7)	122.1(6)
C(10)-C(9)-C(8)	118.5(6)
C(9)-C(10)-C(11)	121.4(6)
C(10)-C(11)-C(12)	117.0(6)
N(3)-C(12)-C(11)	123.4(6)
N(2)-C(13)-C(14)	110.9(6)
C(19)-C(14)-C(15)	119.6(6)
C(19)-C(14)-C(13)	118.9(5)
C(15)-C(14)-C(13)	121.2(6)
C(16)-C(15)-C(14)	120.3(6)
C(15)-C(16)-C(17)	121.7(6)
C(16)-C(17)-C(18)	118.1(6)
C(19)-C(18)-C(17)	120.5(6)
O(1)-C(19)-C(18)	120.4(6)
O(1)-C(19)-C(14)	119.9(6)
C(18)-C(19)-C(14)	119.7(6)
N(5)-C(20)-C(21)	123.3(8)
C(20)-C(21)-C(22)	118.3(7)
C(21)-C(22)-C(23)	118.6(8)
C(24)-C(23)-C(22)	119.2(8)
C(23)-C(24)-N(5)	121.2(6)
C(23)-C(24)-C(25)	122.7(6)
N(5)-C(24)-C(25)	115.9(6)
N(6)-C(25)-C(24)	109.9(5)
N(6)-C(26)-C(27)	114.6(6)
C(27)-N(7)-C(31)	117.8(5)
C(27)-N(7)-Fe(2)	116.6(4)
C(31)-N(7)-Fe(2)	124.1(4)
C(28)-C(27)-N(7)	121.2(6)
C(28)-C(27)-C(26)	124.6(7)
N(7)-C(27)-C(26)	114.0(6)
C(27)-C(28)-C(29)	122.4(8)
C(28)-C(29)-C(30)	115.5(7)
C(31)-C(30)-C(29)	120.7(7)
C(30)-C(31)-N(7)	122.2(7)
C(33)-C(32)-N(6)	114.6(6)
C(34)-C(33)-C(38)	118.8(6)
C(34)-C(33)-C(32)	122.2(7)
C(38)-C(33)-C(32)	118.9(6)
C(33)-C(34)-C(35)	123.4(7)

C(36)-C(35)-C(34)	115.7(7)
C(37)-C(36)-C(35)	122.9(7)
C(36)-C(37)-C(38)	121.1(5)
O(2)-C(38)-C(37)	122.9(5)
O(2)-C(38)-C(33)	119.1(6)
C(37)-C(38)-C(33)	118.0(5)
O(3)-S(1)-O(5)	122.6(8)
O(3)-S(1)-O(4)	113.7(5)
O(5)-S(1)-O(4)	110.6(7)
O(3)-S(1)-C(39)	103.5(5)
O(5)-S(1)-C(39)	100.8(6)
O(4)-S(1)-C(39)	102.1(4)
F(3)-C(39)-F(1)	110.7(9)
F(3)-C(39)-F(2)	107.8(7)
F(1)-C(39)-F(2)	103.5(7)
F(3)-C(39)-S(1)	119.2(6)
F(1)-C(39)-S(1)	106.4(6)
F(2)-C(39)-S(1)	108.1(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, z

Table S22. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$. The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	33(1)	101(1)	42(1)	2(1)	-4(1)	-3(1)
Fe(2)	31(1)	103(1)	39(1)	3(1)	-1(1)	6(1)
O(1)	53(3)	84(3)	45(2)	1(2)	-16(2)	-4(2)
O(2)	31(2)	105(3)	40(2)	1(2)	3(2)	-6(2)
N(1)	41(3)	108(4)	49(3)	0(3)	0(2)	-17(3)
N(2)	41(3)	96(4)	55(3)	-14(3)	-7(2)	6(3)
N(3)	52(3)	55(2)	44(2)	1(2)	-4(2)	5(2)
N(5)	50(3)	99(4)	50(3)	-3(3)	-8(3)	23(3)
N(6)	38(3)	93(4)	56(3)	-16(3)	-1(2)	-3(2)
O(6A)	36(5)	50(5)	47(4)	-6(3)	-6(3)	7(4)
O(6B)	33(5)	40(5)	47(4)	-2(3)	13(3)	-1(4)
N(8A)	36(6)	57(13)	41(6)	-8(5)	-3(4)	1(8)
N(8B)	37(7)	58(14)	34(5)	2(5)	9(5)	0(8)
C(1)	52(4)	100(5)	53(3)	-1(3)	6(3)	-8(3)
C(2)	80(5)	111(6)	64(4)	-17(4)	8(4)	-47(4)
C(3)	68(5)	127(6)	86(6)	-46(5)	19(4)	-28(5)
C(4)	51(4)	123(6)	84(5)	-38(5)	21(4)	-17(4)
C(5)	50(4)	117(6)	62(4)	-27(4)	10(3)	-15(4)
C(6)	49(4)	116(6)	74(5)	-29(4)	-6(3)	4(4)
C(7)	61(4)	90(4)	72(4)	8(4)	-16(4)	13(3)
C(8)	76(4)	75(4)	50(4)	1(3)	-13(3)	17(3)
C(9)	93(5)	82(4)	46(3)	-14(3)	-24(3)	17(3)
C(10)	111(6)	90(4)	37(3)	-6(3)	-9(3)	19(4)
C(11)	71(4)	79(3)	47(3)	-3(3)	0(3)	12(3)
C(12)	47(3)	58(3)	42(3)	0(2)	-6(2)	0(2)
C(13)	34(3)	97(5)	77(4)	-13(4)	-18(3)	15(3)
C(14)	47(4)	107(5)	49(3)	-19(3)	-18(3)	14(3)
C(15)	68(5)	108(5)	61(4)	-11(4)	-35(3)	22(4)
C(16)	85(5)	97(5)	45(3)	-4(3)	-28(3)	8(4)
C(17)	81(5)	101(5)	40(3)	-5(3)	-9(3)	8(4)
C(18)	62(4)	95(5)	41(3)	-7(3)	-5(3)	13(3)
C(19)	45(4)	94(4)	40(3)	-7(3)	-7(3)	6(3)
C(20)	63(4)	112(6)	66(4)	-4(4)	1(3)	45(4)
C(21)	49(4)	139(7)	99(6)	-34(6)	-6(4)	24(4)
C(22)	69(5)	125(6)	107(7)	-37(6)	-24(5)	34(5)
C(23)	70(5)	113(6)	87(6)	-40(5)	-13(4)	23(4)
C(24)	45(4)	99(5)	65(4)	-17(4)	-15(3)	21(3)
C(25)	37(3)	95(4)	75(4)	-30(4)	-15(3)	11(3)
C(26)	40(3)	121(5)	59(4)	-5(4)	4(3)	-25(4)
N(7)	34(2)	92(3)	42(2)	6(2)	-1(2)	-3(2)
C(27)	43(3)	136(6)	51(4)	14(4)	0(3)	-24(4)
C(28)	78(5)	315(15)	78(5)	84(8)	-15(5)	-84(7)
C(29)	90(6)	355(17)	60(5)	70(8)	-16(4)	-88(9)
C(30)	70(5)	198(9)	51(4)	26(5)	-11(4)	-44(5)

C(31)	49(4)	107(5)	46(3)	10(3)	-13(3)	-15(3)
C(32)	38(3)	109(5)	79(5)	-41(4)	8(3)	0(3)
C(33)	42(4)	90(4)	67(4)	-15(3)	13(3)	-10(3)
C(34)	68(5)	120(6)	81(5)	-33(5)	34(4)	-41(4)
C(35)	87(6)	140(7)	80(6)	-37(5)	45(5)	-47(5)
C(36)	59(4)	130(6)	67(4)	-34(5)	11(4)	-42(4)
C(37)	40(3)	110(5)	46(3)	-8(3)	10(3)	-24(3)
C(38)	34(3)	94(4)	49(3)	-8(3)	11(3)	-7(3)
S(1)	110(2)	128(2)	66(1)	-5(1)	-15(1)	30(1)
O(3)	99(5)	178(7)	255(11)	100(7)	71(6)	36(5)
O(4)	165(6)	124(5)	119(5)	22(4)	-1(5)	61(4)
O(5)	311(14)	247(11)	133(7)	-66(7)	-94(8)	-48(10)
C(39)	49(4)	115(6)	109(6)	4(5)	-8(4)	-1(4)
F(1)	159(6)	211(7)	97(4)	28(4)	-41(4)	-51(5)
F(2)	123(4)	116(4)	228(8)	46(5)	28(5)	6(3)
F(3)	71(3)	214(7)	191(6)	8(5)	36(4)	4(4)

Table S23. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$.

	x	y	z	U(eq)
H(1)	5166	3814	5329	82
H(2)	5289	3175	4578	102
H(3)	5790	2942	4541	112
H(4)	6160	3280	5353	103
H(6A)	6230	4215	5777	96
H(6B)	6277	3825	6409	96
H(7A)	5861	3705	7343	89
H(7B)	6082	3972	7950	89
H(9)	5757	3978	9222	89
H(10)	5314	4223	9855	95
H(11)	4927	4547	9076	79
H(12)	4989	4580	7621	59
H(13A)	6269	4789	6613	83
H(13B)	6398	4485	7336	83
H(15)	6371	4778	8714	95
H(16)	6182	5272	9645	91
H(17)	5768	5722	9292	89
H(18)	5546	5661	7935	79
H(20)	5166	6165	6680	96
H(21)	5250	6807	7334	115
H(22)	5757	7072	7413	121
H(23)	6155	6687	6755	108
H(25A)	6299	6119	5734	83
H(25B)	6196	5732	6327	83
H(26A)	6110	5989	4122	88
H(26B)	5895	6284	4690	88
H(28)	5773	6051	2865	188
H(29)	5303	5923	2196	202
H(30)	4915	5575	2992	128
H(31)	4997	5424	4354	81
H(32A)	6406	5493	4745	91
H(32B)	6263	5195	5455	91
H(34)	6408	5187	3437	108
H(35)	6240	4679	2438	123
H(36)	5787	4298	2743	102
H(37)	5552	4346	3996	79

Table S24. Torsion angles [deg] for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{OTf})_2$.

Fe(1)-O(6A)-N(8A)-N(8A)#1	15.8(7)
Fe(1)-O(6A)-N(8A)-Fe(2)#1	-173.1(4)
Fe(2)#1-O(6B)-N(8B)-N(8B)#1	21.3(7)
Fe(2)#1-O(6B)-N(8B)-Fe(1)	-170.3(4)
C(5)-N(1)-C(1)-C(2)	-4.4(10)
Fe(1)-N(1)-C(1)-C(2)	175.1(5)
N(1)-C(1)-C(2)-C(3)	1.5(11)
C(1)-C(2)-C(3)-C(4)	3.7(13)
C(2)-C(3)-C(4)-C(5)	-5.9(14)
C(1)-N(1)-C(5)-C(4)	2.3(11)
Fe(1)-N(1)-C(5)-C(4)	-177.3(6)
C(1)-N(1)-C(5)-C(6)	-178.3(7)
Fe(1)-N(1)-C(5)-C(6)	2.1(9)
C(3)-C(4)-C(5)-N(1)	2.9(13)
C(3)-C(4)-C(5)-C(6)	-176.5(9)
N(1)-C(5)-C(6)-N(2)	27.6(11)
C(4)-C(5)-C(6)-N(2)	-152.9(8)
C(13)-N(2)-C(6)-C(5)	-162.3(7)
C(7)-N(2)-C(6)-C(5)	74.4(8)
Fe(1)-N(2)-C(6)-C(5)	-40.2(8)
C(13)-N(2)-C(7)-C(8)	90.2(7)
C(6)-N(2)-C(7)-C(8)	-148.0(6)
Fe(1)-N(2)-C(7)-C(8)	-35.5(6)
C(12)-N(3)-C(8)-C(9)	-0.2(9)
Fe(1)-N(3)-C(8)-C(9)	163.4(5)
C(12)-N(3)-C(8)-C(7)	176.8(6)
Fe(1)-N(3)-C(8)-C(7)	-19.7(7)
N(2)-C(7)-C(8)-N(3)	38.2(8)
N(2)-C(7)-C(8)-C(9)	-144.8(7)
N(3)-C(8)-C(9)-C(10)	-1.1(11)
C(7)-C(8)-C(9)-C(10)	-177.9(7)
C(8)-C(9)-C(10)-C(11)	0.3(11)
C(9)-C(10)-C(11)-C(12)	1.7(11)
C(8)-N(3)-C(12)-C(11)	2.4(9)
Fe(1)-N(3)-C(12)-C(11)	-159.6(5)
C(10)-C(11)-C(12)-N(3)	-3.1(10)
C(6)-N(2)-C(13)-C(14)	175.5(6)
C(7)-N(2)-C(13)-C(14)	-63.3(7)
Fe(1)-N(2)-C(13)-C(14)	59.1(7)
N(2)-C(13)-C(14)-C(19)	-66.4(9)
N(2)-C(13)-C(14)-C(15)	119.7(8)
C(19)-C(14)-C(15)-C(16)	-0.1(13)
C(13)-C(14)-C(15)-C(16)	173.9(7)
C(14)-C(15)-C(16)-C(17)	-0.5(13)
C(15)-C(16)-C(17)-C(18)	0.0(12)
C(16)-C(17)-C(18)-C(19)	1.1(11)
Fe(1)-O(1)-C(19)-C(18)	-129.7(6)
Fe(2)-O(1)-C(19)-C(18)	53.1(10)

Fe(1)-O(1)-C(19)-C(14)	49.4(8)
Fe(2)-O(1)-C(19)-C(14)	-127.8(7)
C(17)-C(18)-C(19)-O(1)	177.4(6)
C(17)-C(18)-C(19)-C(14)	-1.7(11)
C(15)-C(14)-C(19)-O(1)	-177.9(7)
C(13)-C(14)-C(19)-O(1)	8.0(10)
C(15)-C(14)-C(19)-C(18)	1.2(11)
C(13)-C(14)-C(19)-C(18)	-172.9(7)
C(24)-N(5)-C(20)-C(21)	2.8(12)
Fe(2)-N(5)-C(20)-C(21)	175.8(6)
N(5)-C(20)-C(21)-C(22)	-3.7(14)
C(20)-C(21)-C(22)-C(23)	1.6(15)
C(21)-C(22)-C(23)-C(24)	1.2(14)
C(22)-C(23)-C(24)-N(5)	-2.2(13)
C(22)-C(23)-C(24)-C(25)	-175.5(8)
C(20)-N(5)-C(24)-C(23)	0.2(11)
Fe(2)-N(5)-C(24)-C(23)	-173.7(6)
C(20)-N(5)-C(24)-C(25)	174.0(7)
Fe(2)-N(5)-C(24)-C(25)	0.1(8)
C(26)-N(6)-C(25)-C(24)	70.1(7)
C(32)-N(6)-C(25)-C(24)	-166.2(6)
Fe(2)-N(6)-C(25)-C(24)	-48.4(7)
C(23)-C(24)-C(25)-N(6)	-151.7(8)
N(5)-C(24)-C(25)-N(6)	34.6(9)
C(25)-N(6)-C(26)-C(27)	-146.4(6)
C(32)-N(6)-C(26)-C(27)	90.9(7)
Fe(2)-N(6)-C(26)-C(27)	-30.7(7)
C(31)-N(7)-C(27)-C(28)	2.3(14)
Fe(2)-N(7)-C(27)-C(28)	168.8(10)
C(31)-N(7)-C(27)-C(26)	176.4(7)
Fe(2)-N(7)-C(27)-C(26)	-17.1(9)
N(6)-C(26)-C(27)-C(28)	-153.1(11)
N(6)-C(26)-C(27)-N(7)	33.1(10)
N(7)-C(27)-C(28)-C(29)	2(2)
C(26)-C(27)-C(28)-C(29)	-171.9(13)
C(27)-C(28)-C(29)-C(30)	-4(2)
C(28)-C(29)-C(30)-C(31)	2(2)
C(29)-C(30)-C(31)-N(7)	1.4(17)
C(27)-N(7)-C(31)-C(30)	-3.8(12)
Fe(2)-N(7)-C(31)-C(30)	-169.2(8)
C(26)-N(6)-C(32)-C(33)	-61.7(8)
C(25)-N(6)-C(32)-C(33)	171.9(7)
Fe(2)-N(6)-C(32)-C(33)	58.7(7)
N(6)-C(32)-C(33)-C(34)	119.8(9)
N(6)-C(32)-C(33)-C(38)	-64.2(10)
C(38)-C(33)-C(34)-C(35)	0.0(15)
C(32)-C(33)-C(34)-C(35)	176.0(9)
C(33)-C(34)-C(35)-C(36)	2.2(17)
C(34)-C(35)-C(36)-C(37)	-3.9(16)
C(35)-C(36)-C(37)-C(38)	3.3(15)
Fe(2)-O(2)-C(38)-C(37)	-128.0(6)

Fe(1)-O(2)-C(38)-C(37)	59.8(9)
Fe(2)-O(2)-C(38)-C(33)	50.4(8)
Fe(1)-O(2)-C(38)-C(33)	-121.8(7)
C(36)-C(37)-C(38)-O(2)	177.6(8)
C(36)-C(37)-C(38)-C(33)	-0.8(11)
C(34)-C(33)-C(38)-O(2)	-179.2(8)
C(32)-C(33)-C(38)-O(2)	4.7(10)
C(34)-C(33)-C(38)-C(37)	-0.8(11)
C(32)-C(33)-C(38)-C(37)	-176.9(7)
O(3)-S(1)-C(39)-F(3)	174.5(9)
O(5)-S(1)-C(39)-F(3)	-57.9(10)
O(4)-S(1)-C(39)-F(3)	56.1(9)
O(3)-S(1)-C(39)-F(1)	48.6(8)
O(5)-S(1)-C(39)-F(1)	176.2(8)
O(4)-S(1)-C(39)-F(1)	-69.8(7)
O(3)-S(1)-C(39)-F(2)	-62.0(7)
O(5)-S(1)-C(39)-F(2)	65.5(8)
O(4)-S(1)-C(39)-F(2)	179.6(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,z

Crystal Structure Determination for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$

Single red needle-shaped crystals of $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$ were grown from a benzene/pentane solution of the compound at room temperature. A crystal of dimensions 0.19 x 0.19 x 0.13 mm³ was mounted on a on a dtrek-CrysAlisPro-abstract goniometer imported rigaku-d*trek images diffractometer. The crystal was kept at a steady T = 85 K during data collection. The structure was solved with the ShelXT 2018/2 (Sheldrick, 2018) solution program using dual methods and by using Olex2 1.5-alpha⁸ as the graphical interface. The model was refined with ShelXL 2019/3 (Sheldrick, 2015) using full matrix least squares minimization on F^2 .

