

**Electronic Structures, Spectroscopy, and Electrochemistry of
[M(diimine)(CN-BR₃)₄]²⁻ (M = Fe, Ru; R = Ph, C₆F₅)
Complexes:**

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S.1. NMR Spectroscopy

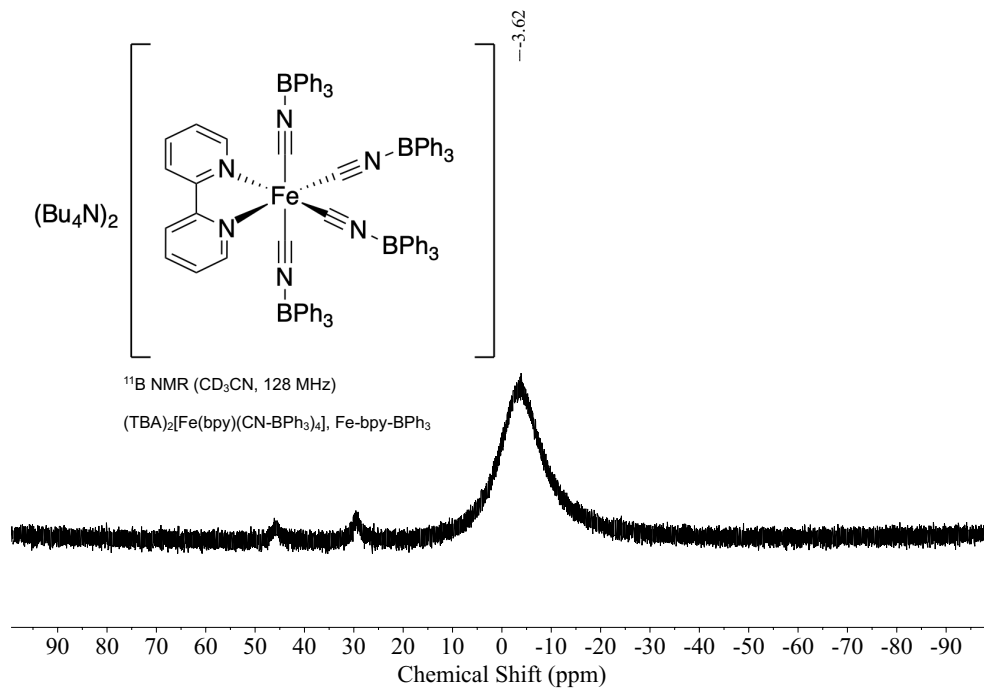


Figure S1. ^{11}B NMR of $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN-BPh}_3)_4]$ (Fe-bpy-BPh₃) in CD_3CN .

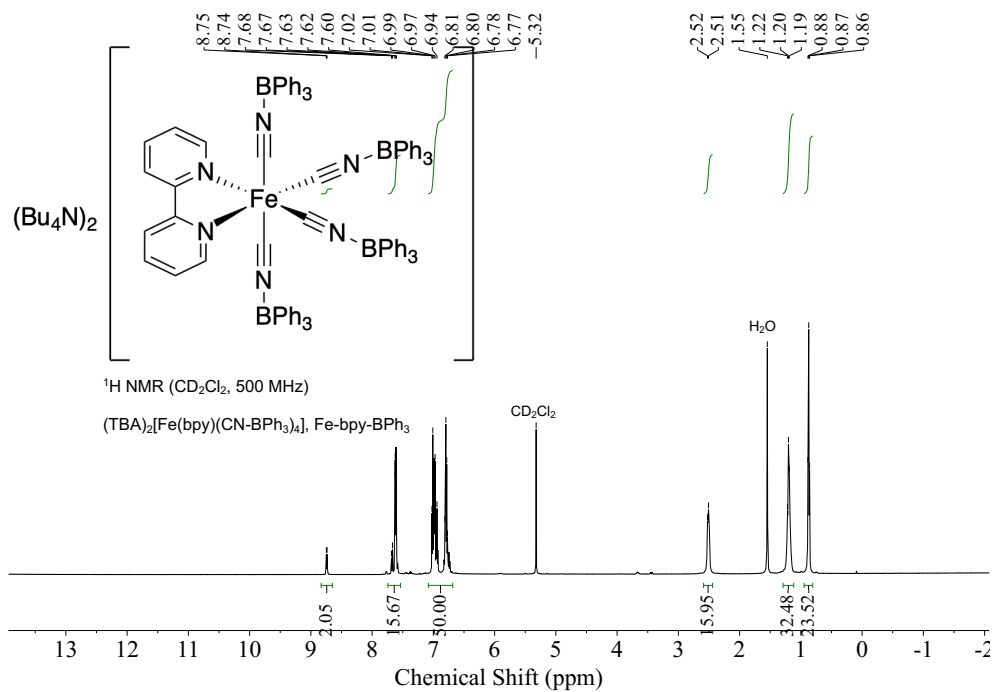


Figure S2. ^1H NMR of $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN-BPh}_3)_4]$ (Fe-bpy-BPh₃) in CD_2Cl_2 .

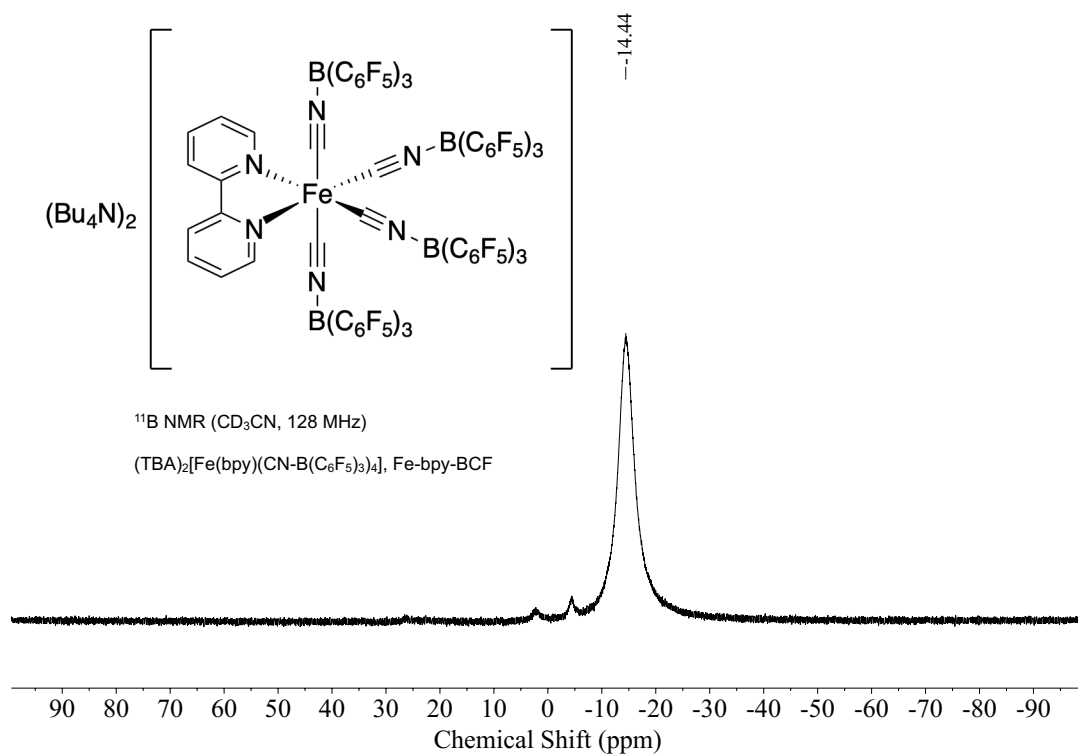


Figure S3. ^{11}B NMR of $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-bpy-BCF**) in CD_3CN .

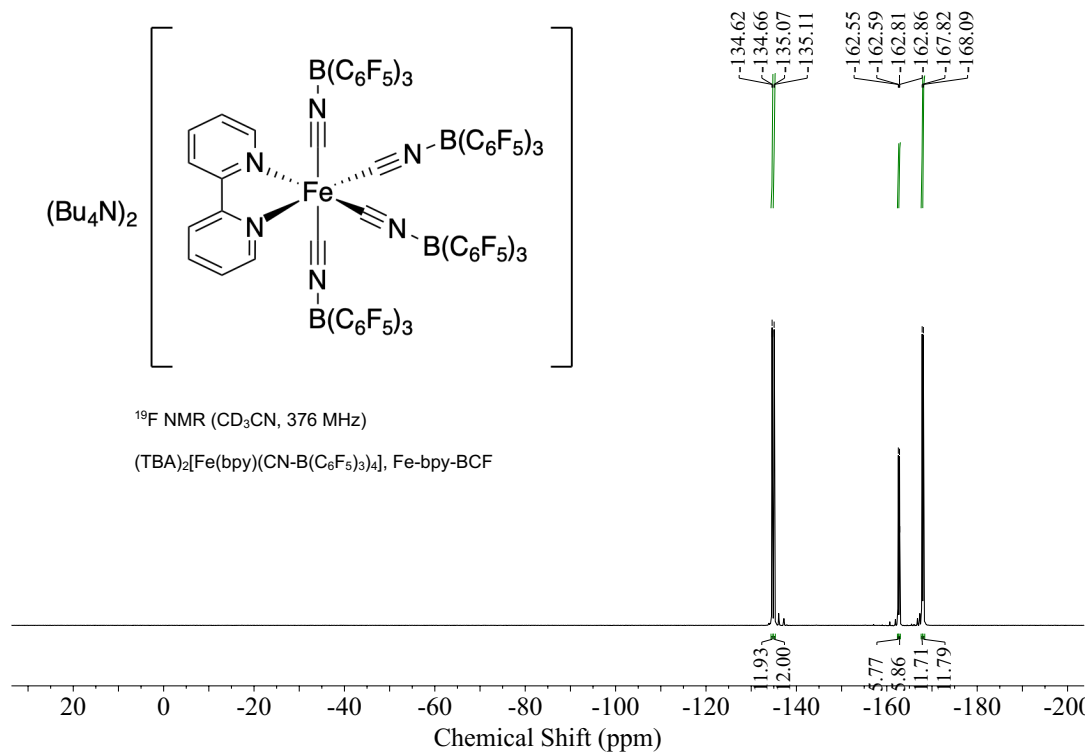


Figure S4. ^{19}F NMR of $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-bpy-BCF**) in CD_3CN .

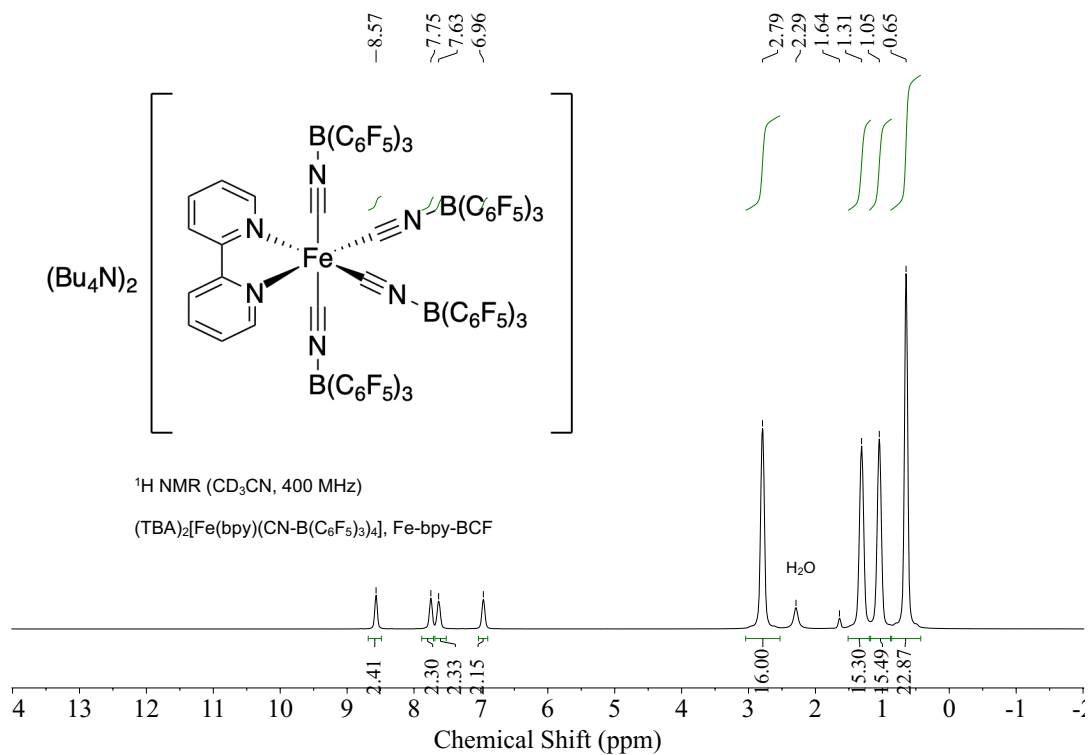


Figure S5. ^1H NMR of $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-bpy-BCF**) in CD_3CN .

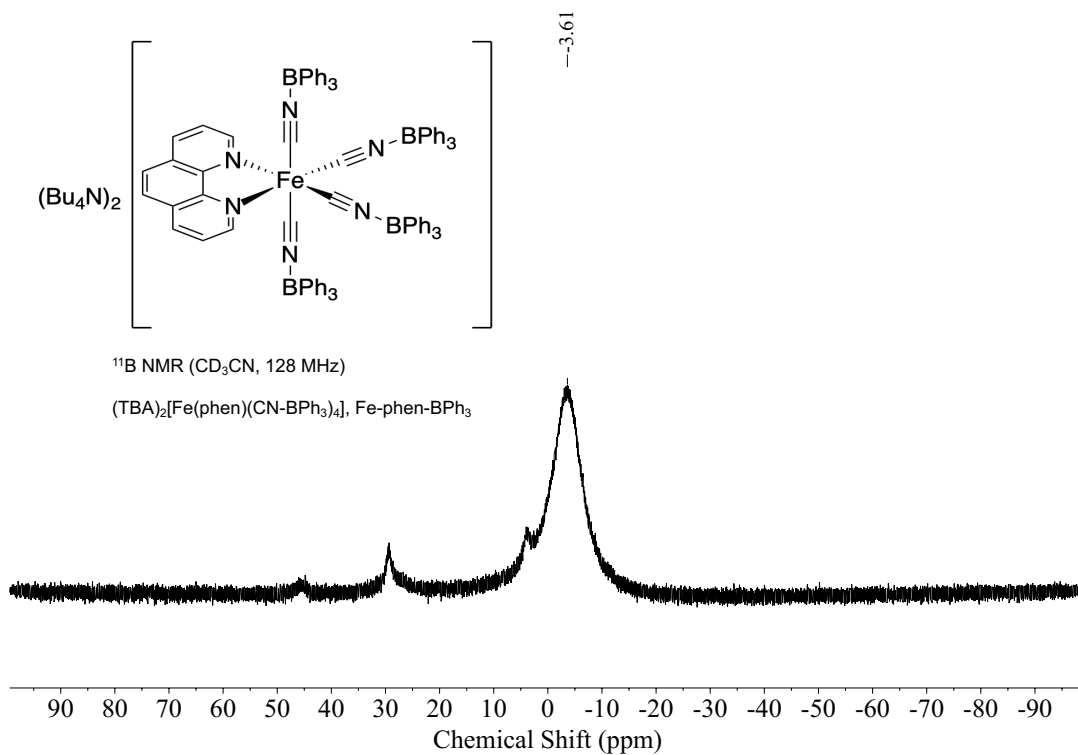


Figure S6. ^{11}B NMR of $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN}-\text{BPh}_3)_4]$ (**Fe-phen-BPh₃**) in CD_3CN .