Crystal Data. C₁₆₅H₁₄₈B₂F₄₈Fe₄N₁₄O₁₁, $M_r = 3659.99$, triclinic, $P-1$ (No. 2), $a = 19.5293(6)$ Å, $b = 21.0724(8)$ Å, $c = 22.8451(6)$ Å, $\alpha = 89.870(2)^\circ$, $\beta = 78.508(2)^\circ$, $\gamma = 62.614(4)^\circ$, $V = 8137.2(5)$ Å³, $T = 85$ K, $Z = 2$, $Z' = 1$, $m(\text{Cu K}\alpha) = 3.851$, 119,013 reflections measured, 29,337 unique ($R_{\text{int}} = 0.0556$) which were used in all calculations. The final wR_2 was 0.1834 (all data) and R_I was 0.0646 ($I \geq 2 \sigma(I)$).

Structure Quality Indicators

Reflections:	d min (CuK α) 2 Θ =139.0°	0.82	I/ σ (I)	24.5	R _{int} m=4.06	5.56%	Full 135.4° 96% to 139.0°	97.4
	Shift	0.002	Max Peak	1.1	Min Peak	-0.8	Goof	1.052

A red needle-shaped crystal with dimensions $0.19 \times 0.19 \times 0.13 \text{ mm}^3$ was mounted. Data were collected using a dtrek-CrysAlisPro-abstract goniometer imported rigaku-d*trek images with the diffractometer operating at $T = 85 \text{ K}$.

Data were measured using w scans with Cu K α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro 1.171.42.99a (Rigaku OD, 2023). The maximum resolution that was achieved was $Q = 69.516^\circ$ ($0.82 \text{ \AA}$).

The unit cell was refined using CrysAlisPro 1.171.42.99a (Rigaku OD, 2023) on 37,602 reflections, 32% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.42.99a (Rigaku OD, 2023). The final completeness is 97.40 % out to 69.516° in Q . A multi-scan absorption correction was performed using CrysAlisPro 1.171.42.99a (Rigaku Oxford Diffraction, 2023). Empirical absorption correction used spherical harmonics, as implemented in SCALE3 ABSPACK scaling algorithm. The absorption coefficient m of this material is 3.851 mm^{-1} at this wavelength ($\lambda = 1.54184 \text{ \AA}$) and the minimum and maximum transmissions are 0.674 and 1.000.

The structure was solved and the space group $P-1$ (# 2) determined by the ShelXT 2018/2 (Sheldrick, 2018) structure solution program using dual methods and refined by full matrix least squares minimization on F^2 using version 2019/3 of ShelXL 2019/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

Refine_special_details: There are disorders at several sites, which are all modelled as two component positional disorder. Strong restraints are used in order to enforce the corresponding

disordered parts to have similar ADPs. Several disordered THF molecules were found in the asymmetric unit. However, they are also disordered. They were eventually "squeezed" out with solvent mask due to the disorders.

Exptl_absorpt_process_details: CrysAlisPro 1.171.42.99a (Rigaku Oxford Diffraction, 2023) using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Smtbx_masks_special_details: A solvent mask was calculated and 399 electrons were found in a volume of 1460 Å³ in 5 voids per unit cell. This is consistent with the presence of 0.6[C₄H₈O], 2.5[C₄H₈O], 0.9[C₄H₈O], 1[C₄H₈O] per formula unit which account for 400 electrons per unit cell.

There is a single formula unit in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1. The moiety formula is C₇₆H₇₂Fe₄N₁₄O₆, 2(C₃₂H₁₂BF₂₄), C₅H₁₂, 0.6[C₄H₈O], 2.5[C₄H₈O], 0.9[C₄H₈O], 1[C₄H₈O].

Table S25. Crystal data and structure refinement for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$.

Identification code	MOL2165
CCDC Deposit Number	2357265
Empirical formula	$\text{C}_{165} \text{H}_{148} \text{B}_2 \text{F}_{48} \text{Fe}_4 \text{N}_{14} \text{O}_{11}$
Formula weight	3659.99
Temperature	85 K
Wavelength	1.54184 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	$a = 19.5293(6) \text{ Å}$ $\alpha = 89.870(2) \text{ deg.}$ $b = 21.0724(8) \text{ Å}$ $\beta = 78.508(2) \text{ deg.}$ $c = 22.8451(6) \text{ Å}$ $\gamma = 62.614(4) \text{ deg.}$
Volume	8137.2(5) Å ³
Z, Calculated density	2, 1.494 Mg/m ³
Absorption coefficient	3.851 mm ⁻¹
F(000)	3740
Crystal size	0.19 x 0.19 x 0.13 mm
Theta range for data collection	1.984 to 69.516 deg.
Limiting indices	$-23 \leq h \leq 23$, $-23 \leq k \leq 20$, $-27 \leq l \leq 27$
Reflections collected / unique	119013 / 29337 [R(int) = 0.0556]
Completeness to theta = 67.684	97.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.674
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	29337 / 138 / 2142
Goodness-of-fit on F ²	1.052
Final R indices [I > 2sigma(I)]	R1 = 0.0646, wR2 = 0.1721
R indices (all data)	R1 = 0.0747, wR2 = 0.1834
Extinction coefficient	n/a
Largest diff. peak and hole	1.153 and -0.768 e.Å ⁻³

Table S26. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	1462(1)	4988(1)	1300(1)	28(1)
Fe(2)	2039(1)	6091(1)	1051(1)	31(1)
Fe(3)	262(1)	6116(1)	3371(1)	37(1)
Fe(4)	1730(1)	6314(1)	3193(1)	37(1)
F(1)	7005(2)	937(2)	5844(2)	97(2)
F(2)	7878(2)	-42(2)	5417(2)	102(2)
F(3)	7991(3)	253(3)	6246(2)	150(2)
F(4)	7628(2)	-2234(2)	5830(2)	80(2)
F(5)	7750(2)	-2217(2)	6741(2)	78(2)
F(6)	6725(2)	-2200(2)	6552(2)	51(1)
F(7)	2259(2)	-2794(2)	8536(2)	62(1)
F(8)	2455(2)	3211(2)	7706(2)	55(1)
F(9)	2661(2)	3588(11)	8493(2)	52(1)
F(10)	5555(2)	1487(2)	8999(2)	93(2)
F(11)	5330(2)	2513(2)	8744(2)	74(2)
F(12)	6227(2)	1573(2)	8168(2)	67(2)
F(13)	4281(2)	-866(2)	5490(2)	90(2)
F(14)	3129(2)	-37(3)	5452(2)	159(2)
F(15)	4105(2)	-275(2)	4742(2)	74(8)
F(16)	3798(3)	2135(2)	4833(2)	128(2)
F(17)	3248(2)	2708(2)	5687(2)	77(2)
F(18)	4470(2)	2299(2)	5379(2)	86(2)
F(19)	5581(2)	-1027(2)	8816(2)	88(2)
F(20)	4932(2)	-1567(2)	8945(2)	115(2)
F(21)	4489(3)	-574(3)	9452(2)	168(3)
F(22)	1919(2)	623(3)	8298(3)	100(2)
F(22A)	2109(6)	-71(7)	8610(6)	101(2)
F(23)	2313(3)	-517(3)	8272(4)	103(2)
F(23A)	2531(6)	-669(6)	7829(7)	98(2)
F(24)	2323(3)	-13(4)	7475(3)	101(2)
F(24A)	2056(6)	398(7)	7708(8)	96(2)
F(25)	-32(2)	8892(2)	9143(2)	100(2)
F(26)	294(2)	9575(2)	8589(2)	91(2)
F(27)	643(2)	9351(2)	9413(2)	97(2)
F(28)	3500(2)	7203(2)	9146(2)	98(2)
F(29)	4093(2)	6998(2)	8222(2)	116(2)
F(30)	3604(2)	8022(2)	8676(2)	107(2)
F(31)	3045(2)	4716(2)	8867(1)	45(1)
F(32)	4098(2)	4029(11)	8222(2)	48(1)
F(33)	3881(2)	5089(2)	8509(1)	46(1)
F(34)	1951(3)	4278(2)	6719(2)	109(2)
F(35)	3157(3)	3632(2)	6571(2)	118(2)
F(36)	2740(5)	4473(3)	6037(2)	178(3)
F(37)	-649(2)	6499(2)	7992(2)	88(1)

F(38)	-1547(2)	7533(2)	7958(2)	99(2)
F(39)	-803(2)	7356(3)	8549(2)	116(2)
F(40)	427(2)	7659(2)	5521(2)	101(2)
F(41)	-431(3)	8641(2)	6023(2)	108(2)
F(42)	-737(2)	7854(2)	5871(2)	80(2)
F(43)	4638(3)	5098(3)	5653(2)	81(2)
F(43A)	3860(5)	5931(5)	5152(4)	141(3)
F(44)	5059(4)	5732(4)	5216(4)	122(2)
F(44A)	4674(4)	5924(4)	5624(4)	108(2)
F(45)	4288(5)	5495(5)	4867(3)	152(3)
F(45A)	4364(6)	6571(5)	4945(4)	148(3)
F(46)	3302(3)	8341(3)	5287(3)	72(2)
F(46A)	2471(4)	9061(3)	5609(3)	72(2)
F(47)	2217(4)	8400(3)	5182(3)	78(2)
F(47A)	2772(5)	9132(4)	6454(3)	99(2)
F(48)	2251(8)	8858(6)	6007(5)	75(3)
F(48A)	1593(4)	9334(3)	6426(3)	102(3)
O(1)	2526(2)	4961(2)	943(1)	32(1)
O(2)	1125(2)	5944(2)	844(2)	33(1)
O(3)	750(2)	5515(2)	2565(2)	28(2)
O(3A)	825(6)	5466(5)	2125(5)	32(3)
O(4)	2040(2)	6130(2)	1917(2)	31(1)
O(4A)	1856(6)	6330(6)	2339(5)	35(3)
O(5)	1345(2)	5673(2)	3670(2)	40(1)
O(6)	486(2)	6981(2)	3424(2)	39(1)
N(1)	1801(2)	4132(2)	545(2)	39(1)
N(2)	369(2)	4941(2)	1318(2)	35(1)
N(3)	2056(2)	3996(2)	1708(2)	27(5)
N(4)	2248(2)	6392(2)	113(2)	33(1)
N(5)	3204(2)	6038(2)	910(2)	40(1)
N(6)	1274(2)	7260(2)	1157(2)	35(1)
N(7)	1249(3)	5644(3)	2136(3)	29(2)
N(7A)	1087(11)	5796(12)	2394(9)	41(6)
N(8)	1553(3)	5982(3)	2342(3)	29(2)
N(8A)	1585(13)	6000(9)	2062(10)	42(6)
N(9)	-697(2)	6662(2)	4210(2)	42(7)
N(10)	-63(3)	5297(2)	3682(2)	46(1)
N(11)	-764(2)	6820(2)	3002(2)	35(1)
N(12)	2111(2)	6513(2)	4012(2)	40(1)
N(13)	1926(2)	7242(2)	3034(2)	43(1)
N(14)	2978(2)	5514(2)	3015(2)	39(1)
C(1)	-269(2)	5180(2)	1782(2)	41(2)
C(1A)	3429(3)	6885(3)	5857(2)	54(2)
C(1B)	3051(3)	6685(2)	6347(2)	40(2)
C(1C)	2437(3)	7207(3)	6776(2)	35(2)
C(1D)	2202(3)	7930(2)	6715(2)	40(2)
C(1E)	2580(3)	8131(2)	6224(2)	50(2)
C(1F)	3193(3)	7608(3)	5796(2)	55(3)
C(1G)	2389(13)	8871(16)	6182(10)	74(8)
C(1H)	4070(6)	6333(6)	5406(4)	65(3)
C(2)	-912(2)	5072(2)	1772(2)	47(2)

C(3)	-901(2)	4700(2)	1273(2)	53(2)
C(4)	-251(2)	4449(2)	796(2)	44(1)
C(5)	367(2)	4586(2)	833(2)	37(1)
C(6)	1081(2)	4355(2)	315(2)	37(1)
C(7)	2031(2)	3431(2)	799(2)	31(1)
C(8)	2386(2)	3390(2)	1337(2)	29(1)
C(9)	2982(2)	2756(2)	1456(2)	35(1)
C(10)	3244(2)	2739(2)	1976(2)	41(1)
C(11)	2898(2)	3360(2)	2369(2)	38(1)
C(12)	2311(2)	3974(2)	2219(2)	31(1)
C(13)	2460(2)	4088(2)	59(2)	32(1)
C(14)	3192(2)	3890(2)	287(2)	31(1)
C(15)	3874(2)	3233(2)	82(2)	37(1)
C(16)	4534(2)	3029(2)	317(2)	46(1)
C(17)	4523(2)	3481(2)	756(2)	46(2)
C(18)	3865(3)	4142(2)	957(2)	36(1)
C(19)	3186(2)	4351(2)	728(2)	29(1)
C(20)	3594(2)	6037(2)	1333(2)	46(2)
C(21)	4342(2)	5993(2)	1192(2)	57(2)
C(22)	4699(2)	5944(2)	603(2)	60(2)
C(23)	4306(2)	5940(2)	162(2)	52(2)
C(24)	3561(2)	5985(2)	329(2)	41(1)
C(25)	3111(2)	5955(2)	-124(2)	39(2)
C(26)	2011(2)	7167(2)	151(2)	42(2)
C(27)	1302(2)	7585(2)	655(2)	41(2)
C(28)	726(3)	8270(2)	614(2)	54(1)
C(29)	114(3)	8639(2)	1102(2)	58(2)
C(30)	85(2)	8307(2)	1625(2)	51(2)
C(31)	674(2)	7619(2)	1630(2)	41(2)
C(32)	1809(2)	6219(2)	-266(2)	36(1)
C(33)	930(2)	6577(2)	-21(2)	36(2)
C(34)	410(2)	7072(2)	-333(2)	45(1)
C(35)	-402(2)	7367(2)	-128(2)	50(1)
C(36)	-701(2)	7162(2)	396(2)	47(1)
C(37)	-193(2)	6669(2)	722(2)	38(1)
C(38)	626(2)	6383(2)	525(2)	31(1)
C(39)	85(3)	4701(2)	3352(2)	54(2)
C(40)	-202(4)	4239(3)	3571(2)	70(2)
C(41)	-659(4)	4381(3)	4145(2)	74(2)
C(42)	-810(3)	4986(3)	4489(2)	64(2)
C(43)	-505(3)	5427(2)	4247(2)	49(2)
C(44)	-632(3)	6088(2)	4601(2)	53(2)
C(45)	-1467(2)	6981(2)	4029(2)	45(2)
C(46)	-1411(2)	7256(2)	3421(2)	41(2)
C(47)	-1993(2)	7892(2)	3284(2)	47(2)
C(48)	-1907(2)	8084(2)	2712(2)	50(2)
C(49)	-1248(2)	7633(2)	2273(2)	42(2)
C(50)	-693(2)	7013(2)	2442(2)	35(2)
C(51)	-593(3)	7220(2)	4523(2)	49(2)
C(52)	-631(2)	7812(2)	4150(2)	45(1)
C(53)	-1210(3)	8518(2)	4329(2)	62(2)

C(54)	-1239(3)	9074(3)	3994(2)	73(2)
C(55)	-666(3)	8925(2)	3469(2)	64(2)
C(56)	-78(2)	8222(2)	3284(2)	47(2)
C(57)	-57(2)	7667(2)	3610(2)	40(1)
C(58)	2027(2)	7507(2)	2501(2)	52(2)
C(59)	2058(3)	8136(3)	2454(2)	68(2)
C(60)	1996(4)	8520(3)	2967(3)	79(2)
C(61)	1890(3)	8255(2)	3521(2)	66(2)
C(62)	1863(2)	7616(2)	3534(2)	49(1)
C(63)	1742(2)	7298(2)	4119(2)	48(2)
C(64)	2988(2)	6187(2)	3865(2)	46(1)
C(65)	3376(2)	5526(2)	3424(2)	44(1)
C(66)	4120(3)	4974(3)	3428(2)	63(2)
C(67)	4460(3)	4390(3)	3002(2)	72(2)
C(68)	4053(2)	4378(2)	2578(2)	57(2)
C(69)	3322(2)	4946(2)	2597(2)	42(1)
C(70)	1833(2)	6205(2)	4536(2)	44(1)
C(71)	2099(2)	5419(2)	4419(2)	44(2)
C(72)	2615(3)	4911(2)	4730(2)	52(2)
C(73)	2819(3)	4194(2)	4643(2)	58(2)
C(74)	2508(3)	3972(2)	4237(2)	52(2)
C(75)	1998(2)	4468(2)	3920(2)	43(1)
C(76)	1800(2)	5189(2)	3994(2)	39(2)
C(77)	5693(2)	27(2)	6801(2)	33(2)
C(78)	6164(2)	335(2)	6530(2)	36(1)
C(79)	6944(2)	-72(2)	6225(2)	35(2)
C(80)	7298(2)	-812(2)	6174(2)	37(1)
C(81)	6845(2)	-1137(2)	6435(2)	34(2)
C(82)	6063(2)	-724(2)	6742(2)	35(1)
C(83)	7420(2)	279(2)	5940(2)	44(1)
C(84)	7227(2)	-1935(2)	6385(2)	42(1)
C(85)	4556(2)	1244(2)	7504(2)	33(1)
C(86)	3794(2)	1829(2)	7645(2)	32(1)
C(87)	3587(2)	2413(2)	8047(2)	34(2)
C(88)	4137(2)	2448(2)	8329(2)	39(2)
C(89)	4897(2)	1878(2)	8203(2)	42(1)
C(90)	5100(2)	1286(2)	7797(2)	38(2)
C(91)	2750(2)	2996(2)	8195(2)	38(1)
C(92)	5495(3)	1870(2)	8517(2)	56(2)
C(93)	4367(2)	728(2)	6489(2)	34(2)
C(94)	4263(2)	218(2)	6177(2)	39(1)
C(95)	4027(2)	334(2)	5636(2)	44(1)
C(96)	3900(2)	961(2)	5369(2)	43(2)
C(97)	4013(2)	1466(2)	5661(2)	41(1)
C(98)	4233(2)	1353(2)	6214(2)	35(1)
C(99)	3882(2)	-204(3)	5334(2)	59(2)
C(100)	3890(2)	2139(2)	5391(2)	51(2)
C(101)	4368(2)	113(2)	7548(2)	37(1)
C(102)	4750(2)	-244(2)	7999(2)	41(1)
C(103)	4416(2)	-538(2)	8440(2)	48(1)
C(104)	3675(2)	-478(2)	8459(2)	55(2)

C(105)	3284(2)	-127(2)	8020(2)	51(1)
C(106)	3631(2)	153(2)	7569(2)	40(2)
C(107)	4849(3)	-909(3)	8915(2)	64(2)
C(108)	2478(3)	-33(3)	8042(3)	67(2)
C(109)	1954(3)	7395(2)	7833(2)	63(2)
C(110)	1281(3)	7975(3)	8168(2)	65(2)
C(111)	1304(3)	8401(3)	8626(3)	67(2)
C(112)	2023(3)	8241(3)	8773(3)	72(2)
C(113)	2701(3)	7665(3)	8443(3)	71(2)
C(114)	2668(3)	7266(3)	7979(3)	68(2)
C(115)	562(3)	9039(3)	8940(3)	78(2)
C(116)	3470(3)	7475(3)	8613(3)	79(3)
C(117)	2341(2)	6056(2)	7377(2)	45(2)
C(118)	2744(2)	5743(2)	7831(2)	37(2)
C(119)	3106(2)	5009(2)	7864(2)	34(1)
C(120)	3074(2)	4545(2)	7459(2)	45(2)
C(121)	2658(2)	4835(3)	7015(2)	55(2)
C(122)	2305(2)	5567(3)	6978(2)	58(2)
C(123)	3531(2)	4714(2)	8359(2)	36(2)
C(124)	2604(3)	4338(4)	6582(2)	92(2)
C(125)	1077(2)	7166(2)	7159(2)	50(2)
C(126)	510(2)	7099(2)	7600(2)	44(2)
C(127)	-248(2)	7308(2)	7530(2)	35(2)
C(128)	-478(2)	7586(2)	7004(2)	35(2)
C(129)	74(2)	7647(2)	6562(2)	36(1)
C(130)	834(2)	7440(2)	6635(2)	46(2)
C(131)	-814(2)	7190(2)	8006(2)	42(2)
C(132)	-151(2)	7950(2)	5998(2)	42(1)
C(133)	2621(3)	6858(2)	6363(2)	31(2)
C(134)	3257(3)	6246(2)	6233(2)	37(2)
C(135)	3706(2)	6305(2)	5702(2)	42(2)
C(136)	3519(3)	6977(3)	5501(2)	45(2)
C(137)	2883(3)	7588(2)	5832(2)	41(2)
C(138)	2434(2)	7529(2)	6363(2)	37(2)
C(139)	4352(6)	5656(5)	5354(3)	53(2)
C(140)	2669(5)	8284(4)	5583(4)	52(3)
C(141)	-2926(4)	9513(4)	8011(3)	104(2)
C(142)	-2150(5)	9402(5)	8080(4)	121(3)
C(143)	-1665(4)	9614(4)	7673(3)	95(2)
C(144)	-867(5)	9462(5)	7720(3)	114(3)
C(145)	-361(5)	9677(5)	7302(4)	127(3)
B(1)	4746(2)	526(2)	7087(2)	34(2)
B(2)	1969(3)	6911(3)	7271(3)	63(2)

Table S27. Bond lengths [Å] and angles [deg] for [$\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$.

Fe(1)-O(1)	2.048(2)
Fe(1)-O(2)	2.150(2)
Fe(1)-O(3A)	2.010(11)
Fe(1)-N(1)	2.264(3)
Fe(1)-N(2)	2.176(3)
Fe(1)-N(3)	2.187(2)
Fe(1)-N(7)	2.214(5)
Fe(2)-O(1)	2.112(2)
Fe(2)-O(2)	2.084(2)
Fe(2)-O(4)	1.981(3)
Fe(2)-N(4)	2.245(3)
Fe(2)-N(5)	2.186(3)
Fe(2)-N(6)	2.198(3)
Fe(2)-N(8A)	2.34(2)
Fe(3)-O(3)	2.026(3)
Fe(3)-O(5)	2.136(2)
Fe(3)-O(6)	2.069(2)
Fe(3)-N(7A)	2.37(2)
Fe(3)-N(9)	2.258(3)
Fe(3)-N(10)	2.169(3)
Fe(3)-N(11)	2.205(3)
Fe(4)-O(4A)	1.919(11)
Fe(4)-O(5)	2.045(2)
Fe(4)-O(6)	2.123(2)
Fe(4)-N(8)	2.211(5)
Fe(4)-N(12)	2.253(3)
Fe(4)-N(13)	2.176(3)
Fe(4)-N(14)	2.184(3)
F(1)-C(83)	1.290(5)
F(2)-C(83)	1.306(5)
F(3)-C(83)	1.309(5)
F(4)-C(84)	1.332(4)
F(5)-C(84)	1.350(4)
F(6)-C(84)	1.331(4)
F(7)-C(91)	1.336(4)
F(8)-C(91)	1.340(4)
F(9)-C(91)	1.346(4)
F(10)-C(92)	1.354(6)
F(11)-C(92)	1.321(5)
F(12)-C(92)	1.340(5)
F(13)-C(99)	1.337(6)
F(14)-C(99)	1.315(5)
F(15)-C(99)	1.322(5)
F(16)-C(100)	1.324(5)
F(17)-C(100)	1.323(5)
F(18)-C(100)	1.318(5)
F(19)-C(107)	1.303(6)

F(20)-C(107)	1.324(6)
F(21)-C(107)	1.304(6)
F(22)-C(108)	1.344(7)
F(22A)-C(108)	1.376(13)
F(23)-C(108)	1.286(7)
F(23A)-C(108)	1.377(13)
F(24)-C(108)	1.383(8)
F(24A)-C(108)	1.283(13)
F(25)-C(115)	1.332(6)
F(26)-C(115)	1.345(5)
F(27)-C(115)	1.338(7)
F(28)-C(116)	1.345(6)
F(29)-C(116)	1.317(8)
F(30)-C(116)	1.308(6)
F(31)-C(123)	1.344(4)
F(32)-C(123)	1.342(4)
F(33)-C(123)	1.340(4)
F(34)-C(124)	1.313(7)
F(35)-C(124)	1.375(8)
F(36)-C(124)	1.279(7)
F(37)-C(131)	1.336(5)
F(38)-C(131)	1.301(4)
F(39)-C(131)	1.297(5)
F(40)-C(132)	1.309(4)
F(41)-C(132)	1.296(5)
F(42)-C(132)	1.334(5)
F(43)-C(139)	1.305(10)
F(43A)-C(1H)	1.279(15)
F(44)-C(139)	1.435(13)
F(44A)-C(1H)	1.296(12)
F(45)-C(139)	1.210(10)
F(45A)-C(1H)	1.309(12)
F(46)-C(140)	1.344(9)
F(46A)-C(1G)	1.37(2)
F(47)-C(140)	1.341(10)
F(47A)-C(1G)	1.35(3)
F(48)-C(140)	1.359(15)
F(48A)-C(1G)	1.39(2)
O(1)-C(19)	1.334(4)
O(2)-C(38)	1.335(4)
O(3)-N(7)	1.358(6)
O(3A)-N(7A)	1.26(3)
O(4)-N(8)	1.358(6)
O(4A)-N(8A)	1.28(3)
O(5)-C(76)	1.343(4)
O(6)-C(57)	1.345(4)
N(1)-C(6)	1.469(4)
N(1)-C(7)	1.485(4)
N(1)-C(13)	1.490(4)
N(2)-C(1)	1.353(4)
N(2)-C(5)	1.342(5)

N(3)-C(8)	1.339(4)
N(3)-C(12)	1.349(4)
N(4)-C(25)	1.482(4)
N(4)-C(26)	1.476(4)
N(4)-C(32)	1.483(4)
N(5)-C(20)	1.344(4)
N(5)-C(24)	1.350(5)
N(6)-C(27)	1.337(5)
N(6)-C(31)	1.343(4)
N(7)-N(8)	1.257(8)
N(7A)-N(8A)	1.34(3)
N(9)-C(44)	1.474(5)
N(9)-C(45)	1.484(5)
N(9)-C(51)	1.489(4)
N(10)-C(39)	1.347(5)
N(10)-C(43)	1.353(5)
N(11)-C(46)	1.346(4)
N(11)-C(50)	1.341(4)
N(12)-C(63)	1.467(5)
N(12)-C(64)	1.486(5)
N(12)-C(70)	1.487(5)
N(13)-C(58)	1.355(5)
N(13)-C(62)	1.342(5)
N(14)-C(65)	1.337(5)
N(14)-C(69)	1.343(5)
C(1)-C(2)	1.378(5)
C(1A)-C(1H)	1.461(10)
C(1C)-B(2)	1.618(5)
C(1E)-C(1G)	1.43(3)
C(2)-C(3)	1.374(6)
C(3)-C(4)	1.384(5)
C(4)-C(5)	1.379(5)
C(5)-C(6)	1.516(5)
C(7)-C(8)	1.512(4)
C(8)-C(9)	1.381(4)
C(9)-C(10)	1.379(5)
C(10)-C(11)	1.387(5)
C(11)-C(12)	1.377(5)
C(13)-C(14)	1.496(4)
C(14)-C(15)	1.403(5)
C(14)-C(19)	1.397(4)
C(15)-C(16)	1.380(5)
C(16)-C(17)	1.374(6)
C(17)-C(18)	1.388(5)
C(18)-C(19)	1.401(4)
C(20)-C(21)	1.390(6)
C(21)-C(22)	1.367(7)
C(22)-C(23)	1.385(6)
C(23)-C(24)	1.386(5)
C(24)-C(25)	1.504(5)
C(26)-C(27)	1.506(5)

C(27)-C(28)	1.381(5)
C(28)-C(29)	1.376(6)
C(29)-C(30)	1.387(6)
C(30)-C(31)	1.377(5)
C(32)-C(33)	1.503(5)
C(33)-C(34)	1.392(5)
C(33)-C(38)	1.415(4)
C(34)-C(35)	1.386(5)
C(35)-C(36)	1.382(5)
C(36)-C(37)	1.401(5)
C(37)-C(38)	1.396(5)
C(39)-C(40)	1.377(7)
C(40)-C(41)	1.376(7)
C(41)-C(42)	1.377(6)
C(42)-C(43)	1.378(6)
C(43)-C(44)	1.505(5)
C(45)-C(46)	1.506(5)
C(46)-C(47)	1.387(5)
C(47)-C(48)	1.368(6)
C(48)-C(49)	1.390(5)
C(49)-C(50)	1.377(5)
C(51)-C(52)	1.490(6)
C(52)-C(53)	1.390(6)
C(52)-C(57)	1.416(5)
C(53)-C(54)	1.383(7)
C(54)-C(55)	1.390(6)
C(55)-C(56)	1.391(6)
C(56)-C(57)	1.375(5)
C(58)-C(59)	1.358(6)
C(59)-C(60)	1.377(8)
C(60)-C(61)	1.399(7)
C(61)-C(62)	1.371(6)
C(62)-C(63)	1.517(5)
C(64)-C(65)	1.505(5)
C(65)-C(66)	1.383(6)
C(66)-C(67)	1.379(7)
C(67)-C(68)	1.378(6)
C(68)-C(69)	1.369(5)
C(70)-C(71)	1.496(5)
C(71)-C(72)	1.399(5)
C(71)-C(76)	1.418(5)
C(72)-C(73)	1.376(6)
C(73)-C(74)	1.393(5)
C(74)-C(75)	1.391(5)
C(75)-C(76)	1.386(5)
C(77)-C(78)	1.404(5)
C(77)-C(82)	1.399(5)
C(77)-B(1)	1.638(5)
C(78)-C(79)	1.384(5)
C(79)-C(80)	1.378(5)
C(79)-C(83)	1.492(5)

C(80)-C(81)	1.397(5)
C(81)-C(82)	1.391(5)
C(81)-C(84)	1.488(5)
C(85)-C(86)	1.400(5)
C(85)-C(90)	1.398(5)
C(85)-B(1)	1.637(5)
C(86)-C(87)	1.387(4)
C(87)-C(88)	1.387(5)
C(87)-C(91)	1.494(5)
C(88)-C(89)	1.385(5)
C(89)-C(90)	1.405(5)
C(89)-C(92)	1.483(5)
C(93)-C(94)	1.402(5)
C(93)-C(98)	1.394(5)
C(93)-B(1)	1.645(5)
C(94)-C(95)	1.385(5)
C(95)-C(96)	1.391(6)
C(95)-C(99)	1.488(5)
C(96)-C(97)	1.381(5)
C(97)-C(98)	1.397(5)
C(97)-C(100)	1.481(6)
C(101)-C(102)	1.403(5)
C(101)-C(106)	1.394(5)
C(101)-B(1)	1.641(5)
C(102)-C(103)	1.391(5)
C(103)-C(104)	1.385(6)
C(103)-C(107)	1.501(6)
C(104)-C(105)	1.385(6)
C(105)-C(106)	1.397(5)
C(105)-C(108)	1.483(6)
C(109)-C(110)	1.390(8)
C(109)-C(114)	1.405(5)
C(109)-B(2)	1.627(8)
C(110)-C(111)	1.402(8)
C(111)-C(112)	1.397(6)
C(111)-C(115)	1.489(8)
C(112)-C(113)	1.387(8)
C(113)-C(114)	1.381(8)
C(113)-C(116)	1.499(6)
C(117)-C(118)	1.405(5)
C(117)-C(122)	1.411(6)
C(117)-B(2)	1.642(7)
C(118)-C(119)	1.383(5)
C(119)-C(120)	1.379(5)
C(119)-C(123)	1.500(4)
C(120)-C(121)	1.388(5)
C(121)-C(122)	1.381(7)
C(121)-C(124)	1.497(7)
C(125)-C(126)	1.400(5)
C(125)-C(130)	1.401(5)
C(125)-B(2)	1.644(5)

C(126)-C(127)	1.380(5)
C(127)-C(128)	1.399(4)
C(127)-C(131)	1.496(5)
C(128)-C(129)	1.374(5)
C(129)-C(130)	1.388(5)
C(129)-C(132)	1.491(5)
C(133)-B(2)	1.816(6)
C(135)-C(139)	1.454(9)
C(137)-C(140)	1.474(8)
C(141)-C(142)	1.464(10)
C(142)-C(143)	1.414(10)
C(143)-C(144)	1.468(10)
C(144)-C(145)	1.457(10)
O(1)-Fe(1)-O(2)	77.15(8)
O(1)-Fe(1)-N(1)	86.03(9)
O(1)-Fe(1)-N(2)	158.21(9)
O(1)-Fe(1)-N(3)	90.75(9)
O(1)-Fe(1)-N(7)	93.97(17)
O(2)-Fe(1)-N(1)	102.23(9)
O(2)-Fe(1)-N(2)	94.25(9)
O(2)-Fe(1)-N(3)	167.86(9)
O(2)-Fe(1)-N(7)	88.74(15)
O(3A)-Fe(1)-O(1)	122.4(3)
O(3A)-Fe(1)-O(2)	97.4(3)
O(3A)-Fe(1)-N(1)	148.6(3)
O(3A)-Fe(1)-N(2)	78.2(3)
O(3A)-Fe(1)-N(3)	88.1(3)
N(2)-Fe(1)-N(1)	76.16(10)
N(2)-Fe(1)-N(3)	97.47(10)
N(2)-Fe(1)-N(7)	105.95(17)
N(3)-Fe(1)-N(1)	77.62(9)
N(3)-Fe(1)-N(7)	91.10(15)
N(7)-Fe(1)-N(1)	168.72(15)
O(1)-Fe(2)-N(4)	104.37(9)
O(1)-Fe(2)-N(5)	92.53(10)
O(1)-Fe(2)-N(6)	166.57(9)
O(1)-Fe(2)-N(8A)	85.4(4)
O(2)-Fe(2)-O(1)	77.24(8)
O(2)-Fe(2)-N(4)	87.09(9)
O(2)-Fe(2)-N(5)	157.44(10)
O(2)-Fe(2)-N(6)	89.55(9)
O(2)-Fe(2)-N(8A)	89.0(6)
O(4)-Fe(2)-O(1)	93.89(11)
O(4)-Fe(2)-O(2)	114.92(12)
O(4)-Fe(2)-N(4)	154.28(12)
O(4)-Fe(2)-N(5)	85.48(13)
O(4)-Fe(2)-N(6)	89.46(11)
N(4)-Fe(2)-N(8A)	168.3(4)
N(5)-Fe(2)-N(4)	75.91(11)
N(5)-Fe(2)-N(6)	100.71(10)