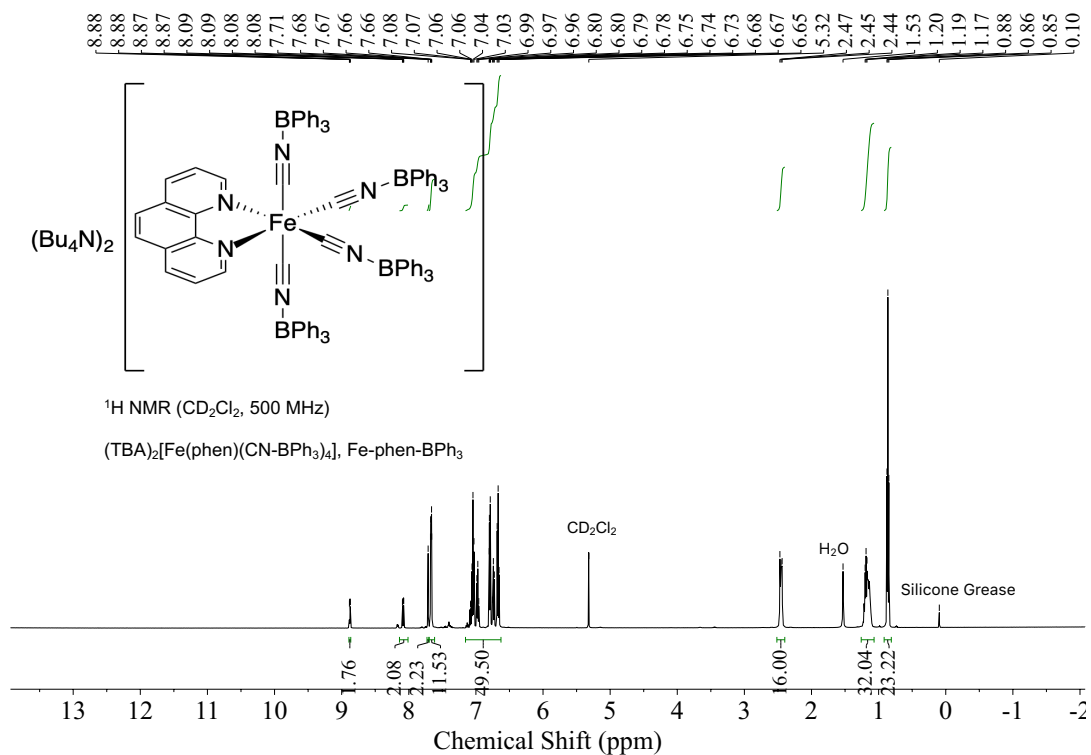


Figure S7. $^1\text{H NMR}$ of $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN-BPh}_3)_4]$ (**Fe-phen-BPh₃**) in CD_2Cl_2 .

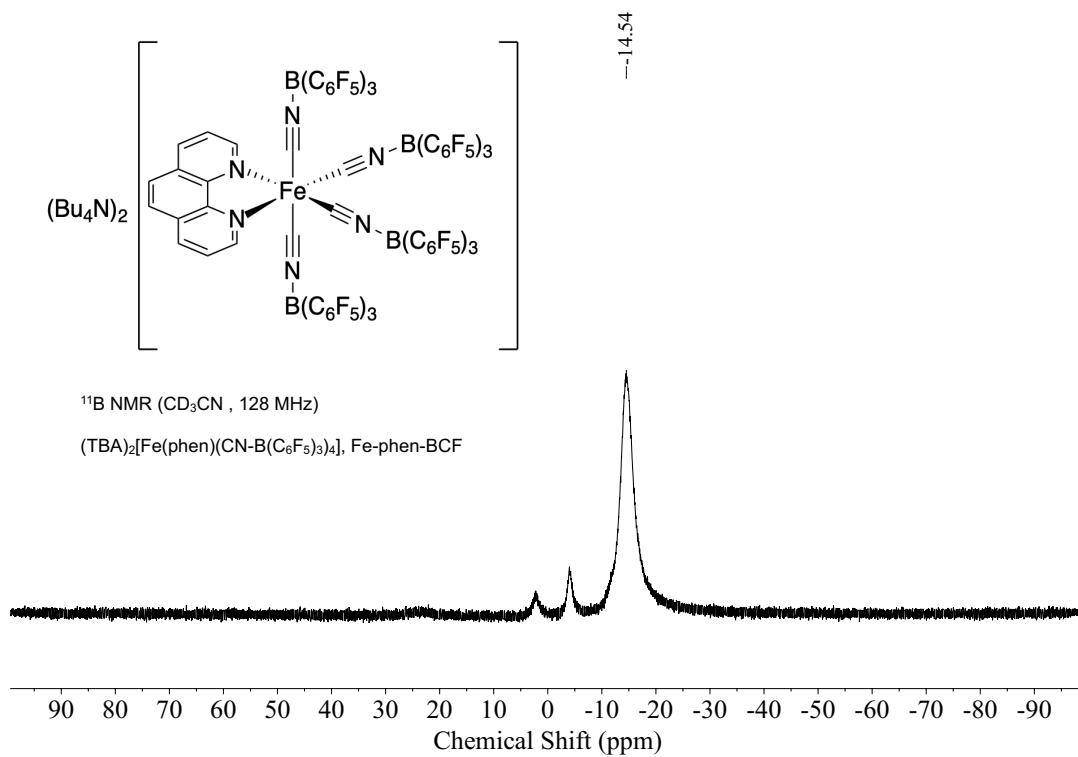


Figure S8. $^{11}\text{B NMR}$ of $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN-B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-phen-BCF**) in CD_3CN .

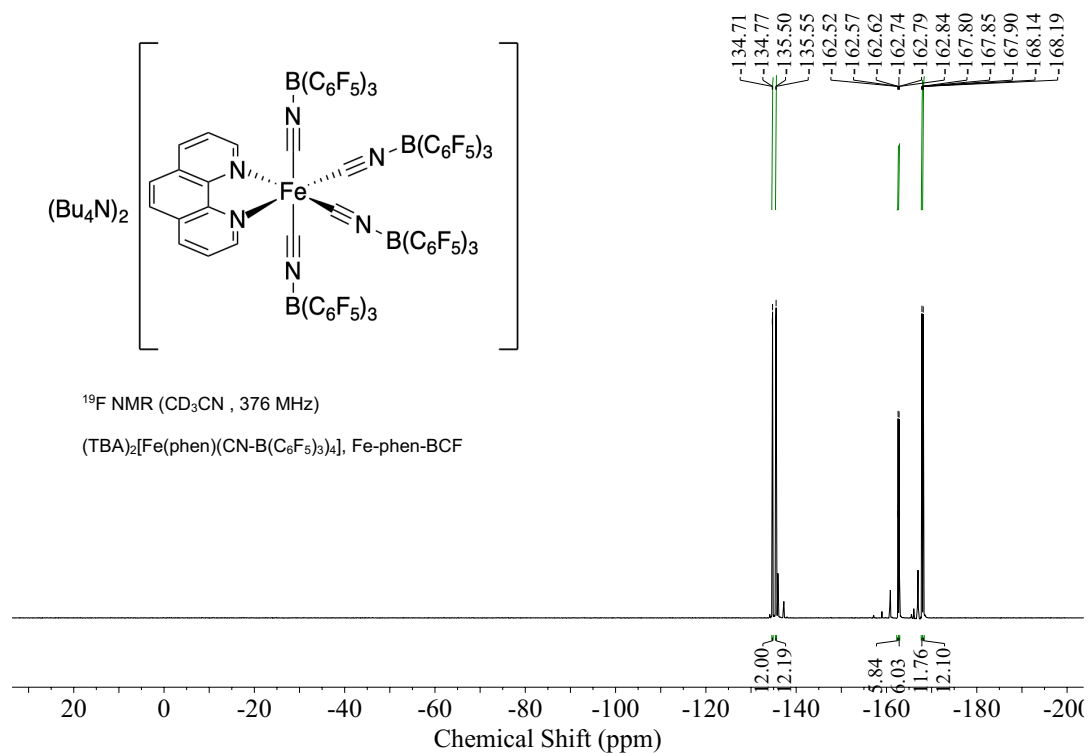


Figure S9. ^{19}F NMR of $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-phen-BCF**) in CD_3CN .

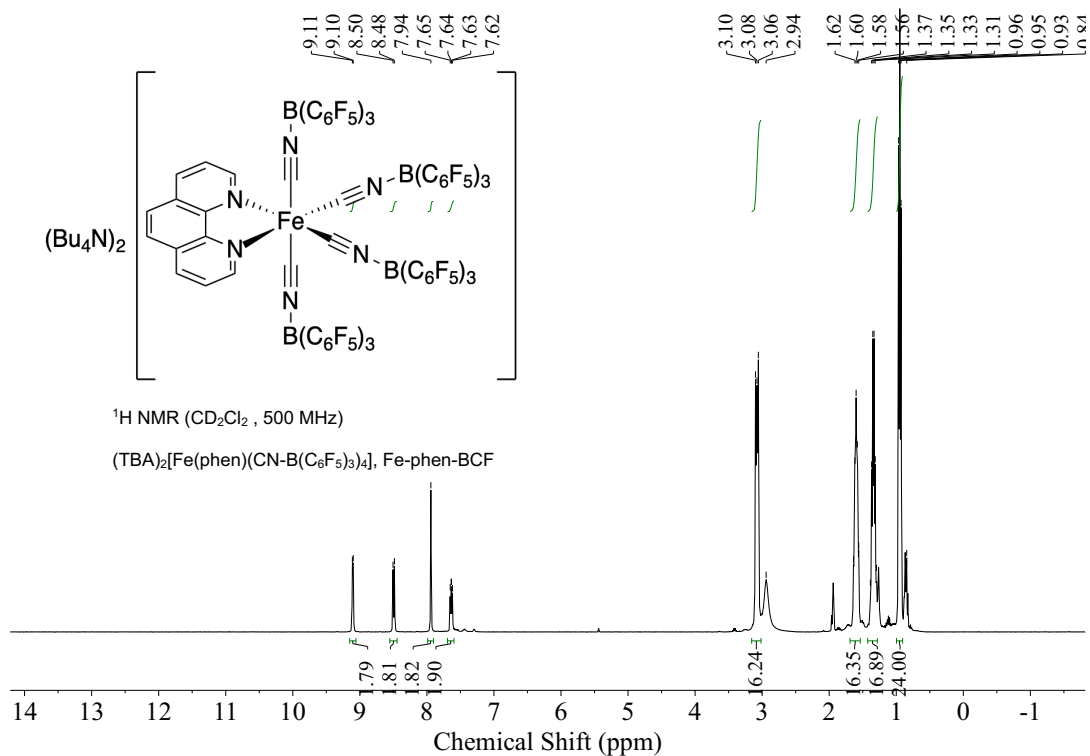


Figure S10. ^1H NMR of $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Fe-phen-BCF**) in CD_2Cl_2 .

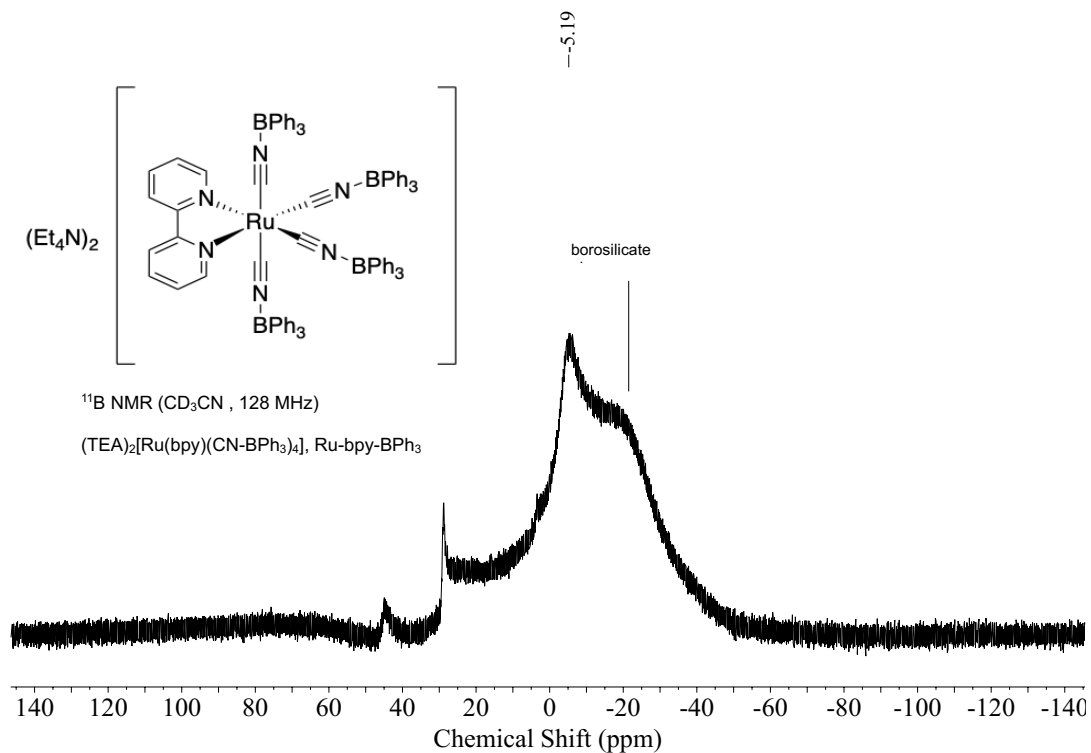


Figure S11. ^{11}B NMR of $(TEA)_2[Ru(bpy)(CN-BPh_3)_4]$ (Ru-bpy-BPh₃) in CD_3CN .