N(5)-Fe(2)-N(8A)	110.5(6)
N(6)-Fe(2)-N(4)	76.99(10)
N(6)-Fe(2)-N(8A)	92.0(4)
O(3)-Fe(3)-O(5)	94.56(10)
O(3)-Fe(3)-O(6)	114.12(12)
O(3)-Fe(3)-N(9)	154.67(12)
O(3)-Fe(3)-N(10)	86.65(12)
O(3)-Fe(3)-N(11)	88.03(10)
O(5)-Fe(3)-N(7A)	84.9(4)
O(5)-Fe(3)-N(9)	105.03(10)
O(5)-Fe(3)-N(10)	95.47(11)
O(5)-Fe(3)-N(11)	163.62(10)
O(6)-Fe(3)-O(5)	76.88(9)
O(6)-Fe(3)-N(7A)	87.0(6)
O(6)-Fe(3)-N(9)	86.32(10)
O(6)-Fe(3)-N(10)	158.13(10)
O(6)-Fe(3)-N(11)	87.30(10)
N(9)-Fe(3)-N(7A)	166.4(5)
N(10)-Fe(3)-N(7A)	113.0(6)
N(10)-Fe(3)-N(9)	75.79(11)
N(10)-Fe(3)-N(11)	100.83(11)
N(11)-Fe(3)-N(7A)	90.1(4)
N(11)-Fe(3)-N(9)	77.73(11)
O(4A)-Fe(4)-O(5)	123.6(3)
O(4A)-Fe(4)-O(6)	97.0(3)
O(4A)-Fe(4)-N(12)	146.2(3)
O(4A)-Fe(4)-N(13)	77.3(3)
O(4A)-Fe(4)-N(14)	86.9(3)
O(5)-Fe(4)-O(6)	77.70(10)
O(5)-Fe(4)-N(8)	92.98(16)
O(5)-Fe(4)-N(12)	87.77(10)
O(5)-Fe(4)-N(13)	157.07(11)
O(5)-Fe(4)-N(14)	94.41(10)
O(6)-Fe(4)-N(8)	86.47(14)
O(6)-Fe(4)-N(12)	102.57(10)
O(6)-Fe(4)-N(13)	91.16(10)
O(6)-Fe(4)-N(14)	172.10(10)
N(8)-Fe(4)-N(12)	170.87(15)
N(13)-Fe(4)-N(8)	106.43(17)
N(13)-Fe(4)-N(12)	75.03(11)
N(13)-Fe(4)-N(14)	96.42(11)
N(14)-Fe(4)-N(8)	93.51(15)
N(14)-Fe(4)-N(12)	77.37(11)
Fe(1)-O(1)-Fe(2)	93.14(8)
C(19)-O(1)-Fe(1)	122.80(19)
C(19)-O(1)-Fe(2)	144.0(2)
Fe(2)-O(2)-Fe(1)	91.04(8)
C(38)-O(2)-Fe(1)	145.6(2)
C(38)-O(2)-Fe(2)	123.3(2)
N(7)-O(3)-Fe(3)	120.5(3)
N(7A)-O(3A)-Fe(1)	115.9(13)

N(8)-O(4)-Fe(2)	123.4(3)
N(8A)-O(4A)-Fe(4)	118.5(14)
Fe(4)-O(5)-Fe(3)	92.96(9)
C(76)-O(5)-Fe(3)	146.5(2)
C(76)-O(5)-Fe(4)	120.5(2)
Fe(3)-O(6)-Fe(4)	92.65(9)
C(57)-O(6)-Fe(3)	126.0(2)
C(57)-O(6)-Fe(4)	141.0(2)
C(6)-N(1)-Fe(1)	104.87(19)
C(6)-N(1)-C(7)	111.1(2)
C(6)-N(1)-C(13)	110.2(2)
C(7)-N(1)-Fe(1)	108.48(16)
C(7)-N(1)-C(13)	110.3(2)
C(13)-N(1)-Fe(1)	111.76(19)
C(1)-N(2)-Fe(1)	126.7(2)
C(5)-N(2)-Fe(1)	115.2(2)
C(5)-N(2)-C(1)	117.9(3)
C(8)-N(3)-Fe(1)	115.24(18)
C(8)-N(3)-C(12)	118.2(3)
C(12)-N(3)-Fe(1)	123.2(2)
C(25)-N(4)-Fe(2)	104.4(2)
C(25)-N(4)-C(32)	110.1(2)
C(26)-N(4)-Fe(2)	108.12(19)
C(26)-N(4)-C(25)	111.1(3)
C(26)-N(4)-C(32)	110.8(3)
C(32)-N(4)-Fe(2)	112.1(2)
C(20)-N(5)-Fe(2)	127.0(3)
C(20)-N(5)-C(24)	118.3(3)
C(24)-N(5)-Fe(2)	114.6(2)
C(27)-N(6)-Fe(2)	115.4(2)
C(27)-N(6)-C(31)	118.5(3)
C(31)-N(6)-Fe(2)	124.1(2)
O(3)-N(7)-Fe(1)	107.1(3)
N(8)-N(7)-Fe(1)	138.0(6)
N(8)-N(7)-O(3)	113.4(6)
O(3A)-N(7A)-Fe(3)	103.4(13)
O(3A)-N(7A)-N(8A)	118(2)
N(8A)-N(7A)-Fe(3)	137(2)
O(4)-N(8)-Fe(4)	103.1(3)
N(7)-N(8)-Fe(4)	141.9(6)
N(7)-N(8)-O(4)	114.2(6)
O(4A)-N(8A)-Fe(2)	102.8(15)
O(4A)-N(8A)-N(7A)	118(2)
N(7A)-N(8A)-Fe(2)	139(2)
C(44)-N(9)-Fe(3)	105.8(2)
C(44)-N(9)-C(45)	110.7(3)
C(44)-N(9)-C(51)	109.9(3)
C(45)-N(9)-Fe(3)	107.46(19)
C(45)-N(9)-C(51)	111.0(3)
C(51)-N(9)-Fe(3)	111.9(2)
C(39)-N(10)-Fe(3)	126.2(3)

C(39)-N(10)-C(43)	117.1(4)
C(43)-N(10)-Fe(3)	116.5(2)
C(46)-N(11)-Fe(3)	114.0(2)
C(50)-N(11)-Fe(3)	122.8(2)
C(50)-N(11)-C(46)	118.4(3)
C(63)-N(12)-Fe(4)	104.3(2)
C(63)-N(12)-C(64)	111.3(3)
C(63)-N(12)-C(70)	111.0(3)
C(64)-N(12)-Fe(4)	108.1(2)
C(64)-N(12)-C(70)	110.7(3)
C(70)-N(12)-Fe(4)	111.2(2)
C(58)-N(13)-Fe(4)	126.9(3)
C(62)-N(13)-Fe(4)	114.4(2)
C(62)-N(13)-C(58)	118.3(3)
C(65)-N(14)-Fe(4)	116.1(2)
C(65)-N(14)-C(69)	118.0(3)
C(69)-N(14)-Fe(4)	124.7(2)
N(2)-C(1)-C(2)	122.6(4)
C(1B)-C(1A)-C(1H)	119.7(5)
C(1F)-C(1A)-C(1H)	120.3(5)
C(1B)-C(1C)-B(2)	115.0(4)
C(1D)-C(1C)-B(2)	124.4(4)
C(1D)-C(1E)-C(1G)	120.5(9)
C(1F)-C(1E)-C(1G)	119.2(9)
F(46A)-C(1G)-F(48A)	101.5(15)
F(46A)-C(1G)-C(1E)	115(2)
F(47A)-C(1G)-F(46A)	104.8(16)
F(47A)-C(1G)-F(48A)	104(2)
F(47A)-C(1G)-C(1E)	117.8(16)
F(48A)-C(1G)-C(1E)	112.3(15)
F(43A)-C(1H)-F(44A)	108.2(9)
F(43A)-C(1H)-F(45A)	102.0(10)
F(43A)-C(1H)-C(1A)	113.4(9)
F(44A)-C(1H)-F(45A)	104.5(10)
F(44A)-C(1H)-C(1A)	112.4(8)
F(45A)-C(1H)-C(1A)	115.5(8)
C(3)-C(2)-C(1)	118.8(3)
C(2)-C(3)-C(4)	119.4(4)
C(5)-C(4)-C(3)	118.8(4)
N(2)-C(5)-C(4)	122.5(3)
N(2)-C(5)-C(6)	115.8(3)
C(4)-C(5)-C(6)	121.6(3)
N(1)-C(6)-C(5)	110.1(2)
N(1)-C(7)-C(8)	112.2(2)
N(3)-C(8)-C(7)	115.8(3)
N(3)-C(8)-C(9)	122.2(3)
C(9)-C(8)-C(7)	121.9(3)
C(10)-C(9)-C(8)	119.3(3)
C(9)-C(10)-C(11)	119.0(3)
C(12)-C(11)-C(10)	118.4(3)
N(3)-C(12)-C(11)	122.8(3)

N(1)-C(13)-C(14)	111.4(2)
C(15)-C(14)-C(13)	120.8(3)
C(19)-C(14)-C(13)	119.6(3)
C(19)-C(14)-C(15)	119.6(3)
C(16)-C(15)-C(14)	121.0(3)
C(17)-C(16)-C(15)	119.3(3)
C(16)-C(17)-C(18)	121.0(3)
C(17)-C(18)-C(19)	120.3(3)
O(1)-C(19)-C(14)	119.6(3)
O(1)-C(19)-C(18)	121.5(3)
C(14)-C(19)-C(18)	118.8(3)
N(5)-C(20)-C(21)	122.2(4)
C(22)-C(21)-C(20)	119.2(4)
C(21)-C(22)-C(23)	119.1(4)
C(22)-C(23)-C(24)	119.2(4)
N(5)-C(24)-C(23)	121.9(3)
N(5)-C(24)-C(25)	115.7(3)
C(23)-C(24)-C(25)	122.3(3)
N(4)-C(25)-C(24)	110.8(3)
N(4)-C(26)-C(27)	111.8(3)
N(6)-C(27)-C(26)	115.8(3)
N(6)-C(27)-C(28)	121.6(3)
C(28)-C(27)-C(26)	122.5(3)
C(29)-C(28)-C(27)	119.7(4)
C(28)-C(29)-C(30)	118.9(4)
C(31)-C(30)-C(29)	118.2(4)
N(6)-C(31)-C(30)	123.0(4)
N(4)-C(32)-C(33)	113.8(3)
C(34)-C(33)-C(32)	121.3(3)
C(34)-C(33)-C(38)	119.6(3)
C(38)-C(33)-C(32)	119.1(3)
C(35)-C(34)-C(33)	121.3(3)
C(36)-C(35)-C(34)	119.2(3)
C(35)-C(36)-C(37)	120.7(3)
C(38)-C(37)-C(36)	120.4(3)
O(2)-C(38)-C(33)	119.5(3)
O(2)-C(38)-C(37)	121.8(3)
C(37)-C(38)-C(33)	118.7(3)
N(10)-C(39)-C(40)	122.3(4)
C(41)-C(40)-C(39)	120.1(4)
C(40)-C(41)-C(42)	118.3(5)
C(41)-C(42)-C(43)	119.1(4)
N(10)-C(43)-C(42)	123.1(4)
N(10)-C(43)-C(44)	114.8(3)
C(42)-C(43)-C(44)	122.1(4)
N(9)-C(44)-C(43)	111.1(3)
N(9)-C(45)-C(46)	111.9(3)
N(11)-C(46)-C(45)	115.1(3)
N(11)-C(46)-C(47)	121.3(3)
C(47)-C(46)-C(45)	123.6(3)
C(48)-C(47)-C(46)	119.6(3)

C(47)-C(48)-C(49)	119.6(3)
C(50)-C(49)-C(48)	117.6(4)
N(11)-C(50)-C(49)	123.4(3)
N(9)-C(51)-C(52)	113.2(3)
C(53)-C(52)-C(51)	121.3(3)
C(53)-C(52)-C(57)	118.4(4)
C(57)-C(52)-C(51)	120.3(3)
C(54)-C(53)-C(52)	121.8(4)
C(53)-C(54)-C(55)	119.2(4)
C(54)-C(55)-C(56)	120.0(5)
C(57)-C(56)-C(55)	120.9(4)
O(6)-C(57)-C(52)	118.6(3)
O(6)-C(57)-C(56)	121.7(3)
C(56)-C(57)-C(52)	119.7(3)
N(13)-C(58)-C(59)	122.7(4)
C(58)-C(59)-C(60)	119.1(4)
C(59)-C(60)-C(61)	119.0(5)
C(62)-C(61)-C(60)	118.8(5)
N(13)-C(62)-C(61)	122.1(4)
N(13)-C(62)-C(63)	116.0(3)
C(61)-C(62)-C(63)	121.8(4)
N(12)-C(63)-C(62)	110.2(3)
N(12)-C(64)-C(65)	112.7(3)
N(14)-C(65)-C(64)	116.5(3)
N(14)-C(65)-C(66)	122.0(4)
C(66)-C(65)-C(64)	121.5(4)
C(67)-C(66)-C(65)	119.3(4)
C(68)-C(67)-C(66)	118.8(4)
C(69)-C(68)-C(67)	118.8(4)
N(14)-C(69)-C(68)	123.1(4)
N(12)-C(70)-C(71)	113.3(3)
C(72)-C(71)-C(70)	121.8(3)
C(72)-C(71)-C(76)	119.4(3)
C(76)-C(71)-C(70)	118.8(3)
C(73)-C(72)-C(71)	121.2(3)
C(72)-C(73)-C(74)	119.4(4)
C(75)-C(74)-C(73)	120.3(4)
C(76)-C(75)-C(74)	121.0(3)
O(5)-C(76)-C(71)	119.1(3)
O(5)-C(76)-C(75)	122.2(3)
C(75)-C(76)-C(71)	118.7(3)
C(78)-C(77)-B(1)	120.9(3)
C(82)-C(77)-C(78)	115.5(3)
C(82)-C(77)-B(1)	123.1(3)
C(79)-C(78)-C(77)	122.7(3)
C(78)-C(79)-C(83)	120.8(3)
C(80)-C(79)-C(78)	120.9(3)
C(80)-C(79)-C(83)	118.3(3)
C(79)-C(80)-C(81)	118.0(3)
C(80)-C(81)-C(84)	118.2(3)
C(82)-C(81)-C(80)	120.8(3)

C(82)-C(81)-C(84)	121.0(3)
C(81)-C(82)-C(77)	122.2(3)
F(1)-C(83)-F(2)	104.6(3)
F(1)-C(83)-F(3)	108.6(4)
F(1)-C(83)-C(79)	114.4(3)
F(2)-C(83)-F(3)	101.9(4)
F(2)-C(83)-C(79)	113.8(3)
F(3)-C(83)-C(79)	112.5(3)
F(4)-C(84)-F(5)	106.1(3)
F(4)-C(84)-C(81)	112.6(3)
F(5)-C(84)-C(81)	112.6(3)
F(6)-C(84)-F(4)	106.6(3)
F(6)-C(84)-F(5)	104.1(3)
F(6)-C(84)-C(81)	114.1(3)
C(86)-C(85)-B(1)	120.8(3)
C(90)-C(85)-C(86)	115.5(3)
C(90)-C(85)-B(1)	123.3(3)
C(87)-C(86)-C(85)	122.6(3)
C(86)-C(87)-C(88)	121.0(3)
C(86)-C(87)-C(91)	119.0(3)
C(88)-C(87)-C(91)	119.9(3)
C(89)-C(88)-C(87)	118.0(3)
C(88)-C(89)-C(90)	120.6(3)
C(88)-C(89)-C(92)	120.1(3)
C(90)-C(89)-C(92)	119.2(3)
C(85)-C(90)-C(89)	122.3(3)
F(7)-C(91)-F(8)	105.3(3)
F(7)-C(91)-F(9)	106.3(3)
F(7)-C(91)-C(87)	112.8(3)
F(8)-C(91)-F(9)	106.2(3)
F(8)-C(91)-C(87)	112.9(3)
F(9)-C(91)-C(87)	112.8(3)
F(10)-C(92)-C(89)	112.8(4)
F(11)-C(92)-F(10)	103.7(3)
F(11)-C(92)-F(12)	107.8(4)
F(11)-C(92)-C(89)	113.6(4)
F(12)-C(92)-F(10)	105.2(4)
F(12)-C(92)-C(89)	113.0(3)
C(94)-C(93)-B(1)	120.1(3)
C(98)-C(93)-C(94)	115.6(3)
C(98)-C(93)-B(1)	123.7(3)
C(95)-C(94)-C(93)	122.1(3)
C(94)-C(95)-C(96)	121.2(3)
C(94)-C(95)-C(99)	120.6(4)
C(96)-C(95)-C(99)	118.3(4)
C(97)-C(96)-C(95)	117.8(3)
C(96)-C(97)-C(98)	120.7(3)
C(96)-C(97)-C(100)	119.7(3)
C(98)-C(97)-C(100)	119.6(3)
C(93)-C(98)-C(97)	122.5(3)
F(13)-C(99)-C(95)	112.6(4)

F(14)-C(99)-F(13)	107.7(5)
F(14)-C(99)-F(15)	105.5(4)
F(14)-C(99)-C(95)	112.2(3)
F(15)-C(99)-F(13)	104.4(3)
F(15)-C(99)-C(95)	113.8(4)
F(16)-C(100)-C(97)	113.5(4)
F(17)-C(100)-F(16)	104.9(4)
F(17)-C(100)-C(97)	112.6(3)
F(18)-C(100)-F(16)	106.5(4)
F(18)-C(100)-F(17)	104.8(4)
F(18)-C(100)-C(97)	113.8(3)
C(102)-C(101)-B(1)	119.9(3)
C(106)-C(101)-C(102)	115.7(3)
C(106)-C(101)-B(1)	124.1(3)
C(103)-C(102)-C(101)	122.3(4)
C(102)-C(103)-C(107)	120.0(4)
C(104)-C(103)-C(102)	120.8(4)
C(104)-C(103)-C(107)	119.1(4)
C(103)-C(104)-C(105)	118.1(4)
C(104)-C(105)-C(106)	120.9(4)
C(104)-C(105)-C(108)	119.1(4)
C(106)-C(105)-C(108)	120.0(4)
C(101)-C(106)-C(105)	122.2(3)
F(19)-C(107)-F(20)	101.9(4)
F(19)-C(107)-F(21)	108.2(5)
F(19)-C(107)-C(103)	114.8(4)
F(20)-C(107)-C(103)	111.9(4)
F(21)-C(107)-F(20)	106.1(5)
F(21)-C(107)-C(103)	113.0(4)
F(22)-C(108)-F(24)	100.5(5)
F(22)-C(108)-C(105)	111.4(5)
F(22A)-C(108)-F(23A)	92.0(8)
F(22A)-C(108)-C(105)	112.0(6)
F(23)-C(108)-F(22)	110.1(5)
F(23)-C(108)-F(24)	104.2(6)
F(23)-C(108)-C(105)	117.3(4)
F(23A)-C(108)-C(105)	109.5(5)
F(24)-C(108)-C(105)	111.9(4)
F(24A)-C(108)-F(22A)	118.4(8)
F(24A)-C(108)-F(23A)	100.2(10)
F(24A)-C(108)-C(105)	119.5(6)
C(110)-C(109)-C(114)	115.2(5)
C(110)-C(109)-B(2)	125.1(4)
C(114)-C(109)-B(2)	119.5(5)
C(109)-C(110)-C(111)	123.0(4)
C(110)-C(111)-C(115)	119.6(4)
C(112)-C(111)-C(110)	120.0(5)
C(112)-C(111)-C(115)	120.3(5)
C(113)-C(112)-C(111)	117.8(5)
C(112)-C(113)-C(116)	117.9(5)
C(114)-C(113)-C(112)	121.3(4)

C(114)-C(113)-C(116)	120.8(5)
C(113)-C(114)-C(109)	122.6(5)
F(25)-C(115)-F(26)	106.4(4)
F(25)-C(115)-F(27)	106.1(5)
F(25)-C(115)-C(111)	113.3(5)
F(26)-C(115)-C(111)	113.0(5)
F(27)-C(115)-F(26)	103.5(4)
F(27)-C(115)-C(111)	113.8(4)
F(28)-C(116)-C(113)	111.9(4)
F(29)-C(116)-F(28)	106.6(4)
F(29)-C(116)-C(113)	113.7(5)
F(30)-C(116)-F(28)	104.5(5)
F(30)-C(116)-F(29)	105.4(4)
F(30)-C(116)-C(113)	114.0(4)
C(118)-C(117)-C(122)	114.7(4)
C(118)-C(117)-B(2)	125.0(4)
C(122)-C(117)-B(2)	120.2(3)
C(119)-C(118)-C(117)	122.2(3)
C(118)-C(119)-C(123)	119.1(3)
C(120)-C(119)-C(118)	121.4(3)
C(120)-C(119)-C(123)	119.4(3)
C(119)-C(120)-C(121)	118.1(4)
C(120)-C(121)-C(124)	118.5(5)
C(122)-C(121)-C(120)	120.4(4)
C(122)-C(121)-C(124)	121.1(4)
C(121)-C(122)-C(117)	123.0(3)
F(31)-C(123)-C(119)	112.4(3)
F(32)-C(123)-F(31)	105.3(3)
F(32)-C(123)-C(119)	113.0(3)
F(33)-C(123)-F(31)	106.1(2)
F(33)-C(123)-F(32)	106.6(3)
F(33)-C(123)-C(119)	112.9(3)
F(34)-C(124)-F(35)	100.1(6)
F(34)-C(124)-C(121)	114.8(4)
F(35)-C(124)-C(121)	113.2(4)
F(36)-C(124)-F(34)	111.5(5)
F(36)-C(124)-F(35)	103.4(5)
F(36)-C(124)-C(121)	112.7(6)
C(126)-C(125)-C(130)	115.7(3)
C(126)-C(125)-B(2)	119.8(3)
C(130)-C(125)-B(2)	124.5(3)
C(127)-C(126)-C(125)	122.3(3)
C(126)-C(127)-C(128)	120.8(3)
C(126)-C(127)-C(131)	119.5(3)
C(128)-C(127)-C(131)	119.6(3)
C(129)-C(128)-C(127)	118.0(3)
C(128)-C(129)-C(130)	121.0(3)
C(128)-C(129)-C(132)	119.6(3)
C(130)-C(129)-C(132)	119.4(3)
C(129)-C(130)-C(125)	122.2(3)
F(37)-C(131)-C(127)	111.9(3)

F(38)-C(131)-F(37)	104.7(3)
F(38)-C(131)-C(127)	114.1(3)
F(39)-C(131)-F(37)	104.4(4)
F(39)-C(131)-F(38)	106.8(4)
F(39)-C(131)-C(127)	114.0(3)
F(40)-C(132)-F(42)	105.0(3)
F(40)-C(132)-C(129)	113.5(3)
F(41)-C(132)-F(40)	108.4(4)
F(41)-C(132)-F(42)	102.8(3)
F(41)-C(132)-C(129)	113.5(3)
F(42)-C(132)-C(129)	112.8(3)
C(134)-C(133)-B(2)	127.6(3)
C(138)-C(133)-B(2)	112.4(3)
C(134)-C(135)-C(139)	119.0(4)
C(136)-C(135)-C(139)	121.0(4)
C(136)-C(137)-C(140)	118.4(4)
C(138)-C(137)-C(140)	121.5(4)
F(43)-C(139)-F(44)	95.6(8)
F(43)-C(139)-C(135)	115.6(6)
F(44)-C(139)-C(135)	109.6(7)
F(45)-C(139)-F(43)	111.9(9)
F(45)-C(139)-F(44)	103.4(8)
F(45)-C(139)-C(135)	117.6(8)
F(46)-C(140)-F(48)	106.7(8)
F(46)-C(140)-C(137)	112.8(6)
F(47)-C(140)-F(46)	104.8(6)
F(47)-C(140)-F(48)	105.2(8)
F(47)-C(140)-C(137)	113.2(6)
F(48)-C(140)-C(137)	113.4(8)
C(143)-C(142)-C(141)	123.4(6)
C(142)-C(143)-C(144)	123.5(6)
C(145)-C(144)-C(143)	124.0(6)
C(77)-B(1)-C(93)	103.1(2)
C(77)-B(1)-C(101)	112.7(3)
C(85)-B(1)-C(77)	112.8(3)
C(85)-B(1)-C(93)	112.2(3)
C(85)-B(1)-C(101)	103.3(2)
C(101)-B(1)-C(93)	113.1(3)
C(1C)-B(2)-C(109)	94.0(4)
C(1C)-B(2)-C(117)	121.7(4)
C(1C)-B(2)-C(125)	109.7(3)
C(109)-B(2)-C(117)	112.1(3)
C(109)-B(2)-C(125)	111.8(4)
C(109)-B(2)-C(133)	116.1(3)
C(117)-B(2)-C(125)	107.1(3)
C(117)-B(2)-C(133)	100.1(4)
C(125)-B(2)-C(133)	108.8(3)

Table S28. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$. The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Fe(1)	30(1)	27(1)	21(1)	3(1)	-4(1)	-8(1)
Fe(2)	36(1)	27(1)	29(1)	1(1)	-13(1)	-10(1)
Fe(3)	40(1)	38(1)	25(1)	-8(1)	-8(1)	-10(1)
Fe(4)	36(1)	38(1)	26(1)	2(1)	-5(1)	-10(1)
F(1)	63(2)	46(2)	144(3)	28(2)	32(2)	-16(2)
F(2)	110(2)	89(2)	94(2)	-26(2)	58(3)	-66(2)
F(3)	219(5)	269(6)	133(3)	133(4)	-124(3)	-224(5)
F(4)	98(2)	42(2)	68(2)	-18(2)	30(2)	-25(2)
F(5)	62(2)	45(2)	134(3)	22(2)	-57(2)	-19(2)
F(6)	44(2)	33(2)	72(2)	2(2)	-5(2)	-17(2)
F(7)	43(2)	57(2)	73(2)	1(2)	5(2)	-20(2)
F(8)	51(2)	41(2)	52(2)	-8(2)	-22(1)	-1(2)
F(9)	50(2)	37(2)	55(2)	-18(2)	-11(2)	-10(2)
F(10)	99(2)	136(3)	73(2)	39(3)	-55(2)	-66(2)
F(11)	64(2)	78(2)	83(3)	-28(2)	-24(2)	-31(2)
F(12)	45(2)	84(3)	68(2)	-19(2)	-15(2)	-27(2)
F(13)	156(3)	88(2)	63(3)	-6(2)	-27(2)	-87(2)
F(14)	55(2)	197(4)	210(4)	-156(4)	52(2)	-78(2)
F(15)	74(3)	82(2)	55(2)	-28(2)	-18(2)	-25(2)
F(16)	257(5)	102(3)	56(2)	36(3)	-78(3)	-93(3)
F(17)	57(2)	47(2)	110(2)	16(2)	-6(2)	-16(2)
F(18)	63(3)	89(2)	115(2)	53(3)	-24(2)	-42(2)
F(19)	73(2)	98(2)	79(3)	39(2)	-31(2)	-24(2)
F(20)	115(3)	94(3)	155(3)	79(3)	-67(3)	-51(2)
F(21)	123(3)	167(4)	49(2)	0(2)	-16(2)	68(3)
F(22)	31(2)	84(3)	156(4)	23(3)	-5(2)	-10(3)
F(22A)	46(2)	94(3)	156(4)	31(3)	-8(3)	-30(3)
F(23)	55(2)	81(3)	169(4)	56(3)	-11(3)	-34(2)
F(23A)	47(3)	93(3)	158(4)	25(3)	-19(3)	-38(2)
F(24)	45(2)	108(3)	152(4)	25(3)	-19(2)	-39(2)
F(24A)	39(3)	87(4)	154(4)	38(4)	-18(3)	-23(3)
F(25)	70(2)	83(2)	159(3)	28(2)	-32(2)	-43(2)
F(26)	96(2)	62(2)	120(3)	45(2)	-63(2)	-26(2)
F(27)	89(2)	83(2)	137(3)	36(2)	-68(2)	-38(3)
F(28)	62(2)	131(3)	138(3)	90(2)	-64(3)	-61(3)
F(29)	49(2)	140(3)	163(4)	9(3)	-50(2)	-38(2)
F(30)	94(2)	99(2)	195(4)	79(3)	-95(3)	-76(2)
F(31)	52(2)	51(2)	27(3)	7(1)	-10(1)	-21(2)
F(32)	41(2)	36(2)	55(2)	-5(2)	-17(1)	-6(2)
F(33)	53(2)	40(2)	55(2)	9(2)	-32(2)	-22(2)
F(34)	132(3)	125(3)	91(2)	-13(2)	-41(2)	-71(3)
F(35)	128(3)	120(3)	86(2)	-39(2)	-45(2)	-32(3)

F(36)	386(9)	187(5)	37(2)	19(2)	-59(3)	-192(6)
F(37)	91(2)	58(3)	97(2)	17(2)	24(3)	-38(2)
F(38)	41(2)	133(3)	112(2)	76(2)	-13(2)	-34(2)
F(39)	143(3)	227(5)	40(2)	3(2)	-1(2)	-145(3)
F(40)	49(2)	159(3)	37(2)	29(2)	-1(2)	-5(3)
F(41)	201(4)	59(3)	68(3)	31(2)	-77(2)	-47(2)
F(42)	79(3)	137(3)	50(2)	28(2)	-36(2)	-63(3)
F(43)	58(3)	79(3)	65(3)	5(2)	3(2)	-6(2)
F(43A)	92(4)	147(6)	95(4)	-73(4)	-43(4)	-27(4)
F(44)	84(3)	98(3)	126(4)	-6(3)	42(3)	-19(3)
F(44A)	70(3)	99(3)	95(3)	-16(3)	5(3)	1(3)
F(45)	111(4)	144(6)	87(4)	-67(4)	-57(3)	49(4)
F(45A)	116(4)	102(4)	132(4)	5(4)	71(4)	-11(3)
F(46)	78(3)	65(3)	84(4)	28(3)	-7(3)	-46(3)
F(46A)	83(4)	58(3)	62(3)	29(3)	3(3)	-30(3)
F(47)	90(4)	71(4)	93(4)	45(3)	-50(3)	-43(3)
F(47A)	143(7)	70(4)	93(5)	20(3)	-25(5)	-58(5)
F(48)	100(7)	37(4)	67(6)	18(4)	-4(4)	-20(4)
F(48A)	83(4)	50(3)	108(5)	32(3)	36(4)	1(3)
O(1)	30(2)	27(2)	34(2)	-1(1)	-4(2)	-10(2)
O(2)	37(2)	30(2)	34(2)	10(2)	-17(1)	-14(1)
O(3)	31(2)	32(2)	21(3)	2(2)	-3(2)	-16(2)
O(3A)	38(6)	23(5)	31(7)	3(4)	-12(4)	-8(4)
O(4)	33(3)	37(2)	26(2)	4(2)	-3(2)	-20(2)
O(4A)	36(5)	38(6)	31(7)	-3(4)	-7(4)	-17(5)
O(5)	46(2)	44(2)	30(2)	6(2)	-14(1)	-19(2)
O(6)	36(2)	35(2)	36(2)	-7(2)	-3(1)	-11(2)
N(1)	29(2)	39(2)	21(2)	6(2)	-6(2)	-16(2)
N(2)	32(2)	34(2)	32(2)	11(2)	-4(1)	-11(2)
N(3)	29(2)	27(2)	23(2)	3(2)	-6(2)	-12(2)
N(4)	33(2)	30(2)	36(2)	1(2)	-7(2)	-14(2)
N(5)	39(2)	29(2)	58(2)	2(2)	-23(2)	-16(2)
N(6)	34(2)	28(2)	41(2)	-1(2)	-10(2)	-12(2)
N(7)	30(3)	31(3)	24(3)	7(2)	-4(2)	-14(2)
N(7A)	21(9)	62(13)	27(9)	17(9)	-5(7)	-10(9)
N(8)	30(3)	29(2)	28(2)	3(2)	-7(2)	-14(3)
N(8A)	44(11)	25(8)	32(9)	5(8)	-7(9)	4(7)
N(9)	54(3)	47(3)	28(2)	-10(2)	-3(2)	-28(2)
N(10)	56(2)	42(2)	41(2)	-3(2)	-21(2)	-20(2)
N(11)	34(2)	32(2)	34(2)	-7(2)	-8(2)	-11(2)
N(12)	49(3)	34(2)	35(2)	2(2)	-8(2)	-19(2)
N(13)	37(2)	38(2)	45(2)	8(2)	-6(2)	-12(2)
N(14)	37(2)	36(2)	37(2)	7(2)	-7(2)	-13(2)
C(1)	33(2)	34(2)	44(2)	10(2)	0(2)	-8(2)
C(1A)	49(5)	57(6)	40(4)	12(4)	-2(4)	-14(4)
C(1B)	25(4)	42(5)	36(4)	2(4)	2(3)	-6(4)
C(1C)	29(3)	41(4)	29(3)	3(3)	-3(3)	-14(3)
C(1D)	34(3)	32(4)	38(4)	0(3)	2(3)	-7(3)
C(1E)	47(4)	46(5)	46(4)	11(3)	7(3)	-19(4)
C(1F)	40(5)	59(6)	45(4)	11(4)	17(4)	-14(4)
C(1G)	60(7)	83(12)	72(13)	54(11)	-3(8)	-32(7)