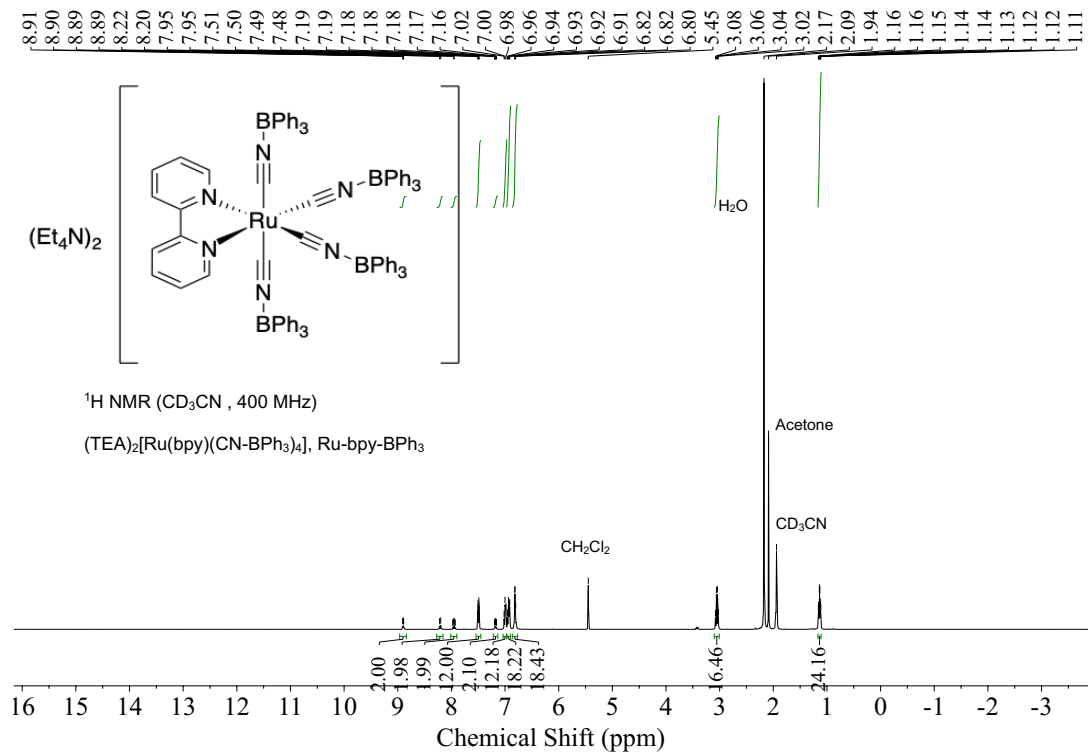


Figure S12. 1H NMR of $(TEA)_2[Ru(bpy)(CN-BPh_3)_4]$ (Ru-bpy-BPh₃) in CD_3CN .

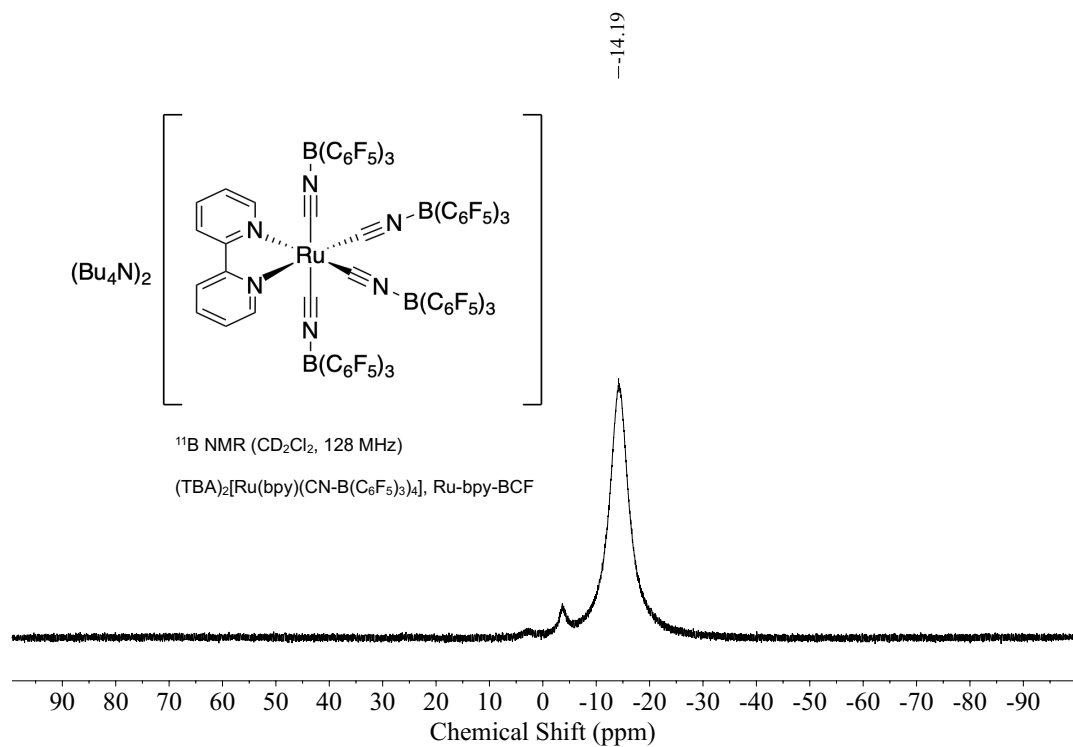


Figure S13. ^{11}B NMR of $(\text{TBA})_2[\text{Ru}(\text{bpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Ru-bpy-BCF**) in CD_2Cl_2 .

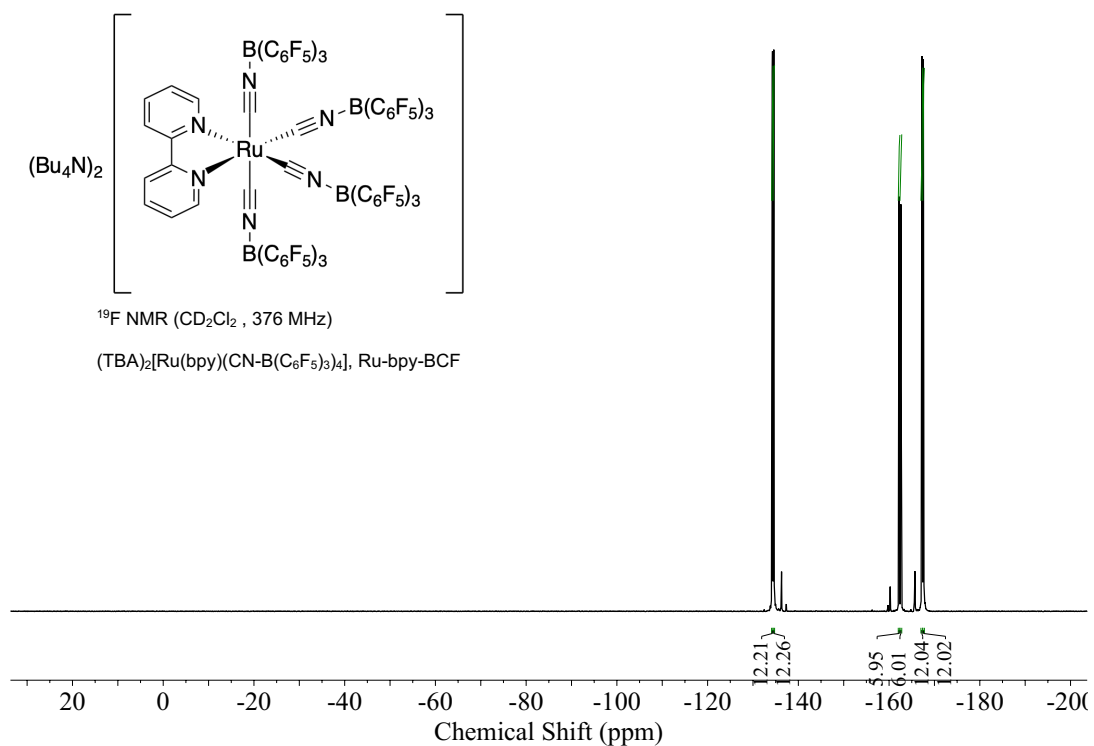


Figure S14. ^{19}F NMR of $(\text{TBA})_2[\text{Ru}(\text{bpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Ru-bpy-BCF**) in CD_2Cl_2 .

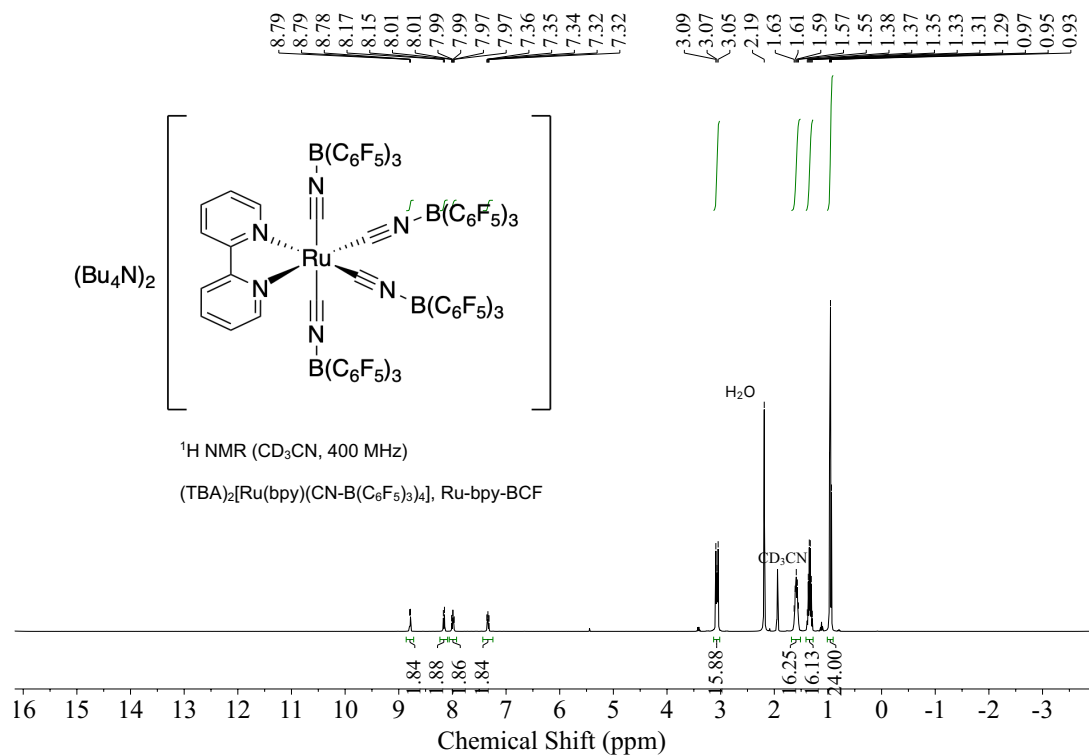


Figure S15. $^1\text{H NMR}$ of $(\text{TBA})_2[\text{Ru}(\text{bpy})(\text{CN-B}(\text{C}_6\text{F}_5)_3)_4]$ (**Ru-bpy-BCF**) in CD_3CN .

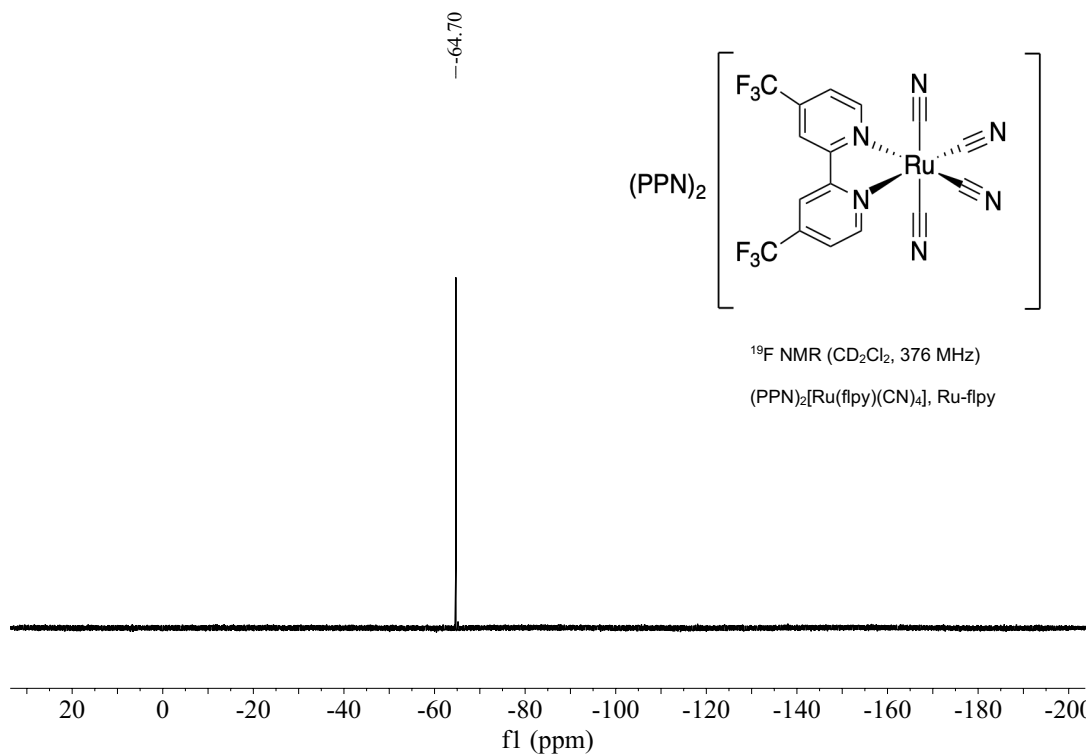


Figure S16. $^{19}\text{F NMR}$ of $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN})_4]$ (**Ru-flpy**) in CD_2Cl_2 .

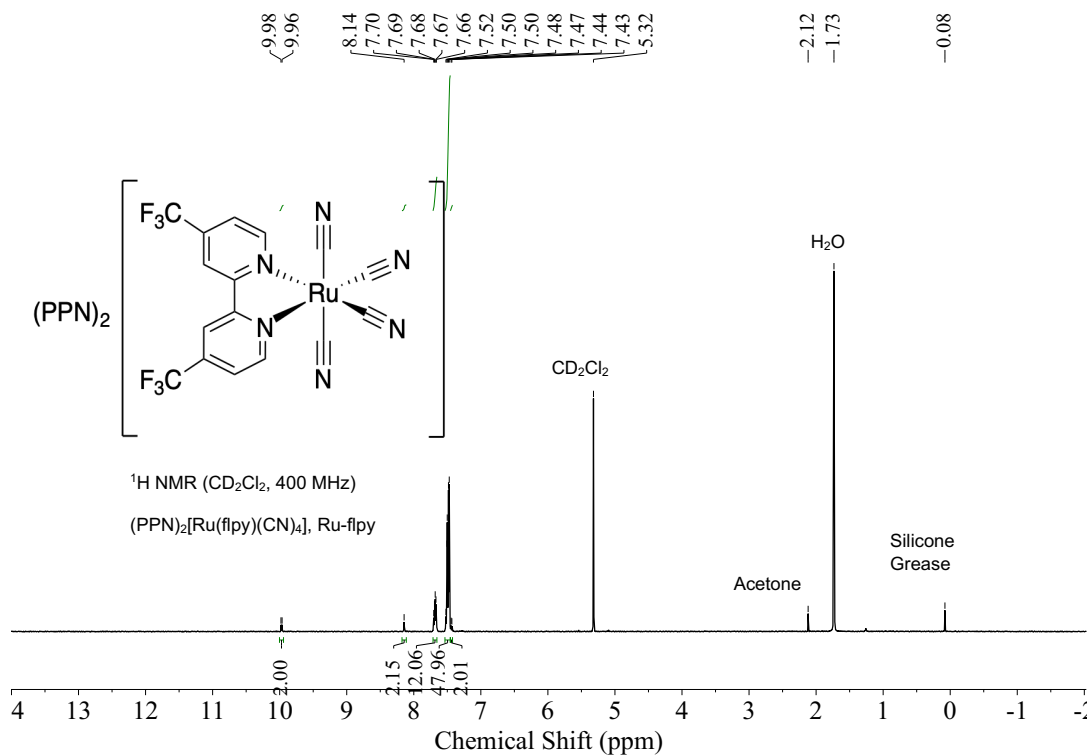


Figure S17. ^1H NMR of $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN})_4]$ (**Ru-flpy**) in CD_2Cl_2 .

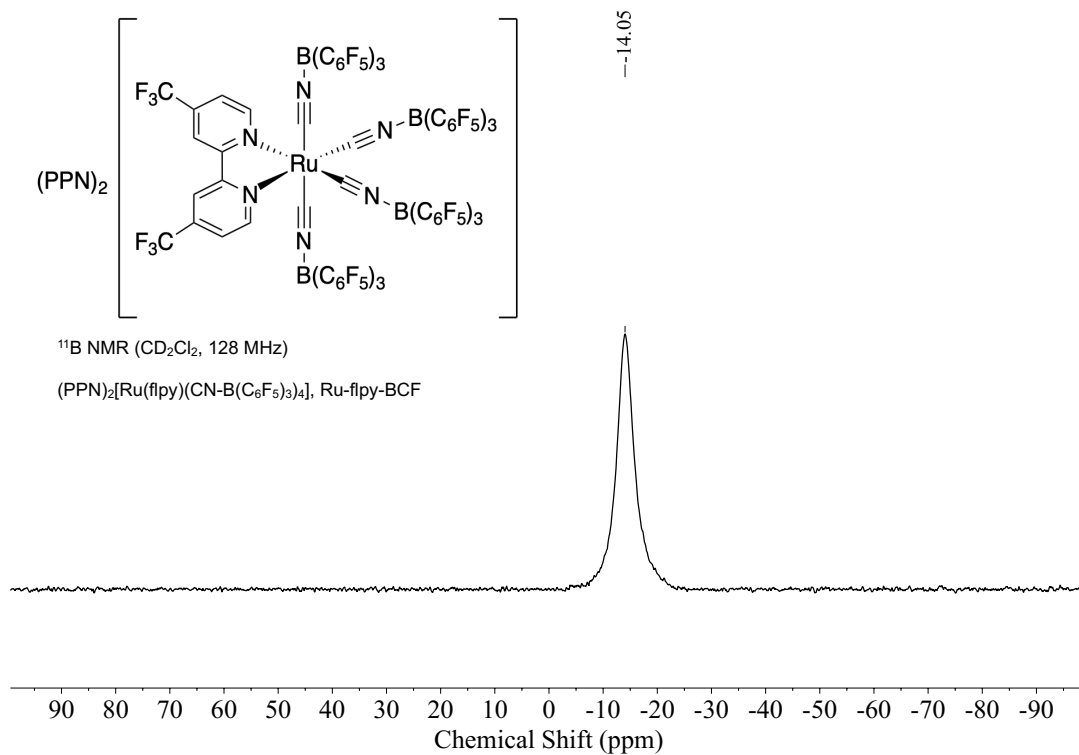


Figure S18. ^{11}B NMR of $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (**Ru-flpy-BCF**) in CD_2Cl_2 .

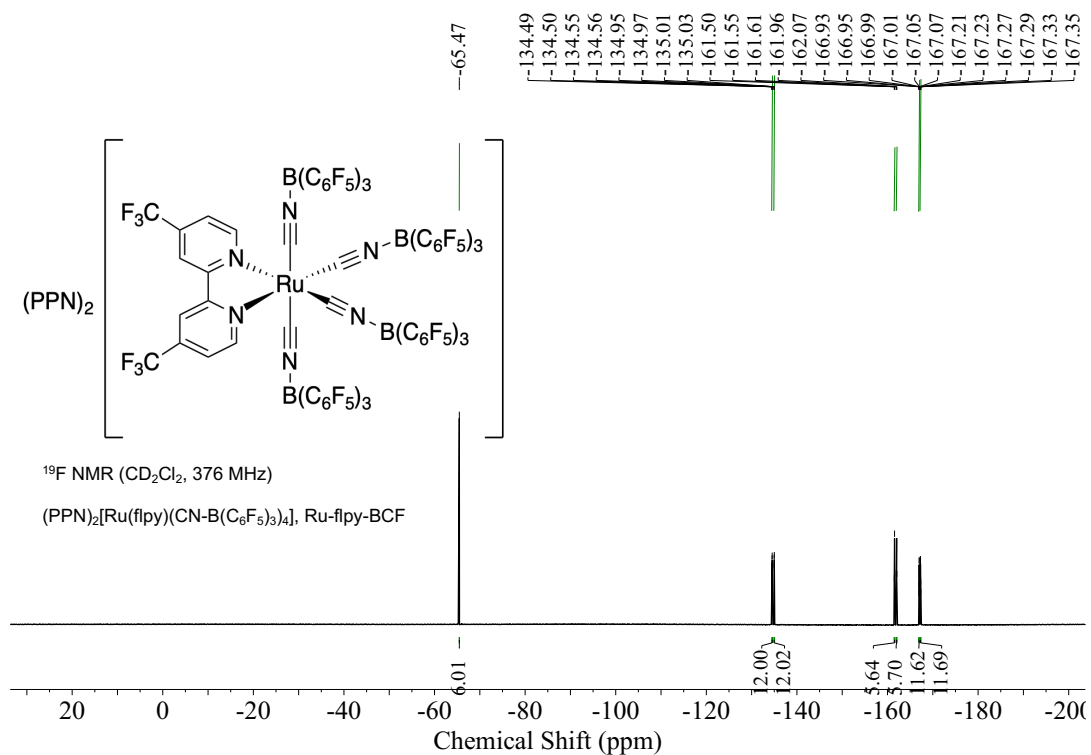


Figure S19. ^{19}F NMR of (PPN) $_2$ [Ru(flpy)(CN-B(C_6F_5) $_3$) $_4$] (**Ru-flpy-BCF**) in CD_2Cl_2 .

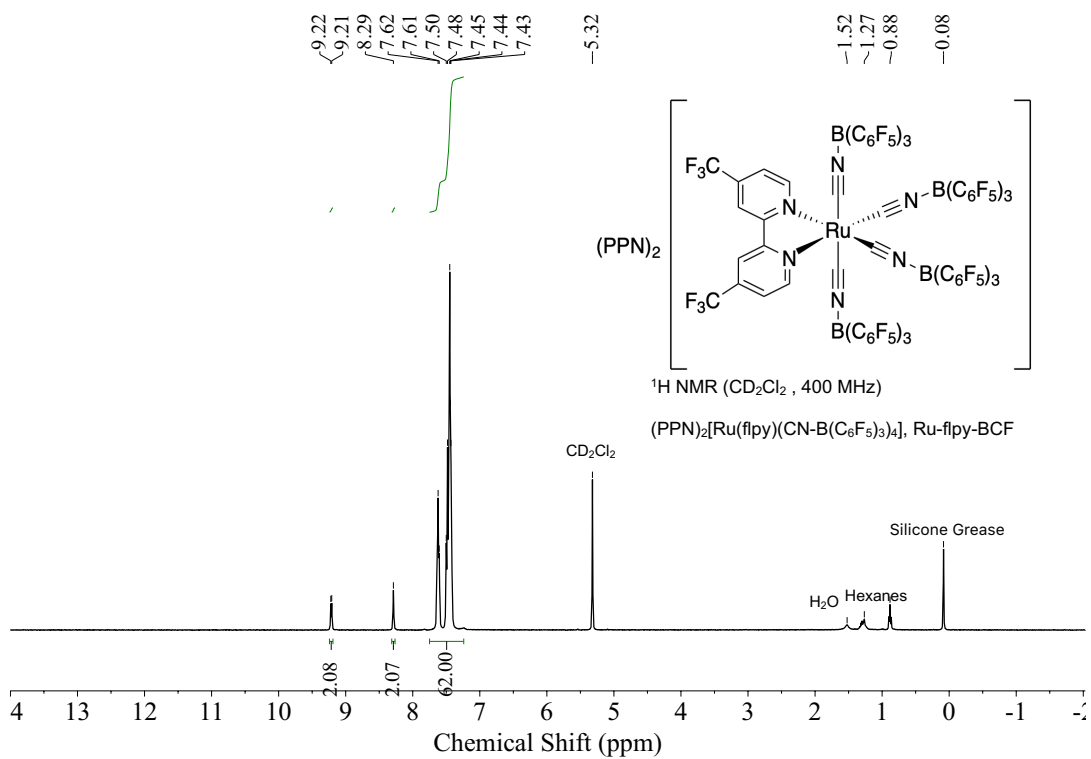


Figure S20. ^1H NMR of (PPN) $_2$ [Ru(flpy)(CN-B(C_6F_5) $_3$) $_4$] (**Ru-flpy-BCF**) in CD_2Cl_2 .

S.2. Solid State ATR-IR Spectroscopy

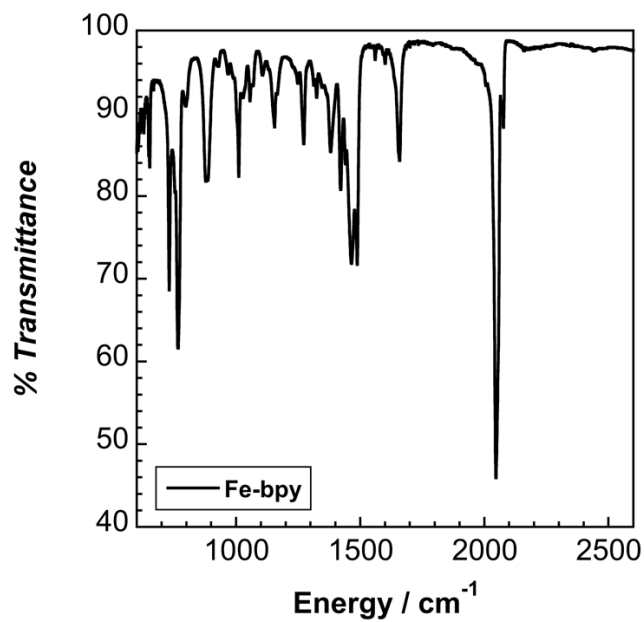


Figure S21. ATR-IR spectrum of Fe-bpy.

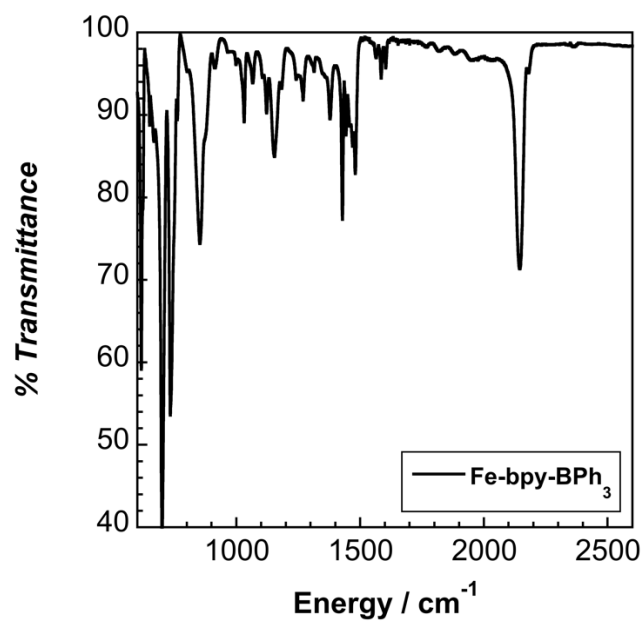


Figure S22. ATR-IR spectrum of Fe-bpy-BPh₃.

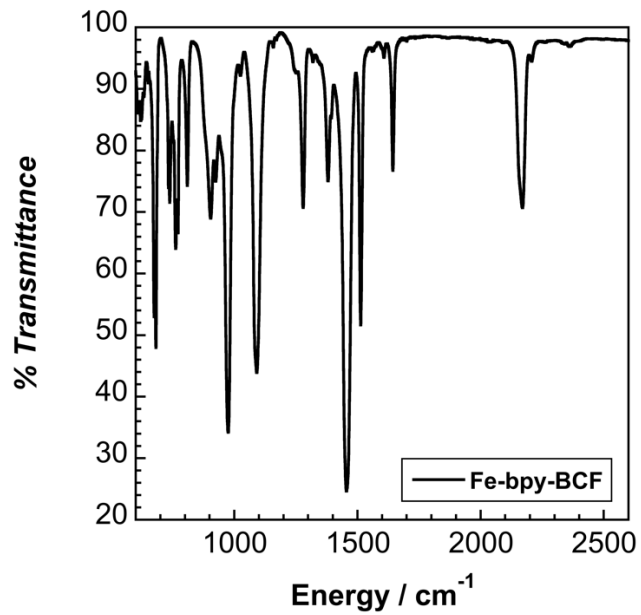


Figure S23. ATR-IR spectrum of **Fe-bpy-BCF**.

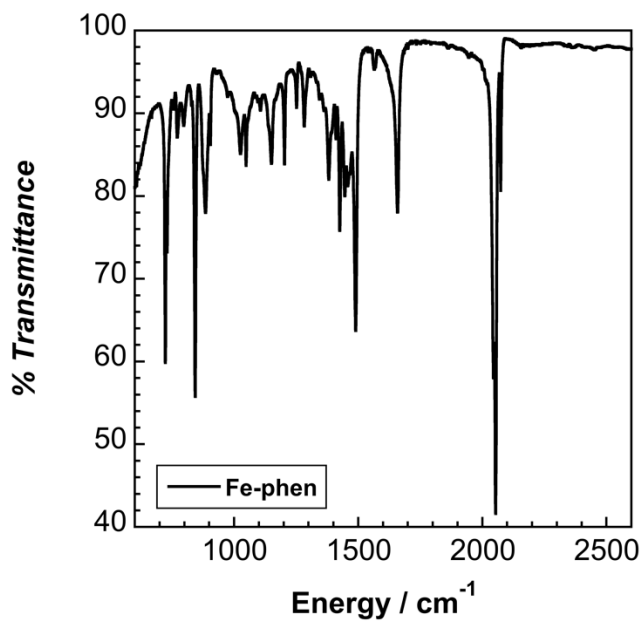


Figure S24. ATR-IR spectrum of **Fe-phen**.