C(1H)	54(5)	62(6)	47(5)	12(4)	8(4)	-7(5)
C(2)	31(3)	46(2)	52(2)	12(2)	-2(2)	-11(2)
C(3)	28(3)	61(3)	70(3)	28(2)	-18(3)	-19(2)
C(4)	34(2)	56(2)	43(3)	16(3)	-16(2)	-19(2)
C(5)	29(2)	44(2)	38(3)	20(2)	-14(2)	-15(2)
C(6)	36(3)	51(2)	28(2)	11(2)	-13(2)	-22(2)
C(7)	34(2)	30(2)	26(2)	2(2)	-6(2)	-14(2)
C(8)	32(2)	30(2)	26(2)	4(2)	-5(2)	-16(2)
C(9)	37(2)	27(2)	34(2)	1(2)	-7(2)	-10(2)
C(10)	42(3)	30(2)	42(2)	6(2)	-16(2)	-7(2)
C(11)	43(2)	38(3)	30(2)	6(2)	-15(2)	-13(2)
C(12)	35(2)	30(3)	26(2)	2(2)	-9(2)	-13(2)
C(13)	35(2)	40(2)	19(2)	3(2)	-1(2)	-19(2)
C(14)	34(2)	32(3)	24(2)	3(2)	-2(2)	-16(2)
C(15)	37(2)	34(2)	32(2)	-3(2)	2(2)	-13(2)
C(16)	34(2)	37(2)	50(2)	-1(2)	3(2)	-7(2)
C(17)	29(3)	53(2)	50(2)	12(3)	-13(2)	-13(2)
C(18)	32(2)	42(3)	32(2)	3(2)	-8(2)	-16(2)
C(19)	28(2)	29(2)	27(2)	4(2)	-4(2)	-11(2)
C(20)	48(2)	35(2)	62(2)	3(2)	-26(2)	-19(2)
C(21)	50(2)	39(2)	91(3)	5(2)	-36(2)	-20(2)
C(22)	40(2)	48(2)	92(3)	0(2)	-19(2)	-21(3)
C(23)	39(3)	45(2)	71(3)	0(2)	-13(3)	-20(3)
C(24)	35(2)	32(3)	55(2)	-2(2)	-10(2)	-14(2)
C(25)	34(2)	36(2)	44(3)	-6(2)	-4(2)	-14(2)
C(26)	49(2)	33(2)	41(3)	5(2)	-10(2)	-18(2)
C(27)	46(3)	32(2)	44(2)	3(2)	-14(2)	-15(2)
C(28)	63(2)	33(2)	54(2)	9(2)	-19(3)	-11(3)
C(29)	55(2)	32(2)	64(2)	2(2)	-15(2)	-1(2)
C(30)	45(2)	34(2)	59(2)	-5(3)	-11(3)	-7(2)
C(31)	39(2)	33(3)	46(3)	-1(2)	-11(2)	-14(2)
C(32)	39(2)	39(3)	30(2)	1(2)	-10(2)	-18(2)
C(33)	38(2)	38(2)	30(2)	5(2)	-10(2)	-17(2)
C(34)	48(2)	52(2)	35(2)	18(2)	-16(2)	-20(2)
C(35)	44(2)	53(2)	44(3)	19(2)	-18(2)	-12(2)
C(36)	35(2)	50(2)	46(2)	13(3)	-13(2)	-10(2)
C(37)	35(2)	41(3)	30(2)	8(2)	-8(2)	-11(2)
C(38)	37(2)	29(3)	27(2)	7(2)	-13(2)	-12(2)
C(39)	69(3)	43(2)	47(2)	-6(2)	-23(2)	-19(2)
C(40)	110(4)	47(3)	65(3)	1(2)	-27(3)	-44(3)
C(41)	128(5)	68(3)	49(2)	9(2)	-21(3)	-65(3)
C(42)	100(4)	67(3)	41(2)	9(3)	-23(2)	-50(3)
C(43)	71(3)	54(2)	32(2)	5(2)	-21(2)	-34(2)
C(44)	78(3)	66(3)	28(2)	-1(2)	-10(3)	-45(2)
C(45)	44(2)	47(2)	39(2)	-13(2)	1(2)	-22(2)
C(46)	34(3)	41(2)	43(3)	-12(2)	-2(2)	-16(2)
C(47)	34(3)	40(2)	61(2)	-11(2)	-1(2)	-15(2)
C(48)	34(3)	33(2)	75(3)	2(2)	-14(2)	-8(2)
C(49)	36(2)	36(3)	50(2)	2(2)	-14(2)	-13(2)
C(50)	34(2)	34(2)	37(2)	-3(2)	-10(2)	-14(2)
C(51)	61(2)	60(2)	29(3)	-18(2)	2(2)	-35(2)

C(52)	49(2)	45(2)	39(2)	-18(2)	3(3)	-26(3)
C(53)	56(2)	52(3)	66(3)	-33(2)	22(2)	-29(2)
C(54)	51(2)	48(3)	98(4)	-32(2)	25(2)	-22(2)
C(55)	51(2)	42(2)	80(3)	-11(2)	10(2)	-16(3)
C(56)	41(3)	40(2)	47(2)	-7(2)	2(2)	-14(2)
C(57)	36(2)	38(3)	38(2)	-13(2)	-1(2)	-13(2)
C(58)	41(2)	50(2)	53(2)	-18(3)	-2(2)	-16(3)
C(59)	79(3)	60(3)	61(3)	18(2)	-6(2)	-33(3)
C(60)	92(4)	45(3)	101(4)	24(3)	-13(3)	-36(3)
C(61)	80(3)	45(3)	71(3)	8(2)	-10(2)	-30(2)
C(62)	45(2)	39(2)	58(2)	10(2)	-7(2)	-17(2)
C(63)	54(2)	37(2)	48(2)	1(2)	-8(3)	-19(2)
C(64)	49(2)	48(2)	44(3)	8(2)	-16(2)	-22(3)
C(65)	48(2)	41(2)	41(2)	8(2)	-13(2)	-18(2)
C(66)	56(2)	62(2)	58(2)	3(2)	-26(2)	-12(2)
C(67)	52(3)	61(3)	71(3)	1(2)	-28(2)	5(2)
C(68)	49(2)	50(2)	50(2)	-1(3)	-14(3)	-2(2)
C(69)	41(2)	38(3)	38(2)	3(2)	-6(2)	-12(2)
C(70)	64(2)	42(2)	30(2)	2(2)	-14(2)	-27(2)
C(71)	64(2)	42(2)	29(2)	4(2)	-16(2)	-27(3)
C(72)	87(3)	47(2)	38(2)	12(2)	-35(2)	-37(2)
C(73)	90(3)	51(2)	47(2)	18(3)	-41(2)	-33(2)
C(74)	79(3)	43(2)	41(3)	8(3)	-26(3)	-28(2)
C(75)	60(2)	46(2)	29(2)	3(2)	-19(2)	-26(2)
C(76)	51(2)	40(2)	27(2)	4(2)	-14(2)	-21(2)
C(77)	36(2)	30(3)	32(2)	2(2)	-8(2)	-14(2)
C(78)	41(2)	27(3)	38(3)	0(2)	-8(2)	-15(2)
C(79)	37(2)	39(3)	32(2)	2(2)	-8(2)	-19(2)
C(80)	33(2)	41(3)	34(3)	0(2)	-7(2)	-15(2)
C(81)	34(2)	32(2)	33(2)	1(2)	-9(2)	-14(2)
C(82)	35(2)	35(2)	33(2)	1(2)	-7(2)	-15(2)
C(83)	46(2)	45(2)	42(2)	4(2)	-8(2)	-23(2)
C(84)	38(3)	34(2)	50(2)	-1(2)	-6(2)	-14(2)
C(85)	39(2)	32(2)	28(2)	3(2)	-6(2)	-18(2)
C(86)	37(2)	30(2)	31(2)	2(2)	-9(2)	-16(2)
C(87)	40(2)	29(2)	28(2)	2(2)	-5(2)	-14(2)
C(88)	47(2)	35(2)	35(2)	-1(2)	-12(2)	-19(3)
C(89)	45(3)	42(2)	36(2)	-1(2)	-13(2)	-17(3)
C(90)	36(2)	36(3)	38(2)	-1(2)	-11(2)	-11(2)
C(91)	41(2)	31(2)	37(2)	-6(2)	-8(2)	-12(2)
C(92)	53(2)	58(3)	57(2)	-8(2)	-17(3)	-23(2)
C(93)	32(2)	30(2)	32(2)	-6(2)	-3(2)	-11(2)
C(94)	35(2)	38(3)	40(2)	-6(2)	-4(2)	-16(2)
C(95)	33(2)	55(2)	38(2)	-18(3)	0(2)	-19(2)
C(96)	37(2)	54(2)	30(2)	-6(2)	-4(2)	-17(2)
C(97)	34(2)	46(2)	32(2)	-1(2)	-4(2)	-14(2)
C(98)	31(2)	35(3)	33(2)	-4(2)	-5(2)	-11(2)
C(99)	43(2)	73(3)	59(2)	-27(2)	1(2)	-29(2)
C(100)	52(2)	60(3)	38(2)	8(2)	-15(2)	-23(2)
C(101)	36(2)	24(2)	40(3)	-3(2)	-3(2)	-7(2)
C(102)	38(2)	34(3)	38(2)	0(2)	-4(2)	-9(2)

C(103)	43(2)	35(2)	45(3)	4(2)	0(2)	-5(2)
C(104)	50(2)	36(2)	59(2)	10(3)	5(2)	-11(2)
C(105)	37(3)	36(2)	66(2)	7(2)	-1(2)	-12(2)
C(106)	33(2)	27(3)	51(2)	3(2)	-4(2)	-7(2)
C(107)	53(3)	59(3)	51(2)	18(2)	-3(3)	-6(2)
C(108)	41(2)	63(3)	93(4)	37(3)	-9(2)	-24(2)
C(109)	49(2)	61(3)	109(4)	60(3)	-47(2)	-38(2)
C(110)	55(2)	62(3)	113(4)	60(3)	-56(3)	-41(2)
C(111)	56(3)	60(3)	111(4)	57(3)	-53(3)	-37(2)
C(112)	69(3)	68(3)	122(4)	66(3)	-66(3)	-51(3)
C(113)	56(3)	68(3)	129(4)	73(3)	-60(3)	-47(3)
C(114)	54(2)	67(3)	117(4)	63(3)	-52(3)	-45(2)
C(115)	68(3)	75(3)	112(4)	51(3)	-58(3)	-37(3)
C(116)	67(3)	81(4)	135(5)	73(4)	-67(3)	-57(3)
C(117)	31(2)	71(3)	35(3)	21(2)	-10(2)	-24(3)
C(118)	31(2)	48(2)	30(2)	10(2)	-7(2)	-17(2)
C(119)	30(2)	43(3)	26(2)	1(2)	-4(2)	-15(2)
C(120)	42(3)	60(2)	29(3)	-3(2)	-6(2)	-21(3)
C(121)	53(2)	83(3)	27(3)	-1(3)	-8(2)	-29(2)
C(122)	46(2)	98(4)	30(2)	18(3)	-16(2)	-32(2)
C(123)	35(2)	32(3)	36(2)	-1(2)	-10(2)	-12(2)
C(124)	69(3)	147(6)	44(3)	-31(3)	-22(2)	-34(4)
C(125)	42(2)	64(3)	58(2)	36(2)	-25(2)	-31(3)
C(126)	46(2)	53(2)	44(3)	27(2)	-23(2)	-29(3)
C(127)	38(2)	35(2)	34(2)	7(2)	-11(2)	-19(2)
C(128)	33(2)	34(2)	35(2)	2(2)	-10(2)	-13(2)
C(129)	37(2)	35(2)	34(2)	6(2)	-12(2)	-13(2)
C(130)	39(3)	53(2)	49(2)	26(2)	-14(2)	-24(3)
C(131)	40(2)	50(2)	41(2)	13(2)	-14(2)	-23(2)
C(132)	41(2)	45(2)	34(3)	4(2)	-11(2)	-14(3)
C(133)	30(4)	31(3)	33(3)	6(2)	-11(3)	-13(3)
C(134)	38(4)	35(3)	33(3)	5(3)	-8(2)	-14(3)
C(135)	41(4)	48(4)	35(3)	9(3)	-8(3)	-20(3)
C(136)	40(3)	53(4)	45(4)	16(3)	-13(3)	-24(3)
C(137)	39(4)	50(4)	41(3)	15(3)	-17(3)	-23(3)
C(138)	34(3)	35(3)	47(3)	12(3)	-13(2)	-18(3)
C(139)	76(6)	47(5)	29(3)	6(3)	-1(4)	-29(4)
C(140)	55(4)	49(5)	57(4)	14(4)	-10(4)	-30(4)
C(141)	74(4)	119(5)	98(4)	12(4)	-39(3)	-20(4)
C(142)	153(7)	154(7)	113(6)	61(5)	-69(5)	-103(6)
C(143)	89(4)	91(4)	71(3)	25(3)	-27(3)	-12(3)
C(144)	136(6)	150(7)	105(5)	36(5)	-62(5)	-93(6)
C(145)	92(5)	162(8)	110(5)	49(5)	-18(4)	-47(5)
B(1)	34(2)	28(3)	34(3)	0(2)	-6(2)	-11(2)
B(2)	45(2)	89(4)	75(3)	56(3)	-32(2)	-41(3)

Table S29. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\{\text{Fe}_2(\text{BMPA-PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$.

	x	y	z	U(eq)
H(1)	-275	5431	2129	50
H(1B)	3212	6191	6389	48
H(1D)	1782	8288	7008	48
H(1F)	3452	7745	5461	67
H(2)	-1354	5252	2103	56
H(3)	-1335	4617	1257	64
H(4)	-230	4188	449	53
H(6A)	1136	3950	56	45
H(6B)	1007	4759	68	45
H(7A)	2420	3040	485	37
H(7B)	1558	3358	918	37
H(9)	3209	2336	1182	42
H(10)	3656	2308	2064	49
H(11)	3062	3361	2733	46
H(12)	2075	4400	2487	37
H(13A)	2296	4558	-106	38
H(13B)	2574	3724	-270	38
H(15)	3881	2924	-224	45
H(16)	4991	2581	178	55
H(17)	4974	3338	924	55
H(18)	3874	4454	1251	43
H(20)	3350	6068	1743	55
H(21)	4602	5996	1501	68
H(22)	5210	5914	497	71
H(23)	4544	5906	-250	62
H(25A)	3274	6138	-498	47
H(25B)	3239	5450	-223	47
H(26A)	1885	7352	-234	50
H(26B)	2458	7238	214	50
H(28)	751	8486	251	65
H(29)	-282	9114	1082	70
H(30)	-329	8548	1970	61
H(31)	655	7388	1986	49
H(32A)	2011	5692	-308	43
H(32B)	1917	6366	-672	43
H(34)	616	7210	-695	54
H(35)	-750	7706	-345	60
H(36)	-1257	7358	536	56
H(37)	-406	6529	1079	45
H(39)	398	4595	2955	65
H(40)	-84	3823	3326	84
H(41)	-864	4069	4299	89
H(42)	-1120	5097	4888	77
H(44A)	-1121	6263	4920	64

H(44B) -183	5966	4796	64
H(45A) -1865	7382	4332	54
H(45B) -1649	6614	4020	54
H(47) -2447	8192	3585	57
H(48) -2297	8524	2616	60
H(49) -1182	7749	1870	50
H(50) -235	6705	2147	42
H(51A) -75	6990	4637	59
H(51B) -1010	7426	4896	59
H(53) -1597	8622	4691	74
H(54) -1645	9552	4121	88
H(55) -676	9302	3237	77
H(56) 316	8125	2928	56
H(58) 2079	7241	2145	62
H(59) 2121	8309	2073	82
H(60) 2025	8957	2944	95
H(61) 1837	8513	3882	80
H(63A) 1978	7434	4409	57
H(63B) 1169	7494	4292	57
H(64A) 3182	6060	4239	55
H(64B) 3144	6547	3696	55
H(66) 4393	4998	3722	76
H(67) 4967	4002	3001	86
H(68) 4275	3984	2277	69
H(69) 3045	4937	2302	50
H(70A) 1248	6464	4647	53
H(70B) 2031	6283	4881	53
H(72) 2829	5062	5006	62
H(73) 3168	3855	4859	70
H(74) 2644	3478	4176	63
H(75) 1783	4311	3649	52
H(78) 5938	844	6555	43
H(80) 7833	-1092	5966	44
H(82) 5771	-960	6918	42
H(86) 3403	1825	7458	39
H(88) 3997	2850	8602	47
H(90) 5625	902	7718	46
H(94) 4356	-221	6342	47
H(96) 3741	1039	4997	51
H(98) 4293	1715	6409	42
H(102) 5255	-285	8003	49
H(104) 3443	-672	8764	65
H(106) 3354	378	7267	48
H(110) 784	8088	8082	78
H(112) 2048	8518	9088	86
H(114) 3149	6891	7751	81
H(118) 2768	6045	8125	45
H(120) 3330	4041	7482	55
H(122) 2024	5751	6670	69
H(126) 651	6904	7958	52
H(128) -998	7728	6955	41

H(130) 1202	7486	6319	55
H(134) 3385	5787	6370	44
H(136) 3826	7017	5138	54
H(138) 1999	7947	6588	45
H(14A) -3172	9948	7810	156
H(14B) -3264	9568	8407	156
H(14C) -2861	9098	7768	156
H(14D) -2237	9642	8480	146
H(14E) -1830	8881	8100	146
H(14F) -1971	10142	7676	113
H(14G) -1612	9404	7269	113
H(14H) -922	9673	8125	137
H(14I) -563	8935	7719	137
H(14J) -547	9778	6928	191
H(14K) 184	9287	7218	191
H(14L) -381	10109	7481	191

Table S30. Torsion angles [deg] for [$\{\text{Fe}_2(\text{BMPA}-\text{PhO})_2\}_2(\mu\text{-N}_2\text{O}_2)](\text{BArF})_2$.