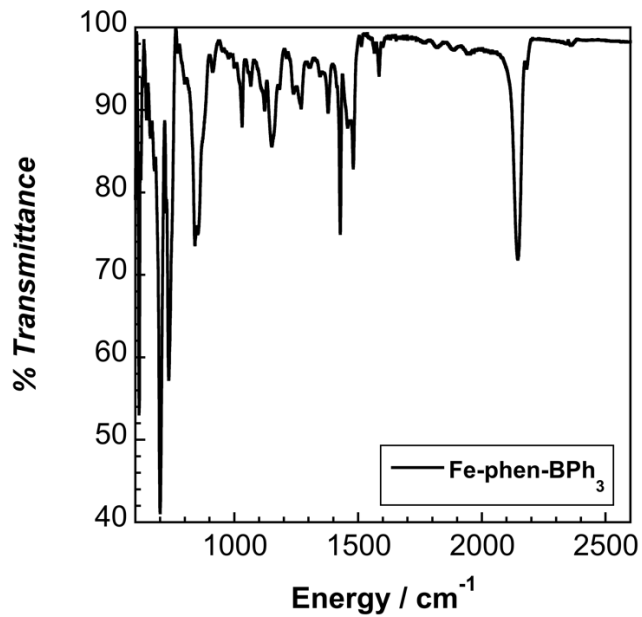


Figure S25. ATR-IR spectrum of **Fe-phen-BPh₃**.

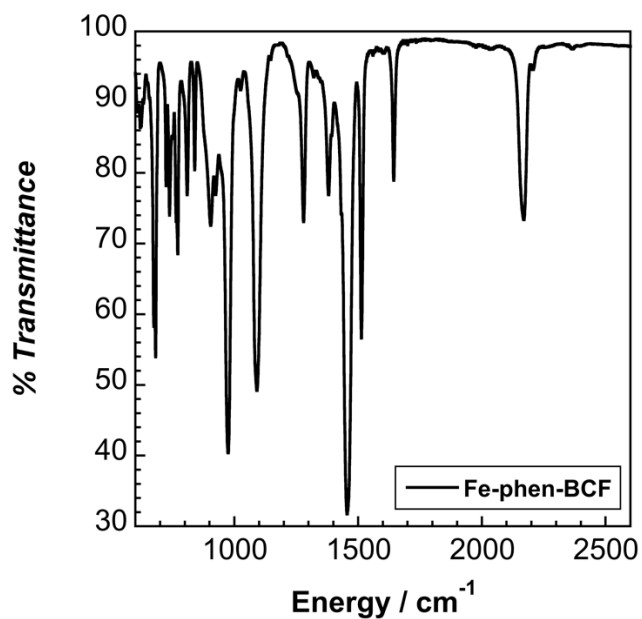


Figure S26. ATR-IR spectrum of **Fe-phen-BCF**.

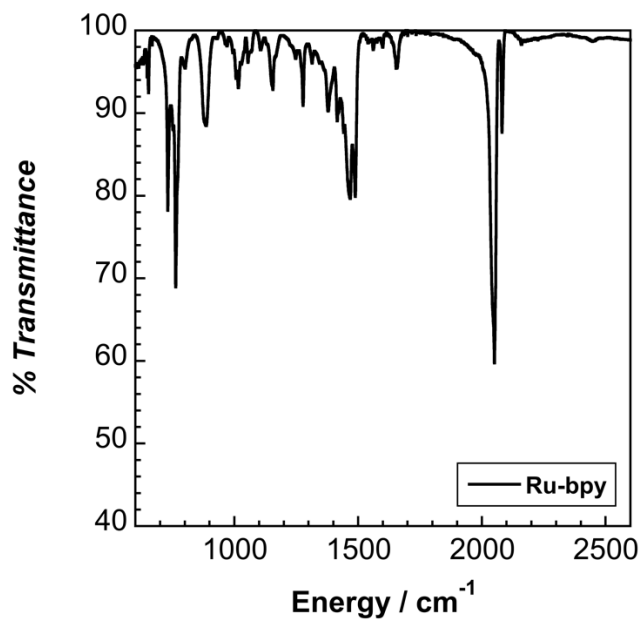


Figure S27. ATR-IR spectrum of **Ru-bpy**.

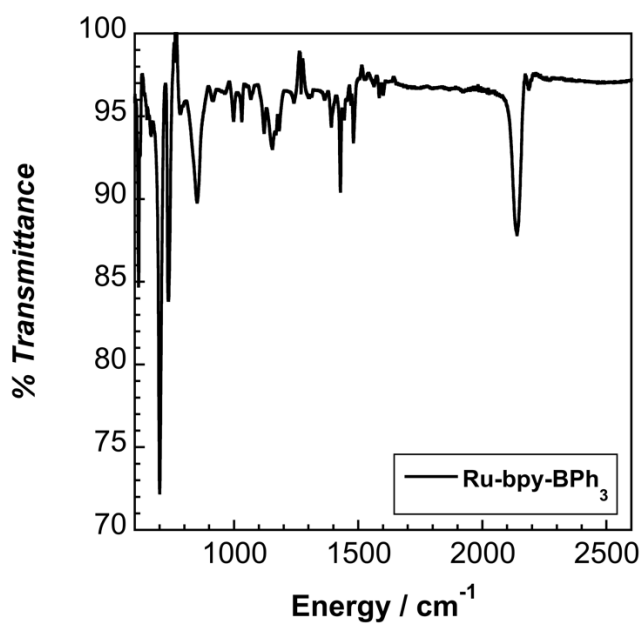


Figure S28. ATR-IR spectrum of **Ru-bpy-BPh₃**.

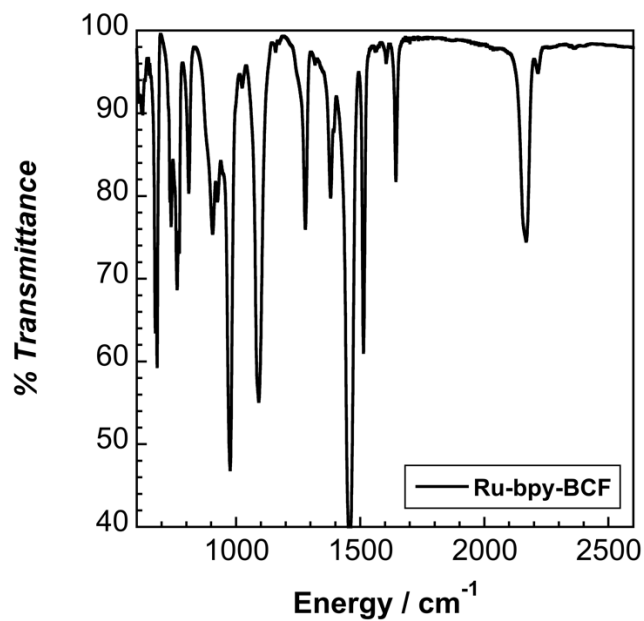


Figure S29. ATR-IR spectrum of **Ru-bpy-BCF**.

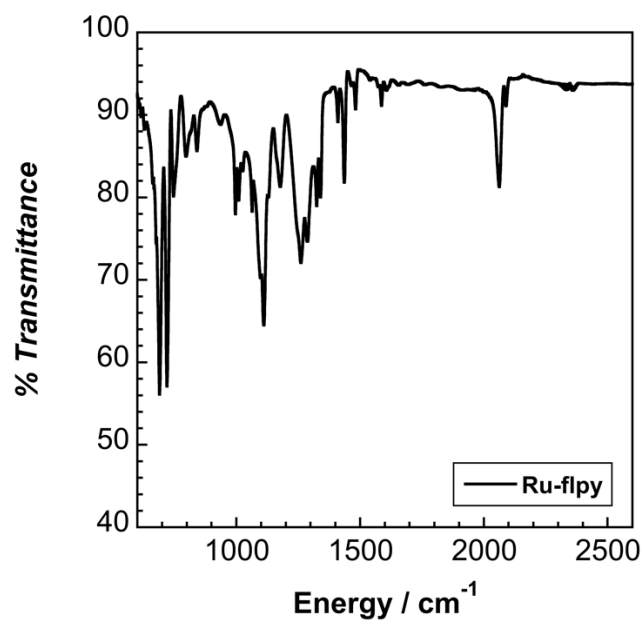


Figure S30. ATR-IR spectrum of **Ru-flpy**.

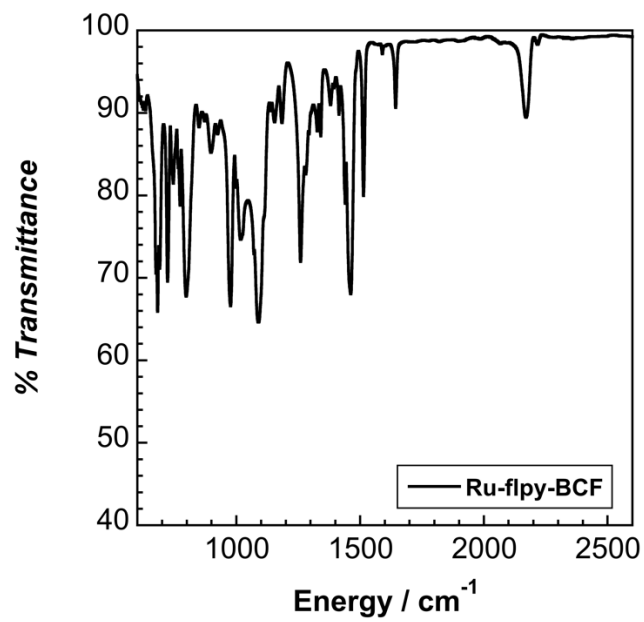


Figure S31. ATR-IR spectrum of **Ru-flpy-BCF**.

S.3. UV-Vis Spectroscopy and Transient Absorption Spectroscopy

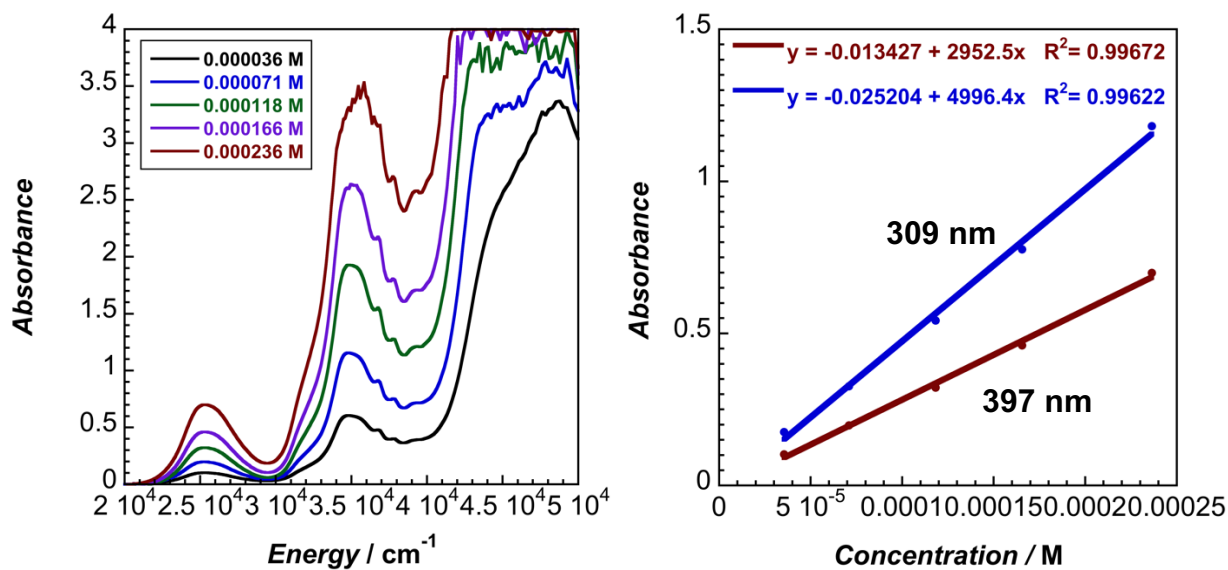


Figure S32. UV-visible absorption spectra and metal-to-ligand charge transfer linear fits for **Ru-bpy-BPh₃** in MeCN using a 1 cm path length cuvette.

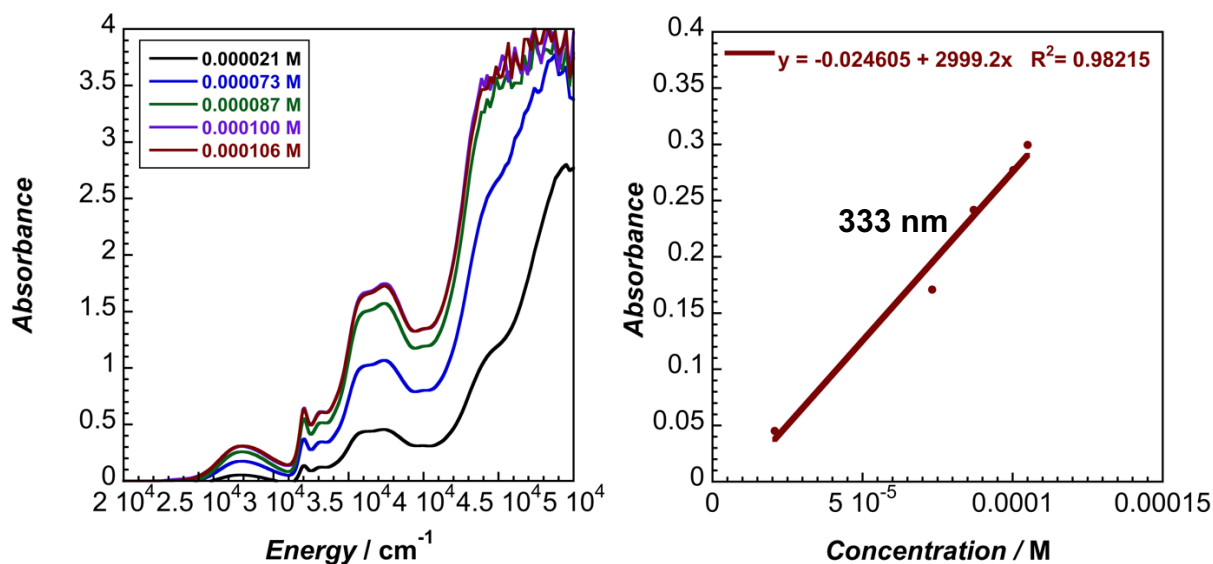


Figure S33. UV-visible absorption spectra and metal-to-ligand charge transfer linear fit for **Ru-bpy-BCF** in MeCN using a 1 cm path length cuvette.

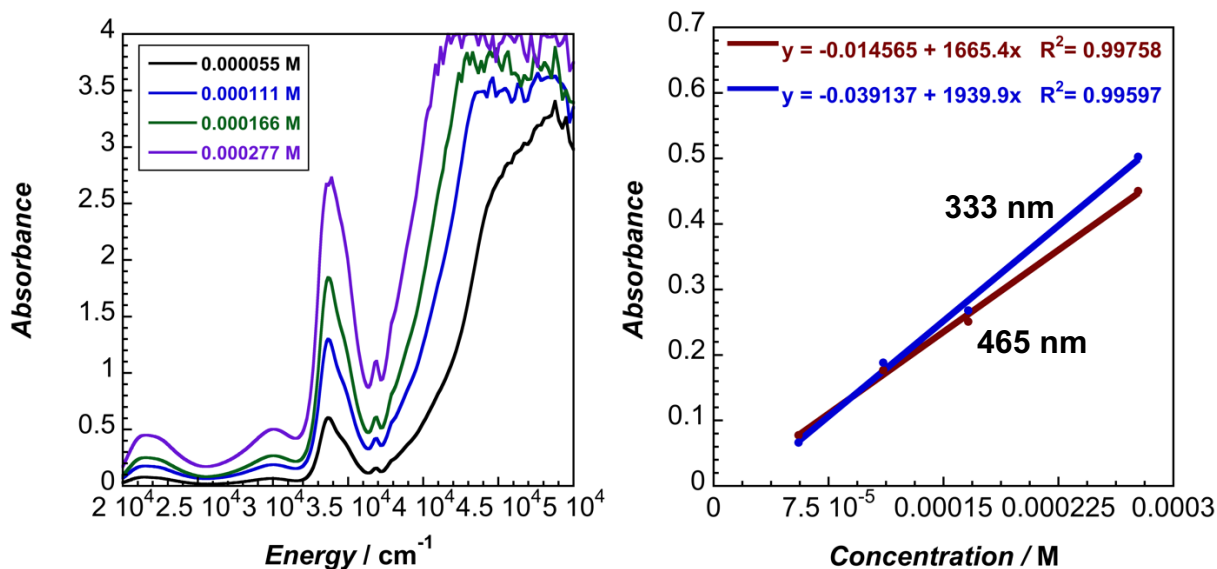


Figure S34. UV-visible absorption spectra and metal-to-ligand charge transfer linear fits for **Fe-bpy-BPh₃** in MeCN using a 1 cm path length cuvette.

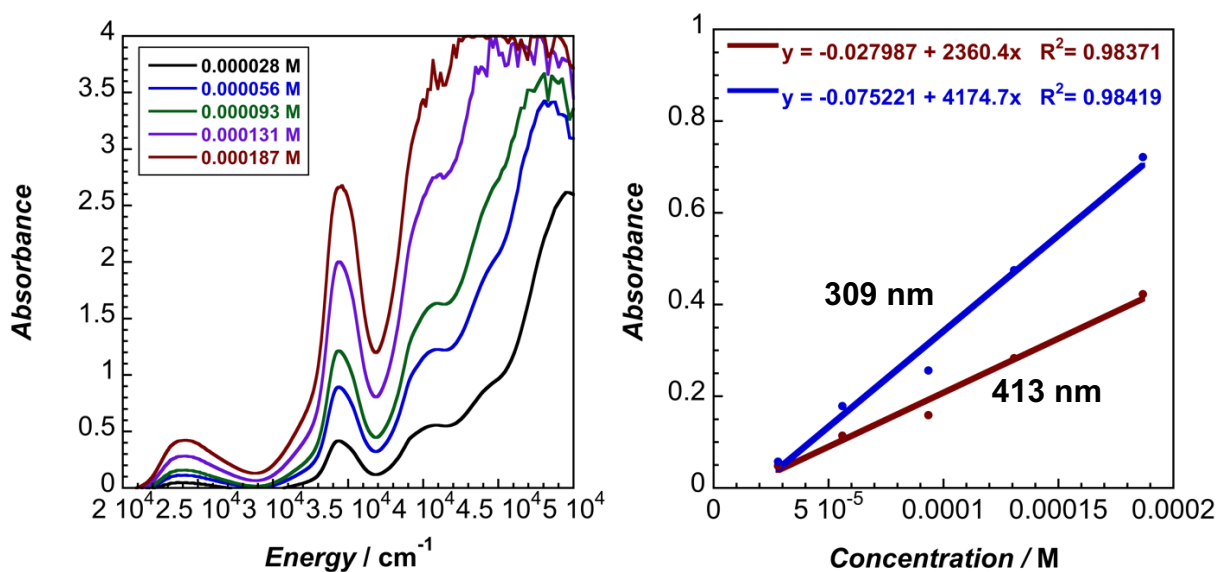


Figure S35. UV-visible absorption spectra and metal-to-ligand charge transfer linear fits for **Fe-bpy-BCF** in MeCN using a 1 cm path length cuvette.

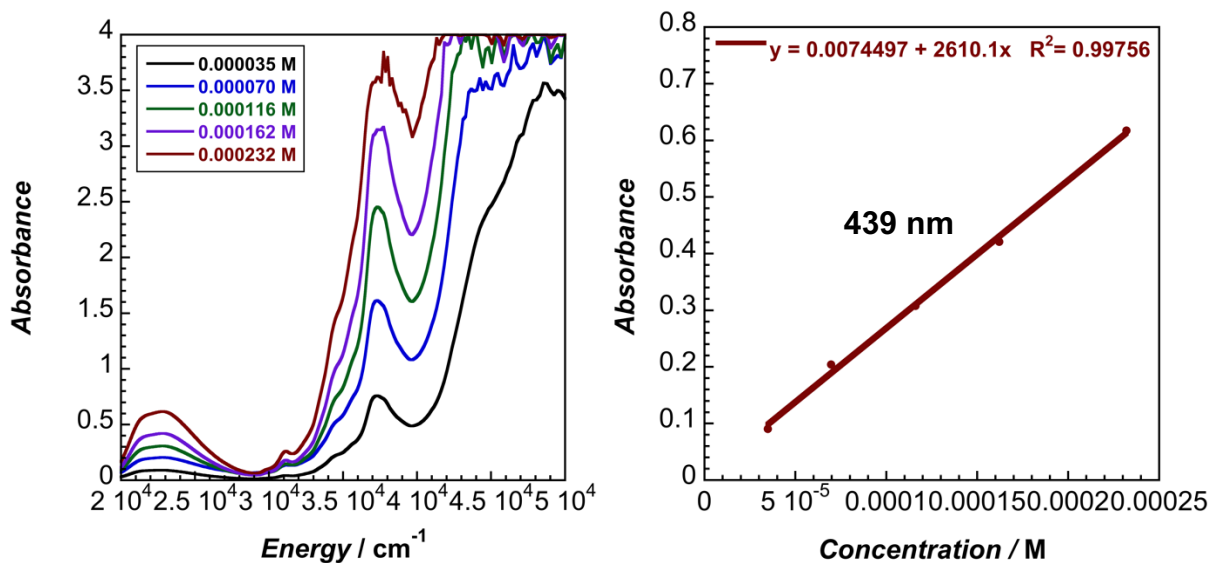


Figure S36. UV-visible absorption spectra and metal-to-ligand charge transfer linear fit for **Fe-phen-BPh₃** in MeCN using a 1 cm path length cuvette.

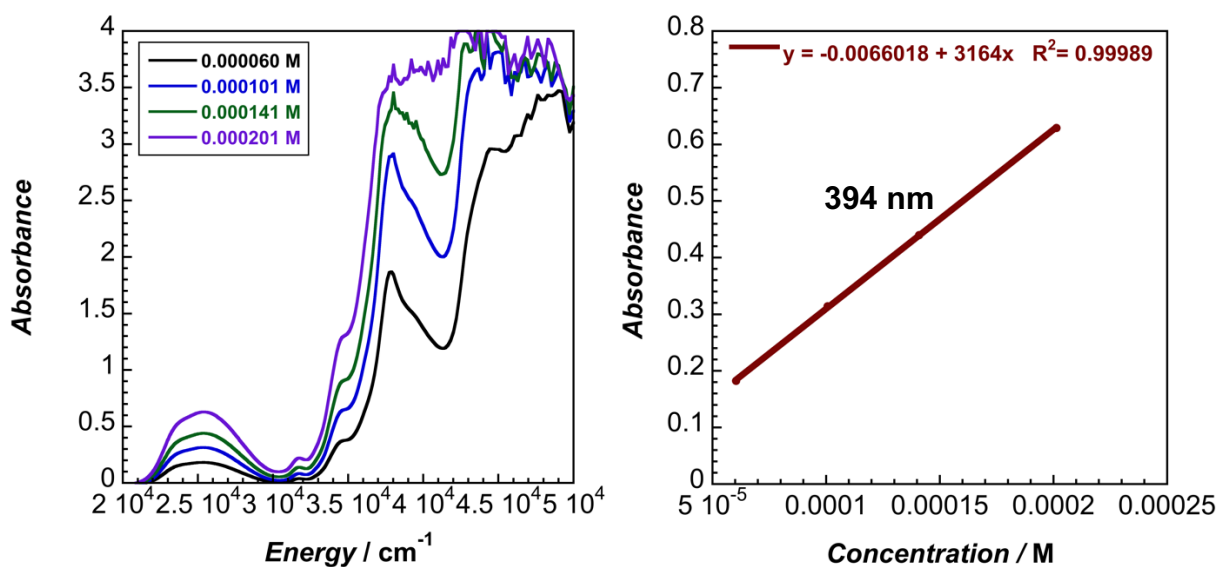


Figure S37. UV-visible absorption spectra and metal-to-ligand charge transfer linear fit for **Fe-phen-BCF** in MeCN using a 1 cm path length cuvette.

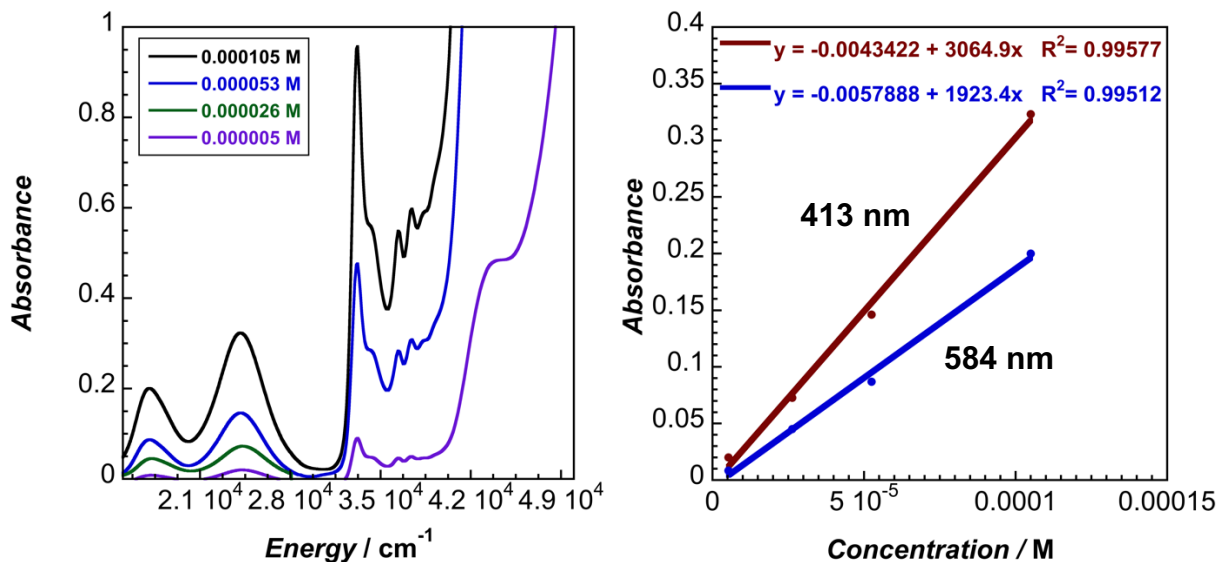


Figure S38. UV-visible absorption spectra and metal-to-ligand charge transfer linear fits for **Ru-flpy** in MeCN using a 0.5 cm path length cuvette.

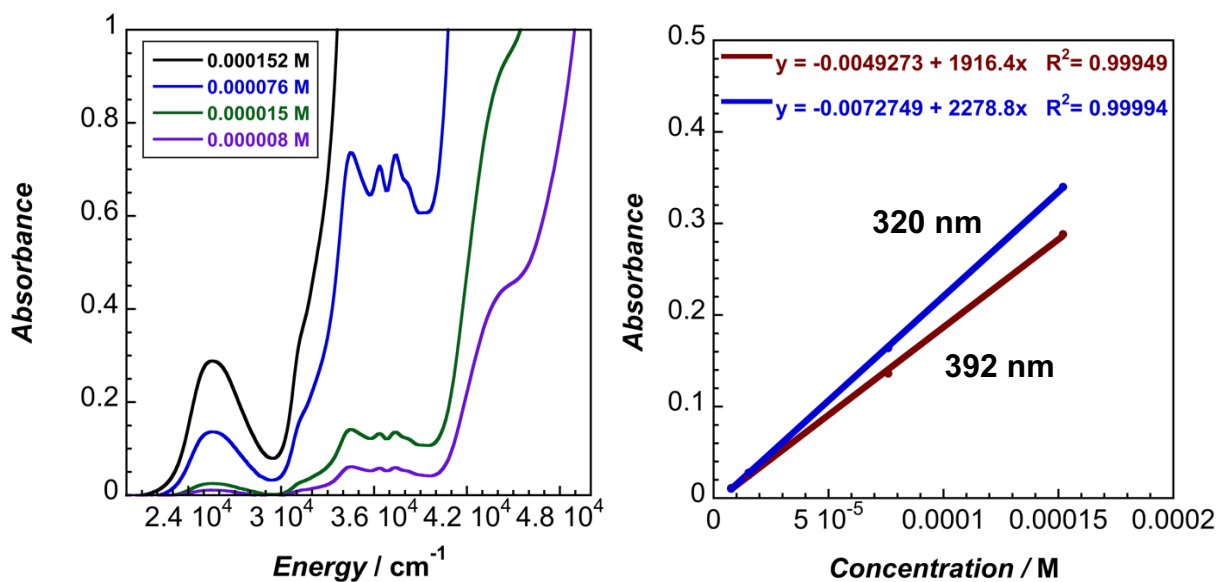


Figure S39. UV-visible absorption spectra and metal-to-ligand charge transfer linear fits for **Ru-flpy-BCF** in MeCN using a 0.5 cm path length cuvette.