Fe(1)-O(1)-C(19)-C(14)	54.8(3)
Fe(1)-O(1)-C(19)-C(18)	-121.8(3)
Fe(1)-O(2)-C(38)-C(33)	-129.9(3)
Fe(1)-O(2)-C(38)-C(37)	51.4(5)
Fe(1)-O(3A)-N(7A)-Fe(3)	-172.4(5)
Fe(1)-O(3A)-N(7A)-N(8A)	21(2)
Fe(1)-N(1)-C(6)-C(5)	-45.0(3)
Fe(1)-N(1)-C(7)-C(8)	-30.1(3)
Fe(1)-N(1)-C(13)-C(14)	61.6(3)
Fe(1)-N(2)-C(1)-C(2)	-174.3(3)
Fe(1)-N(2)-C(5)-C(4)	173.9(3)
Fe(1)-N(2)-C(5)-C(6)	-7.5(4)
Fe(1)-N(3)-C(8)-C(7)	-24.9(3)
Fe(1)-N(3)-C(8)-C(9)	158.7(2)
Fe(1)-N(3)-C(12)-C(11)	-157.5(3)
Fe(1)-N(7)-N(8)-Fe(4)	-149.6(5)
Fe(1)-N(7)-N(8)-O(4)	17.9(8)
Fe(2)-O(1)-C(19)-C(14)	-120.8(3)
Fe(2)-O(1)-C(19)-C(18)	62.6(4)
Fe(2)-O(2)-C(38)-C(33)	48.6(4)
Fe(2)-O(2)-C(38)-C(37)	-130.1(3)
Fe(2)-O(4)-N(8)-Fe(4)	-170.47(17)
Fe(2)-O(4)-N(8)-N(7)	17.4(6)
Fe(2)-N(4)-C(25)-C(24)	-45.7(3)
Fe(2)-N(4)-C(26)-C(27)	-35.8(3)
Fe(2)-N(4)-C(32)-C(33)	58.0(3)
Fe(2)-N(5)-C(20)-C(21)	179.2(3)
Fe(2)-N(5)-C(24)-C(23)	-179.4(3)
Fe(2)-N(5)-C(24)-C(25)	-1.3(4)

Fe(2)-N(6)-C(27)-C(26)	-18.2(4)
Fe(2)-N(6)-C(27)-C(28)	163.7(3)
Fe(2)-N(6)-C(31)-C(30)	-163.2(3)
Fe(3)-O(3)-N(7)-Fe(1)	-170.68(15)
Fe(3)-O(3)-N(7)-N(8)	20.8(5)
Fe(3)-O(5)-C(76)-C(71)	-129.4(4)
Fe(3)-O(5)-C(76)-C(75)	51.7(6)
Fe(3)-O(6)-C(57)-C(52)	47.8(4)
Fe(3)-O(6)-C(57)-C(56)	-130.8(3)
Fe(3)-N(7A)-N(8A)-Fe(2)	-148.9(14)
Fe(3)-N(7A)-N(8A)-O(4A)	20(3)
Fe(3)-N(9)-C(44)-C(43)	-43.2(4)
Fe(3)-N(9)-C(45)-C(46)	-35.1(3)
Fe(3)-N(9)-C(51)-C(52)	61.4(4)
Fe(3)-N(10)-C(39)-C(40)	-174.3(3)
Fe(3)-N(10)-C(43)-C(42)	174.6(3)
Fe(3)-N(10)-C(43)-C(44)	-6.4(4)
Fe(3)-N(11)-C(46)-C(45)	-26.8(4)
Fe(3)-N(11)-C(46)-C(47)	156.1(3)
Fe(3)-N(11)-C(50)-C(49)	-154.3(3)
Fe(4)-O(4A)-N(8A)-Fe(2)	-173.6(5)
Fe(4)-O(4A)-N(8A)-N(7A)	13.8(19)
Fe(4)-O(5)-C(76)-C(71)	53.3(4)
Fe(4)-O(5)-C(76)-C(75)	-125.6(3)
Fe(4)-O(6)-C(57)-C(52)	-123.2(3)
Fe(4)-O(6)-C(57)-C(56)	58.2(5)
Fe(4)-N(12)-C(63)-C(62)	-45.9(3)
Fe(4)-N(12)-C(64)-C(65)	-32.1(3)
Fe(4)-N(12)-C(70)-C(71)	56.1(4)
Fe(4)-N(13)-C(58)-C(59)	172.4(3)
Fe(4)-N(13)-C(62)-C(61)	-173.3(3)
Fe(4)-N(13)-C(62)-C(63)	5.3(4)
Fe(4)-N(14)-C(65)-C(64)	-14.9(4)
Fe(4)-N(14)-C(65)-C(66)	167.8(3)
Fe(4)-N(14)-C(69)-C(68)	-166.1(3)
O(3)-N(7)-N(8)-Fe(4)	14.0(8)
O(3)-N(7)-N(8)-O(4)	-178.6(4)
O(3A)-N(7A)-N(8A)-Fe(2)	12(3)
O(3A)-N(7A)-N(8A)-O(4A)	-179.3(15)
N(1)-C(7)-C(8)-N(3)	37.8(4)
N(1)-C(7)-C(8)-C(9)	-145.7(3)
N(1)-C(13)-C(14)-C(15)	114.1(3)
N(1)-C(13)-C(14)-C(19)	-63.0(4)
N(2)-C(1)-C(2)-C(3)	0.8(5)
N(2)-C(5)-C(6)-N(1)	37.2(4)
N(3)-C(8)-C(9)-C(10)	0.7(5)
N(4)-C(26)-C(27)-N(6)	37.3(4)
N(4)-C(26)-C(27)-C(28)	-144.7(4)
N(4)-C(32)-C(33)-C(34)	116.8(4)
N(4)-C(32)-C(33)-C(38)	-65.8(4)
N(5)-C(20)-C(21)-C(22)	-0.4(6)

N(5)-C(24)-C(25)-N(4)	33.3(4)
N(6)-C(27)-C(28)-C(29)	1.5(6)
N(9)-C(45)-C(46)-N(11)	42.9(4)
N(9)-C(45)-C(46)-C(47)	-140.1(3)
N(9)-C(51)-C(52)-C(53)	118.5(4)
N(9)-C(51)-C(52)-C(57)	-63.4(5)
N(10)-C(39)-C(40)-C(41)	0.2(8)
N(10)-C(43)-C(44)-N(9)	34.8(5)
N(11)-C(46)-C(47)-C(48)	-0.3(5)
N(12)-C(64)-C(65)-N(14)	32.5(5)
N(12)-C(64)-C(65)-C(66)	-150.1(4)
N(12)-C(70)-C(71)-C(72)	115.2(4)
N(12)-C(70)-C(71)-C(76)	-66.7(5)
N(13)-C(58)-C(59)-C(60)	1.0(7)
N(13)-C(62)-C(63)-N(12)	29.3(5)
N(14)-C(65)-C(66)-C(67)	-0.6(7)
C(1)-N(2)-C(5)-C(4)	-0.9(5)
C(1)-N(2)-C(5)-C(6)	177.7(3)
C(1)-C(2)-C(3)-C(4)	-0.5(6)
C(1A)-C(1B)-C(1C)-C(1D)	0
C(1A)-C(1B)-C(1C)-B(2)	171.9(4)
C(1B)-C(1A)-C(1F)-C(1E)	0
C(1B)-C(1A)-C(1H)-F(43A)	59.4(10)
C(1B)-C(1A)-C(1H)-F(44A)	-63.7(11)
C(1B)-C(1A)-C(1H)-F(45A)	176.6(9)
C(1B)-C(1C)-C(1D)-C(1E)	0
C(1B)-C(1C)-B(2)-C(109)	135.8(3)
C(1B)-C(1C)-B(2)-C(117)	16.7(6)
C(1B)-C(1C)-B(2)-C(125)	-109.3(4)
C(1C)-C(1D)-C(1E)-C(1F)	0
C(1C)-C(1D)-C(1E)-C(1G)	-174.6(12)
C(1D)-C(1C)-B(2)-C(109)	-52.7(4)
C(1D)-C(1C)-B(2)-C(117)	-171.8(4)
C(1D)-C(1C)-B(2)-C(125)	62.1(6)
C(1D)-C(1E)-C(1F)-C(1A)	0
C(1D)-C(1E)-C(1G)-F(46A)	-149.7(11)
C(1D)-C(1E)-C(1G)-F(47A)	86.0(17)
C(1D)-C(1E)-C(1G)-F(48A)	-34(2)
C(1F)-C(1A)-C(1B)-C(1C)	0
C(1F)-C(1A)-C(1H)-F(43A)	-120.2(8)
C(1F)-C(1A)-C(1H)-F(44A)	116.7(8)
C(1F)-C(1A)-C(1H)-F(45A)	-3.0(13)
C(1F)-C(1E)-C(1G)-F(46A)	35.6(19)
C(1F)-C(1E)-C(1G)-F(47A)	-88.7(17)
C(1F)-C(1E)-C(1G)-F(48A)	150.9(11)
C(1G)-C(1E)-C(1F)-C(1A)	174.7(12)
C(1H)-C(1A)-C(1B)-C(1C)	-179.6(7)
C(1H)-C(1A)-C(1F)-C(1E)	179.6(7)
C(2)-C(3)-C(4)-C(5)	-0.6(6)
C(3)-C(4)-C(5)-N(2)	1.3(5)
C(3)-C(4)-C(5)-C(6)	-177.3(3)

C(4)-C(5)-C(6)-N(1)	-144.1(3)
C(5)-N(2)-C(1)-C(2)	-0.2(5)
C(6)-N(1)-C(7)-C(8)	-144.9(3)
C(6)-N(1)-C(13)-C(14)	177.7(3)
C(7)-N(1)-C(6)-C(5)	72.1(3)
C(7)-N(1)-C(13)-C(14)	-59.2(3)
C(7)-C(8)-C(9)-C(10)	-175.5(3)
C(8)-N(3)-C(12)-C(11)	0.8(5)
C(8)-C(9)-C(10)-C(11)	0.4(5)
C(9)-C(10)-C(11)-C(12)	-0.9(5)
C(10)-C(11)-C(12)-N(3)	0.3(5)
C(12)-N(3)-C(8)-C(7)	175.1(3)
C(12)-N(3)-C(8)-C(9)	-1.3(4)
C(13)-N(1)-C(6)-C(5)	-165.4(3)
C(13)-N(1)-C(7)-C(8)	92.6(3)
C(13)-C(14)-C(15)-C(16)	-176.0(3)
C(13)-C(14)-C(19)-O(1)	0.3(4)
C(13)-C(14)-C(19)-C(18)	176.9(3)
C(14)-C(15)-C(16)-C(17)	-0.5(5)
C(15)-C(14)-C(19)-O(1)	-176.9(3)
C(15)-C(14)-C(19)-C(18)	-0.2(4)
C(15)-C(16)-C(17)-C(18)	-1.1(6)
C(16)-C(17)-C(18)-C(19)	2.1(5)
C(17)-C(18)-C(19)-O(1)	175.3(3)
C(17)-C(18)-C(19)-C(14)	-1.4(5)
C(19)-C(14)-C(15)-C(16)	1.1(5)
C(20)-N(5)-C(24)-C(23)	-0.8(5)
C(20)-N(5)-C(24)-C(25)	177.3(3)
C(20)-C(21)-C(22)-C(23)	-0.1(6)
C(21)-C(22)-C(23)-C(24)	0.1(6)
C(22)-C(23)-C(24)-N(5)	0.4(6)
C(22)-C(23)-C(24)-C(25)	-177.6(4)
C(23)-C(24)-C(25)-N(4)	-148.6(3)
C(24)-N(5)-C(20)-C(21)	0.8(5)
C(25)-N(4)-C(26)-C(27)	-149.7(3)
C(25)-N(4)-C(32)-C(33)	173.7(3)
C(26)-N(4)-C(25)-C(24)	70.6(4)
C(26)-N(4)-C(32)-C(33)	-62.9(4)
C(26)-C(27)-C(28)-C(29)	-176.5(4)
C(27)-N(6)-C(31)-C(30)	0.1(5)
C(27)-C(28)-C(29)-C(30)	-0.8(7)
C(28)-C(29)-C(30)-C(31)	0.0(7)
C(29)-C(30)-C(31)-N(6)	0.4(6)
C(31)-N(6)-C(27)-C(26)	177.0(3)
C(31)-N(6)-C(27)-C(28)	-1.1(5)
C(32)-N(4)-C(25)-C(24)	-166.2(3)
C(32)-N(4)-C(26)-C(27)	87.5(3)
C(32)-C(33)-C(34)-C(35)	175.7(4)
C(32)-C(33)-C(38)-O(2)	6.9(5)
C(32)-C(33)-C(38)-C(37)	-174.3(3)
C(33)-C(34)-C(35)-C(36)	-0.3(6)

C(34)-C(33)-C(38)-O(2)	-175.7(3)
C(34)-C(33)-C(38)-C(37)	3.1(5)
C(34)-C(35)-C(36)-C(37)	0.8(6)
C(35)-C(36)-C(37)-C(38)	0.7(6)
C(36)-C(37)-C(38)-O(2)	176.1(3)
C(36)-C(37)-C(38)-C(33)	-2.7(5)
C(38)-C(33)-C(34)-C(35)	-1.6(6)
C(39)-N(10)-C(43)-C(42)	-0.7(6)
C(39)-N(10)-C(43)-C(44)	178.3(4)
C(39)-C(40)-C(41)-C(42)	-0.7(8)
C(40)-C(41)-C(42)-C(43)	0.5(8)
C(41)-C(42)-C(43)-N(10)	0.3(7)
C(41)-C(42)-C(43)-C(44)	-178.7(5)
C(42)-C(43)-C(44)-N(9)	-146.2(4)
C(43)-N(10)-C(39)-C(40)	0.5(6)
C(44)-N(9)-C(45)-C(46)	-150.1(3)
C(44)-N(9)-C(51)-C(52)	178.6(3)
C(45)-N(9)-C(44)-C(43)	72.9(4)
C(45)-N(9)-C(51)-C(52)	-58.6(4)
C(45)-C(46)-C(47)-C(48)	-177.2(3)
C(46)-N(11)-C(50)-C(49)	-0.2(5)
C(46)-C(47)-C(48)-C(49)	1.3(6)
C(47)-C(48)-C(49)-C(50)	-1.6(5)
C(48)-C(49)-C(50)-N(11)	1.1(5)
C(50)-N(11)-C(46)-C(45)	176.9(3)
C(50)-N(11)-C(46)-C(47)	-0.2(5)
C(51)-N(9)-C(44)-C(43)	-164.1(3)
C(51)-N(9)-C(45)-C(46)	87.6(3)
C(51)-C(52)-C(53)-C(54)	178.3(4)
C(51)-C(52)-C(57)-O(6)	4.4(5)
C(51)-C(52)-C(57)-C(56)	-177.0(3)
C(52)-C(53)-C(54)-C(55)	-1.0(8)
C(53)-C(52)-C(57)-O(6)	-177.6(3)
C(53)-C(52)-C(57)-C(56)	1.1(5)
C(53)-C(54)-C(55)-C(56)	0.5(8)
C(54)-C(55)-C(56)-C(57)	0.8(7)
C(55)-C(56)-C(57)-O(6)	177.0(4)
C(55)-C(56)-C(57)-C(52)	-1.6(6)
C(57)-C(52)-C(53)-C(54)	0.2(6)
C(58)-N(13)-C(62)-C(61)	0.8(6)
C(58)-N(13)-C(62)-C(63)	179.4(3)
C(58)-C(59)-C(60)-C(61)	-1.1(8)
C(59)-C(60)-C(61)-C(62)	1.0(8)
C(60)-C(61)-C(62)-N(13)	-0.9(7)
C(60)-C(61)-C(62)-C(63)	-179.4(4)
C(61)-C(62)-C(63)-N(12)	-152.1(4)
C(62)-N(13)-C(58)-C(59)	-0.8(6)
C(63)-N(12)-C(64)-C(65)	-146.0(3)
C(63)-N(12)-C(70)-C(71)	171.7(3)
C(64)-N(12)-C(63)-C(62)	70.5(4)
C(64)-N(12)-C(70)-C(71)	-64.1(4)

C(64)-C(65)-C(66)-C(67)	-177.9(4)
C(65)-N(14)-C(69)-C(68)	0.9(6)
C(65)-C(66)-C(67)-C(68)	1.0(8)
C(66)-C(67)-C(68)-C(69)	-0.4(8)
C(67)-C(68)-C(69)-N(14)	-0.5(7)
C(69)-N(14)-C(65)-C(64)	177.1(3)
C(69)-N(14)-C(65)-C(66)	-0.3(6)
C(70)-N(12)-C(63)-C(62)	-165.7(3)
C(70)-N(12)-C(64)-C(65)	89.9(3)
C(70)-C(71)-C(72)-C(73)	176.1(4)
C(70)-C(71)-C(76)-O(5)	6.0(5)
C(70)-C(71)-C(76)-C(75)	-175.1(3)
C(71)-C(72)-C(73)-C(74)	0.3(7)
C(72)-C(71)-C(76)-O(5)	-175.9(4)
C(72)-C(71)-C(76)-C(75)	3.0(6)
C(72)-C(73)-C(74)-C(75)	0.2(7)
C(73)-C(74)-C(75)-C(76)	1.0(6)
C(74)-C(75)-C(76)-O(5)	176.3(4)
C(74)-C(75)-C(76)-C(71)	-2.6(6)
C(76)-C(71)-C(72)-C(73)	-1.9(6)
C(77)-C(78)-C(79)-C(80)	0.2(5)
C(77)-C(78)-C(79)-C(83)	179.6(3)
C(78)-C(77)-C(82)-C(81)	0.0(5)
C(78)-C(77)-B(1)-C(85)	-46.5(4)
C(78)-C(77)-B(1)-C(93)	74.7(4)
C(78)-C(77)-B(1)-C(101)	-163.0(3)
C(78)-C(79)-C(80)-C(81)	0.2(5)
C(78)-C(79)-C(83)-F(1)	-19.8(5)
C(78)-C(79)-C(83)-F(2)	-140.0(4)
C(78)-C(79)-C(83)-F(3)	104.7(5)
C(79)-C(80)-C(81)-C(82)	-0.6(5)
C(79)-C(80)-C(81)-C(84)	-179.4(3)
C(80)-C(79)-C(83)-F(1)	159.6(4)
C(80)-C(79)-C(83)-F(2)	39.4(5)
C(80)-C(79)-C(83)-F(3)	-75.9(5)
C(80)-C(81)-C(82)-C(77)	0.4(5)
C(80)-C(81)-C(84)-F(4)	-47.2(4)
C(80)-C(81)-C(84)-F(5)	72.7(4)
C(80)-C(81)-C(84)-F(6)	-168.9(3)
C(82)-C(77)-C(78)-C(79)	-0.4(5)
C(82)-C(77)-B(1)-C(85)	141.8(3)
C(82)-C(77)-B(1)-C(93)	-97.0(3)
C(82)-C(77)-B(1)-C(101)	25.3(4)
C(82)-C(81)-C(84)-F(4)	134.0(3)
C(82)-C(81)-C(84)-F(5)	-106.1(4)
C(82)-C(81)-C(84)-F(6)	12.3(5)
C(83)-C(79)-C(80)-C(81)	-179.2(3)
C(84)-C(81)-C(82)-C(77)	179.2(3)
C(85)-C(86)-C(87)-C(88)	0.4(5)
C(85)-C(86)-C(87)-C(91)	-176.8(3)
C(86)-C(85)-C(90)-C(89)	-0.2(5)

C(86)-C(85)-B(1)-C(77)	161.7(3)
C(86)-C(85)-B(1)-C(93)	45.8(4)
C(86)-C(85)-B(1)-C(101)	-76.3(4)
C(86)-C(87)-C(88)-C(89)	-0.6(5)
C(86)-C(87)-C(91)-F(7)	71.6(4)
C(86)-C(87)-C(91)-F(8)	-47.5(4)
C(86)-C(87)-C(91)-F(9)	-167.9(3)
C(87)-C(88)-C(89)-C(90)	0.4(5)
C(87)-C(88)-C(89)-C(92)	-176.8(4)
C(88)-C(87)-C(91)-F(7)	-105.6(4)
C(88)-C(87)-C(91)-F(8)	135.2(3)
C(88)-C(87)-C(91)-F(9)	14.8(4)
C(88)-C(89)-C(90)-C(85)	0.0(6)
C(88)-C(89)-C(92)-F(10)	96.2(5)
C(88)-C(89)-C(92)-F(11)	-21.4(6)
C(88)-C(89)-C(92)-F(12)	-144.6(4)
C(90)-C(85)-C(86)-C(87)	0.0(5)
C(90)-C(85)-B(1)-C(77)	-25.7(4)
C(90)-C(85)-B(1)-C(93)	-141.6(3)
C(90)-C(85)-B(1)-C(101)	96.2(4)
C(90)-C(89)-C(92)-F(10)	-81.0(5)
C(90)-C(89)-C(92)-F(11)	161.4(4)
C(90)-C(89)-C(92)-F(12)	38.2(5)
C(91)-C(87)-C(88)-C(89)	176.6(3)
C(92)-C(89)-C(90)-C(85)	177.2(4)
C(93)-C(94)-C(95)-C(96)	1.5(5)
C(93)-C(94)-C(95)-C(99)	-176.8(3)
C(94)-C(93)-C(98)-C(97)	-0.3(5)
C(94)-C(93)-B(1)-C(77)	77.1(4)
C(94)-C(93)-B(1)-C(85)	-161.3(3)
C(94)-C(93)-B(1)-C(101)	-44.9(4)
C(94)-C(95)-C(96)-C(97)	-0.3(5)
C(94)-C(95)-C(99)-F(13)	-24.7(5)
C(94)-C(95)-C(99)-F(14)	97.0(6)
C(94)-C(95)-C(99)-F(15)	-143.3(4)
C(95)-C(96)-C(97)-C(98)	-1.2(5)
C(95)-C(96)-C(97)-C(100)	179.5(3)
C(96)-C(95)-C(99)-F(13)	157.0(3)
C(96)-C(95)-C(99)-F(14)	-81.3(6)
C(96)-C(95)-C(99)-F(15)	38.4(5)
C(96)-C(97)-C(98)-C(93)	1.5(5)
C(96)-C(97)-C(100)-F(16)	-10.0(6)
C(96)-C(97)-C(100)-F(17)	109.1(4)
C(96)-C(97)-C(100)-F(18)	-131.9(4)
C(98)-C(93)-C(94)-C(95)	-1.2(5)
C(98)-C(93)-B(1)-C(77)	-93.8(3)
C(98)-C(93)-B(1)-C(85)	27.8(4)
C(98)-C(93)-B(1)-C(101)	144.2(3)
C(98)-C(97)-C(100)-F(16)	170.7(4)
C(98)-C(97)-C(100)-F(17)	-70.2(4)
C(98)-C(97)-C(100)-F(18)	48.8(5)

C(99)-C(95)-C(96)-C(97)	178.1(3)
C(100)-C(97)-C(98)-C(93)	-179.2(3)
C(101)-C(102)-C(103)-C(104)	-1.2(6)
C(101)-C(102)-C(103)-C(107)	-179.5(4)
C(102)-C(101)-C(106)-C(105)	1.6(5)
C(102)-C(101)-B(1)-C(77)	48.4(4)
C(102)-C(101)-B(1)-C(85)	-73.6(4)
C(102)-C(101)-B(1)-C(93)	164.9(3)
C(102)-C(103)-C(104)-C(105)	1.0(6)
C(102)-C(103)-C(107)-F(19)	-10.6(6)
C(102)-C(103)-C(107)-F(20)	-126.2(4)
C(102)-C(103)-C(107)-F(21)	114.1(5)
C(103)-C(104)-C(105)-C(106)	0.5(6)
C(103)-C(10)-C(105)-C(108)	-177.9(4)
C(104)-C(103)-C(107)-F(19)	171.0(4)
C(104)-C(103)-C(107)-F(20)	55.5(5)
C(104)-C(103)-C(107)-F(21)	-64.2(7)
C(104)-C(105)-C(106)-C(101)	-1.8(6)
C(104)-C(105)-C(108)-F(22)	97.9(5)
C(104)-C(105)-C(108)-F(22A)	22.6(9)
C(104)-C(105)-C(108)-F(23)	-30.2(8)
C(104)-C(105)-C(108)-F(23A)	-77.9(8)
C(104)-C(105)-C(108)-F(24)	-150.5(5)
C(104)-C(105)-C(108)-F(24A)	167.4(10)
C(106)-C(101)-C(102)-C(103)	-0.1(5)
C(106)-C(101)-B(1)-C(77)	-139.0(3)
C(106)-C(101)-B(1)-C(85)	99.0(4)
C(106)-C(101)-B(1)-C(93)	-22.5(4)
C(106)-C(105)-C(108)-F(22)	-80.4(6)
C(106)-C(105)-C(108)-F(22A)	-155.7(7)
C(106)-C(105)-C(108)-F(23)	151.5(6)
C(106)-C(105)-C(108)-F(23A)	103.7(8)
C(106)-C(105)-C(108)-F(24)	31.2(7)
C(106)-C(105)-C(108)-F(24A)	-10.9(12)
C(107)-C(103)-C(104)-C(105)	179.3(4)
C(108)-C(105)-C(106)-C(101)	176.5(4)
C(109)-C(110)-C(111)-C(112)	-1.4(6)
C(109)-C(110)-C(111)-C(115)	176.4(4)
C(110)-C(109)-C(114)-C(113)	3.0(6)
C(110)-C(109)-B(2)-C(1C)	110.5(4)
C(110)-C(109)-B(2)-C(117)	-122.8(4)
C(110)-C(109)-B(2)-C(125)	-2.6(5)
C(110)-C(109)-B(2)-C(133)	123.1(4)
C(110)-C(111)-C(112)-C(113)	1.4(6)
C(110)-C(111)-C(115)-F(25)	51.2(6)
C(110)-C(111)-C(115)-F(26)	-69.8(6)
C(110)-C(111)-C(115)-F(27)	172.5(4)
C(111)-C(112)-C(113)-C(114)	0.8(6)
C(111)-C(112)-C(113)-C(116)	-177.8(4)
C(112)-C(111)-C(115)-F(25)	-131.0(5)
C(112)-C(111)-C(115)-F(26)	108.0(5)

C(112)-C(111)-C(115)-F(27)	-9.7(6)
C(112)-C(113)-C(114)-C(109)	-3.1(6)
C(112)-C(113)-C(116)-F(28)	69.2(6)
C(112)-C(113)-C(116)-F(29)	-170.0(4)
C(112)-C(113)-C(116)-F(30)	-49.1(7)
C(114)-C(109)-C(110)-C(111)	-0.8(6)
C(114)-C(109)-B(2)-C(1C)	-64.8(4)
C(114)-C(109)-B(2)-C(117)	61.9(5)
C(114)-C(109)-B(2)-C(125)	-177.8(3)
C(114)-C(109)-B(2)-C(133)	-52.2(5)
C(114)-C(113)-C(116)-F(28)	-109.4(6)
C(114)-C(113)-C(116)-F(29)	11.4(6)
C(114)-C(113)-C(116)-F(30)	132.3(5)
C(115)-C(111)-C(112)-C(113)	-176.4(4)
C(116)-C(113)-C(114)-C(109)	175.4(4)
C(117)-C(118)-C(119)-C(120)	-1.6(5)
C(117)-C(118)-C(119)-C(123)	179.4(3)
C(118)-C(117)-C(122)-C(121)	-2.1(5)
C(118)-C(117)-B(2)-C(1C)	98.0(5)
C(118)-C(117)-B(2)-C(109)	-11.9(5)
C(118)-C(117)-B(2)-C(125)	-134.8(4)
C(118)-C(117)-B(2)-C(133)	111.8(4)
C(118)-C(119)-C(120)-C(121)	-0.7(5)
C(118)-C(119)-C(123)-F(31)	85.7(4)
C(118)-C(119)-C(123)-F(32)	-155.2(3)
C(118)-C(119)-C(123)-F(33)	-34.2(4)
C(119)-C(120)-C(121)-C(122)	1.5(6)
C(119)-C(120)-C(121)-C(124)	-178.5(4)
C(120)-C(119)-C(123)-F(31)	-93.4(4)
C(120)-C(119)-C(123)-F(32)	25.7(4)
C(120)-C(119)-C(123)-F(33)	146.7(3)
C(120)-C(121)-C(122)-C(117)	0.0(6)
C(120)-C(121)-C(124)-F(34)	96.8(6)
C(120)-C(121)-C(124)-F(35)	-17.3(7)
C(120)-C(121)-C(124)-F(36)	-134.2(6)
C(122)-C(117)-C(118)-C(119)	2.9(5)
C(122)-C(117)-B(2)-C(1C)	-78.8(5)
C(122)-C(117)-B(2)-C(109)	171.3(3)
C(122)-C(117)-B(2)-C(125)	48.4(5)
C(122)-C(117)-B(2)-C(133)	-65.0(4)
C(122)-C(121)-C(124)-F(34)	-83.3(7)
C(122)-C(121)-C(124)-F(35)	162.7(5)
C(122)-C(121)-C(124)-F(36)	45.8(7)
C(123)-C(119)-C(120)-C(121)	178.3(3)
C(124)-C(121)-C(122)-C(117)	-180.0(4)
C(125)-C(126)-C(127)-C(128)	1.2(6)
C(125)-C(126)-C(127)-C(131)	177.1(4)
C(126)-C(125)-C(130)-C(129)	1.4(6)
C(126)-C(125)-B(2)-C(1C)	-167.2(4)
C(126)-C(125)-B(2)-C(109)	-64.3(5)
C(126)-C(125)-B(2)-C(117)	58.8(6)

C(126)-C(125)-B(2)-C(133)	166.2(4)
C(126)-C(127)-C(128)-C(129)	-0.2(5)
C(126)-C(127)-C(131)-F(37)	-74.7(4)
C(126)-C(127)-C(131)-F(38)	166.6(4)
C(126)-C(127)-C(131)-F(39)	43.5(5)
C(127)-C(128)-C(129)-C(130)	-0.1(5)
C(127)-C(128)-C(129)-C(132)	-179.2(3)
C(128)-C(127)-C(131)-F(37)	101.4(4)
C(128)-C(127)-C(131)-F(38)	-17.4(5)
C(128)-C(127)-C(131)-F(39)	-140.5(4)
C(128)-C(129)-C(130)-C(125)	-0.5(6)
C(128)-C(129)-C(132)-F(40)	-145.8(4)
C(128)-C(129)-C(132)-F(41)	89.9(5)
C(128)-C(129)-C(132)-F(42)	-26.5(5)
C(130)-C(125)-C(126)-C(127)	-1.7(6)
C(130)-C(125)-B(2)-C(1C)	14.4(7)
C(130)-C(125)-B(2)-C(109)	117.3(5)
C(130)-C(125)-B(2)-C(117)	-119.6(4)
C(130)-C(125)-B(2)-C(133)	-12.3(7)
C(130)-C(129)-C(132)-F(40)	35.1(5)
C(130)-C(129)-C(132)-F(41)	-89.3(5)
C(130)-C(129)-C(132)-F(42)	154.4(4)
C(131)-C(127)-C(128)-C(129)	-176.2(3)
C(132)-C(129)-C(130)-C(125)	178.6(4)
C(133)-C(134)-C(135)-C(136)	0
C(133)-C(134)-C(135)-C(139)	-178.0(6)
C(134)-C(133)-C(138)-C(137)	0
C(134)-C(133)-B(2)-C(109)	119.7(4)
C(134)-C(133)-B(2)-C(117)	-1.1(5)
C(134)-C(133)-B(2)-C(125)	-113.2(4)
C(134)-C(135)-C(136)-C(137)	0
C(134)-C(135)-C(139)-F(43)	-22.8(10)
C(134)-C(135)-C(139)-F(44)	-129.4(6)
C(134)-C(135)-C(139)-F(45)	113.1(9)
C(135)-C(136)-C(137)-C(138)	0
C(135)-C(136)-C(137)-C(140)	-175.8(5)
C(136)-C(135)-C(139)-F(43)	159.3(6)
C(136)-C(135)-C(139)-F(44)	52.7(8)
C(136)-C(135)-C(139)-F(45)	-64.9(11)
C(136)-C(137)-C(138)-C(133)	0
C(136)-C(137)-C(140)-F(46)	-36.4(8)
C(136)-C(137)-C(140)-F(47)	82.3(7)
C(136)-C(137)-C(140)-F(48)	-157.9(8)
C(138)-C(133)-C(134)-C(135)	0
C(138)-C(133)-B(2)-C(109)	-59.1(4)
C(138)-C(133)-B(2)-C(117)	-179.9(3)
C(138)-C(133)-B(2)-C(125)	68.0(5)
C(138)-C(137)-C(140)-F(46)	147.9(5)
C(138)-C(137)-C(140)-F(47)	-93.4(7)
C(138)-C(137)-C(140)-F(48)	26.4(10)
C(139)-C(135)-C(136)-C(137)	177.9(6)

C(140)-C(137)-C(138)-C(133)	175.6(6)
C(141)-C(142)-C(143)-C(144)	-175.9(8)
C(142)-C(143)-C(144)-C(145)	179.9(9)
B(1)-C(77)-C(78)-C(79)	-172.7(3)
B(1)-C(77)-C(82)-C(81)	172.1(3)
B(1)-C(85)-C(86)-C(87)	173.1(3)
B(1)-C(85)-C(90)-C(89)	-173.1(3)
B(1)-C(93)-C(94)-C(95)	-172.8(3)
B(1)-C(93)-C(98)-C(97)	170.9(3)
B(1)-C(101)-C(102)-C(103)	173.1(3)
B(1)-C(101)-C(106)-C(105)	-171.3(3)
B(2)-C(1C)-C(1D)-C(1E)	-171.1(5)
B(2)-C(109)-C(110)-C(111)	-176.2(4)
B(2)-C(109)-C(114)-C(113)	178.7(4)
B(2)-C(117)-C(118)-C(119)	-174.0(3)
B(2)-C(117)-C(122)-C(121)	175.0(4)
B(2)-C(125)-C(126)-C(127)	179.7(4)
B(2)-C(125)-C(130)-C(129)	179.9(4)
B(2)-C(133)-C(134)-C(135)	-178.7(4)
B(2)-C(133)-C(138)-C(137)	178.9(4)

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