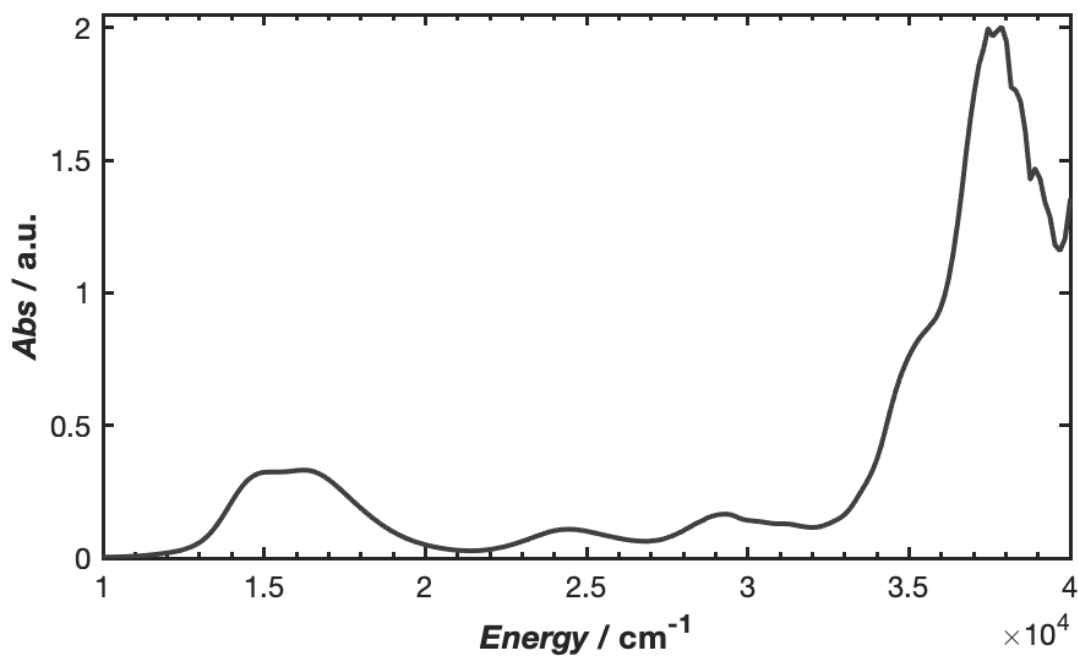


Figure S40. UV-vis absorption spectrum of 0.34 mM **Fe-phen** in MeCN. Spectrum recorded in a 2 mm path length cuvette. For this sample, the optical density is 0.25 a.u. at the intended excitation wavelength.

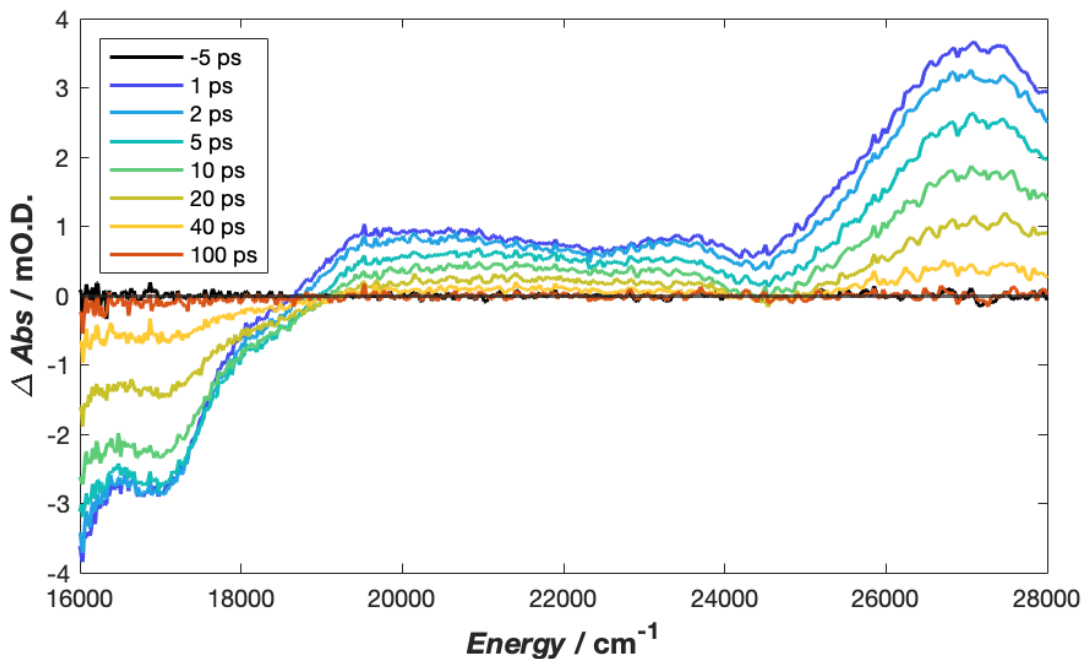


Figure S41. Transient absorption spectra of **Fe-phen** in MeCN after 700 nm / 14,300 cm^{-1} excitation, depicting traces from -5 to 100 ps time delay.

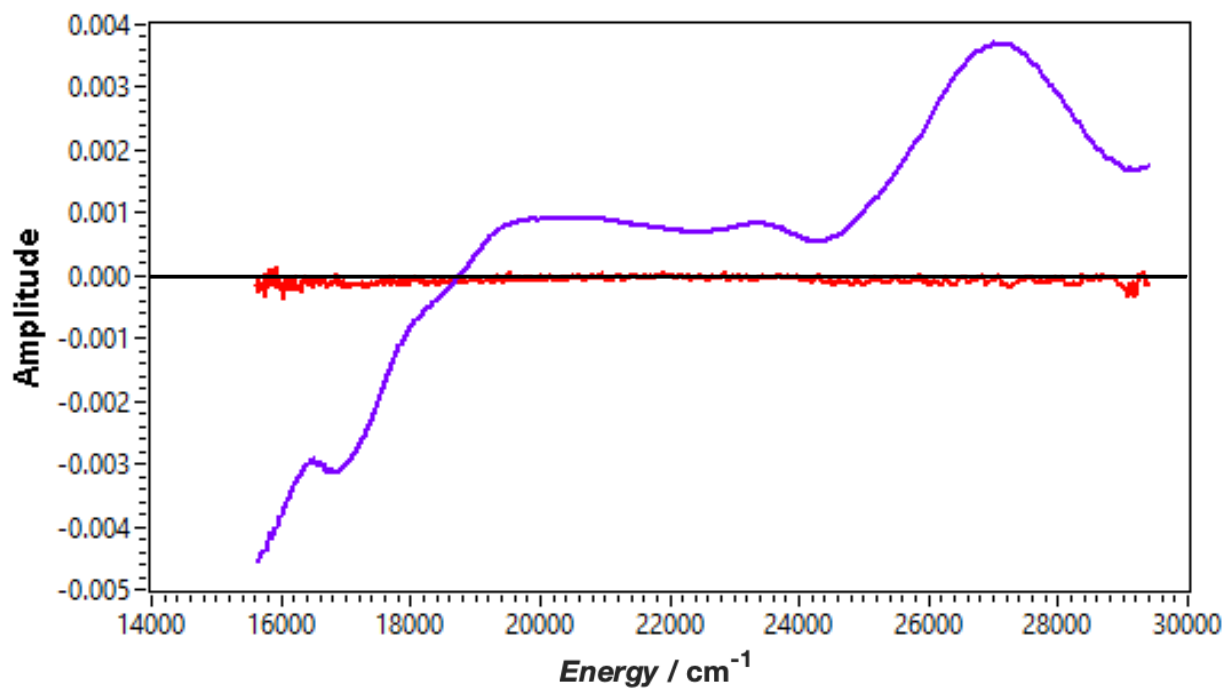


Figure S42. Principal components from a global analysis of the transient absorption data for **Fe-phen**. The red trace, associated with instrument noise, has an infinite lifetime. Single exponent decay kinetics of the purple trace are reported.

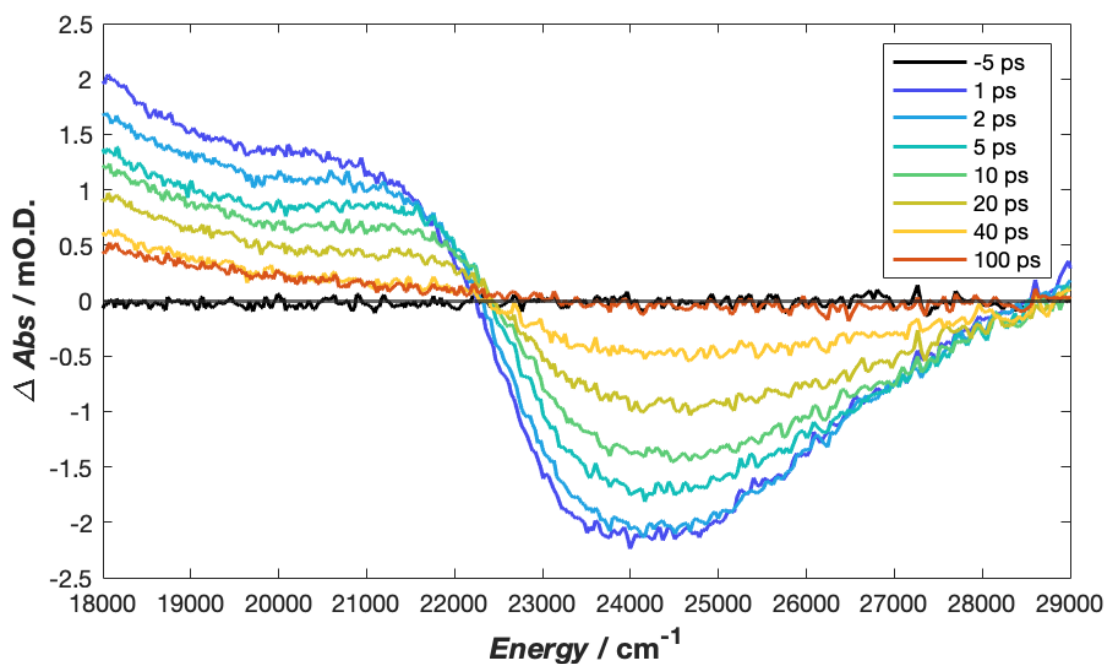


Figure S43. Transient absorption spectra of **Fe-bpy-BCF** after 290 nm / 34,500 cm^{-1} excitation, depicting traces at -5 ps to 100 ps time delay.

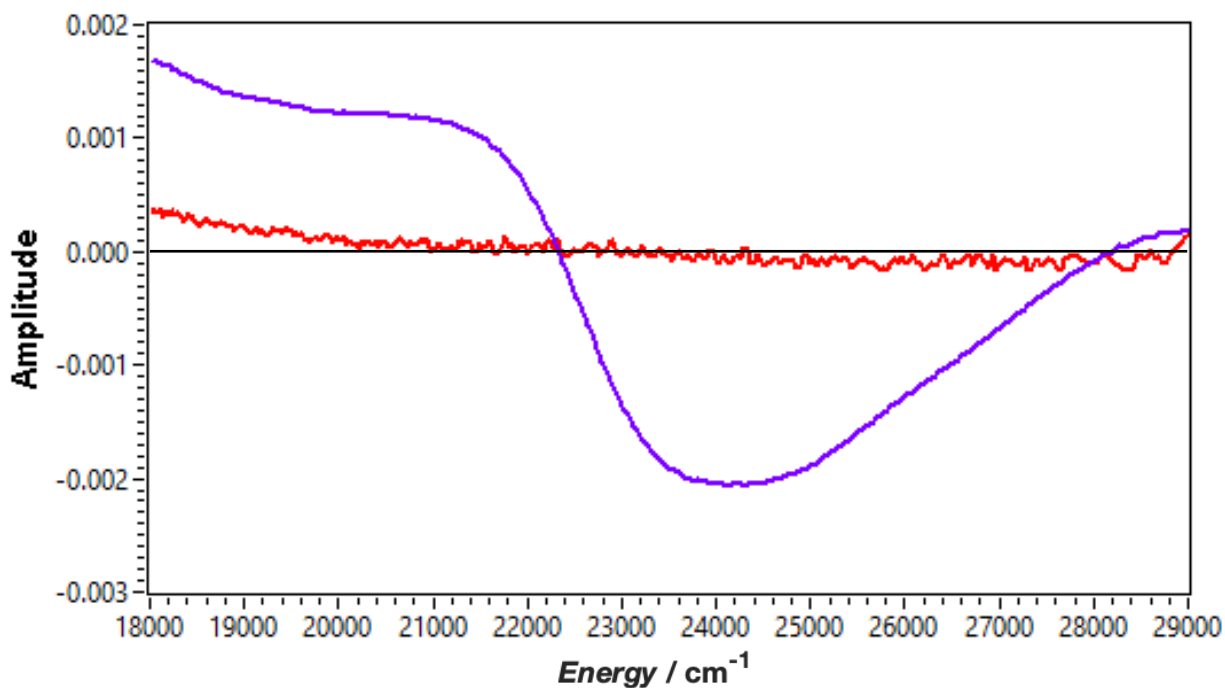


Figure S44. Principal components from a global analysis of the transient absorption data for **Fe-bpy-BCF**. The red trace corresponding to generation of $[(\text{MeCN})_2]^-$ in solution has an infinite lifetime over the experimental time scale. Single exponent decay kinetics of the purple trace are reported.

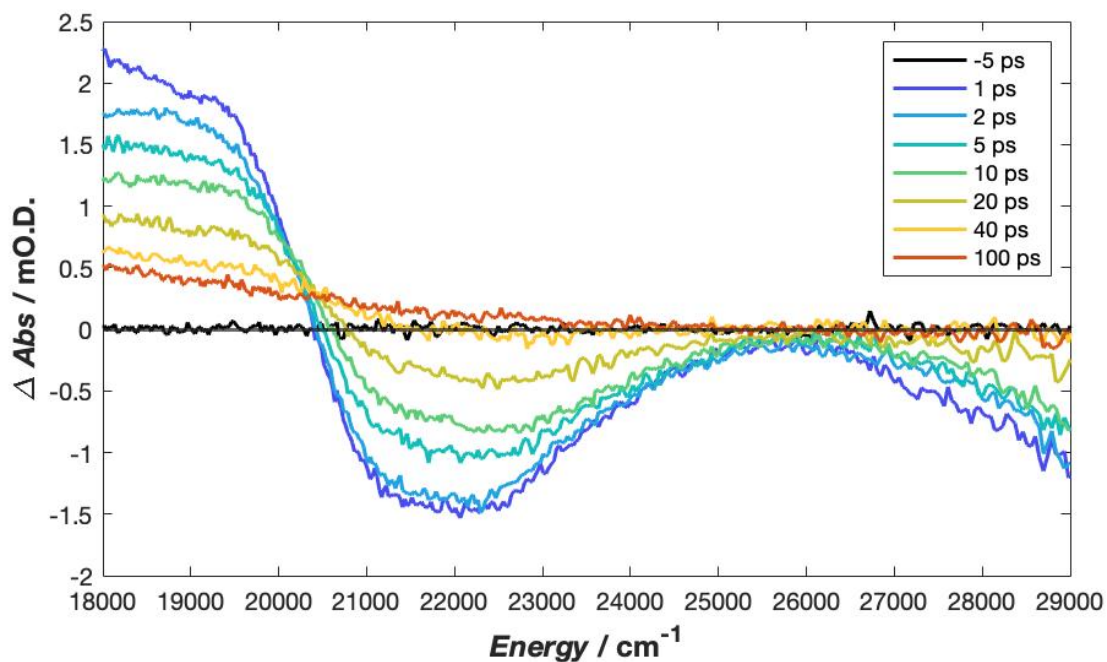


Figure S45. Transient absorption spectra of **Fe-bpy-BPh₃** after 290 nm / 34,500 cm^{-1} excitation, depicting traces at -5 ps to 100 ps time delay.

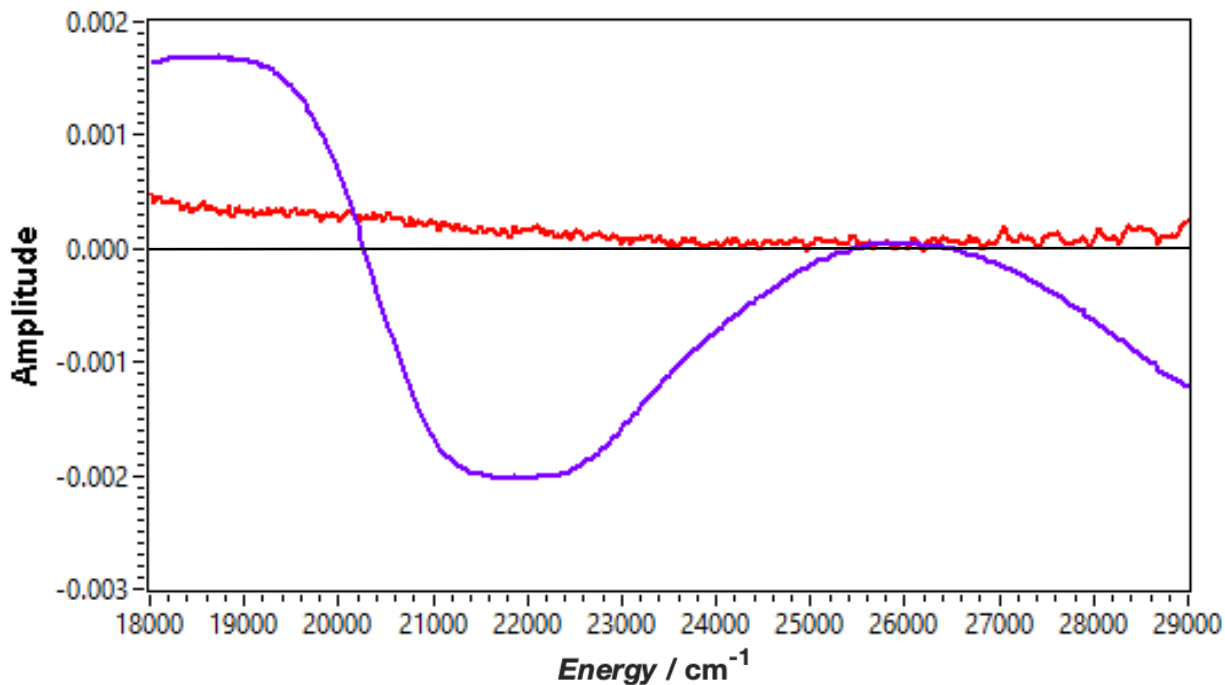


Figure S46. Principal components from a global analysis of the transient absorption data for **Fe-bpy-BPh₃**. The red trace corresponding to generation of [(MeCN)₂]⁻ in solution has an infinite lifetime over the experimental time scale. Single exponent decay kinetics of the purple trace are reported.

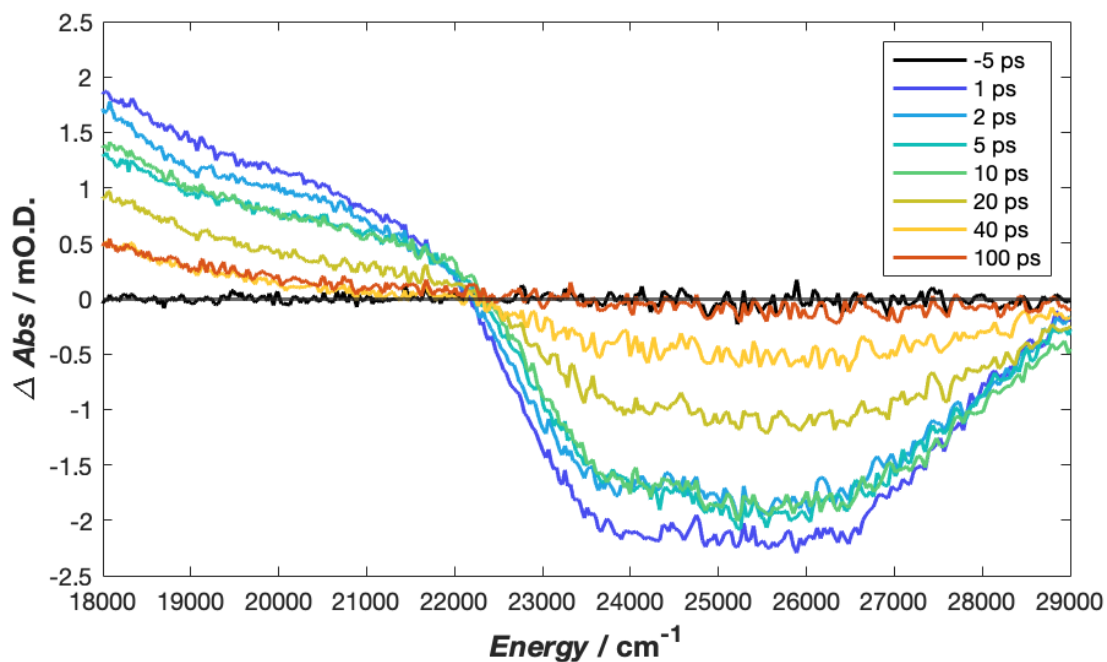


Figure S47. Transient absorption spectra of **Fe-phen-BCF** after 290 nm / 34,500 cm⁻¹ excitation, depicting traces at -5 ps to 100 ps time delay.

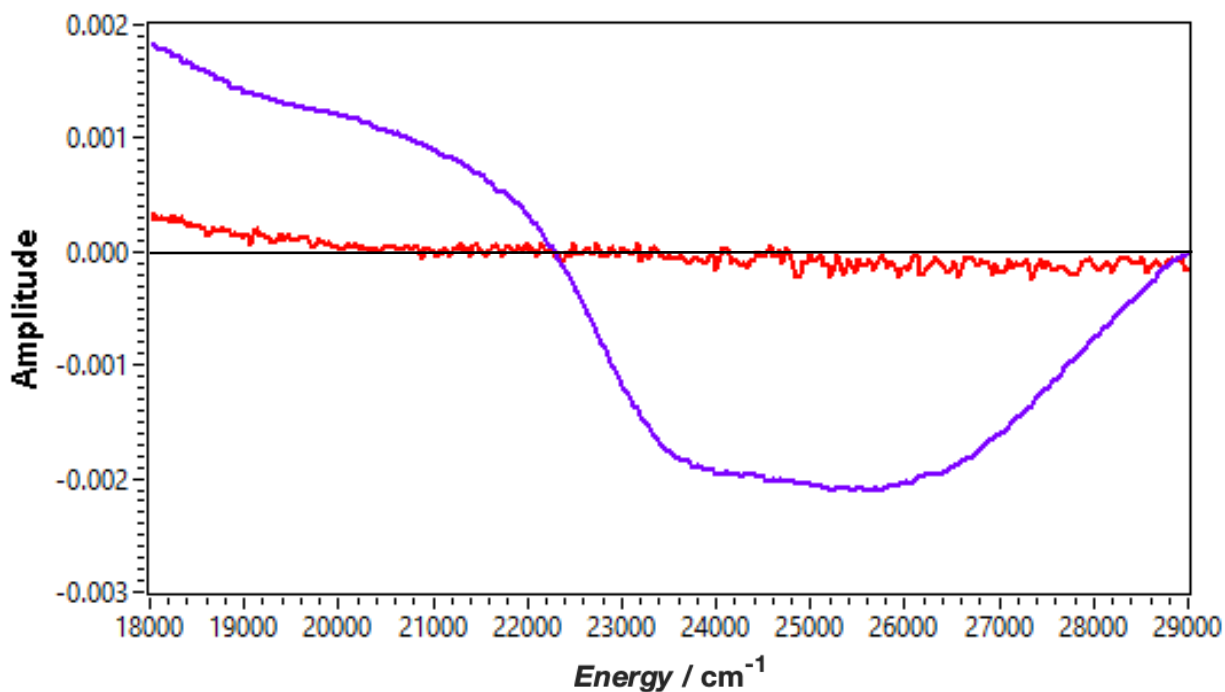


Figure S48. Principal components from a global analysis of the transient absorption data for **Fe-phen-BCF**. The red trace corresponding to $[(\text{MeCN})_2]^-$ in solution has an infinite lifetime over the experimental time scale. Single exponent decay kinetics of the purple trace are reported.

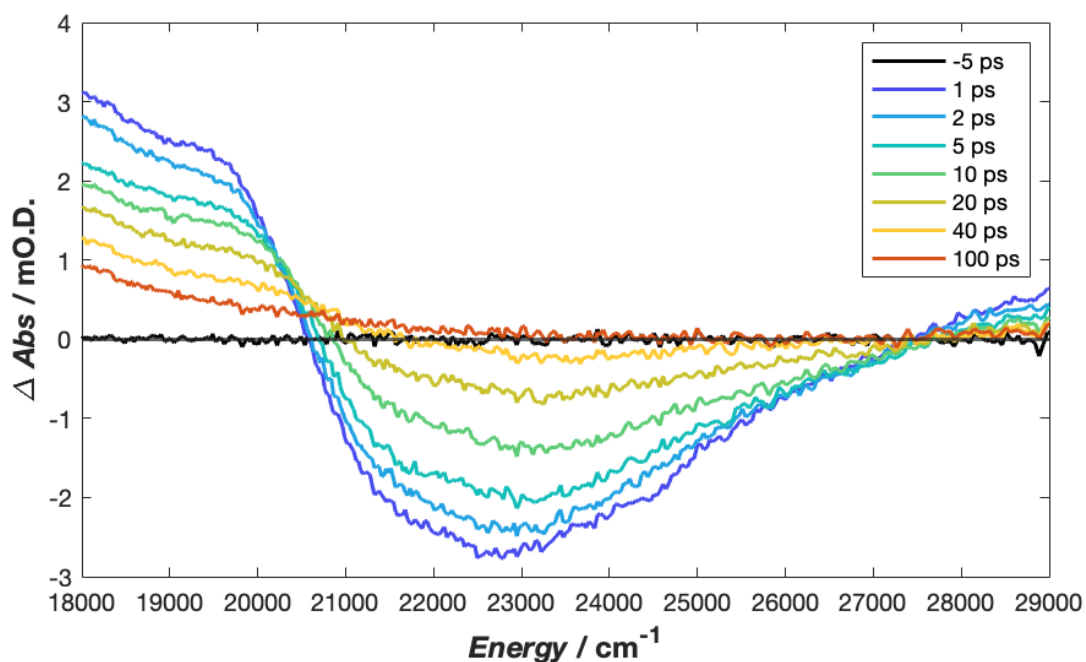


Figure S49. Transient absorption spectra of **Fe-phen-BPh₃** after 290 nm / 34,500 cm^{-1} excitation, depicting traces at -5 ps to 100 ps time delay.

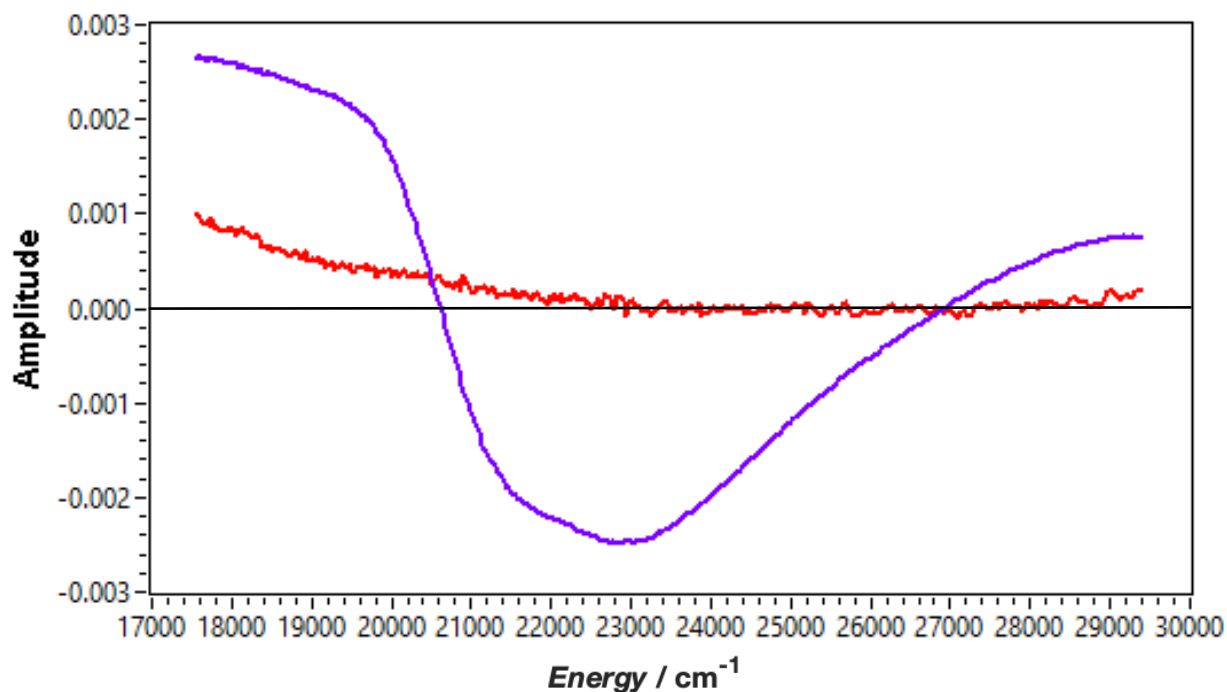


Figure S50. Principal components from a global analysis of the transient absorption data for **Fe-phen-BPh₃**. The red trace corresponding to [(MeCN)₂]⁻ in solution has an infinite lifetime over the experimental time scale. Single exponent decay kinetics of the purple trace are reported.

Table S1. Kinetic lifetimes for [Fe(diimine)(CN)₄]²⁻ and [Fe(diimine)(CN-BR₃)₄]²⁻ in MeCN. Spectra fit using SVD/global analysis.

Species	τ (ps)
Fe-bpy	18.1 ps ¹
Fe-bpy-BPh₃	18.5 ± 2.1 ps
Fe-bpy-BCF	22.4 ± 2.3 ps
Fe-phen	19.5 ± 1.3 ps
Fe-phen-BPh₃	17.9 ± 1.7 ps
Fe-phen-BCF	25.1 ± 2.3 ps

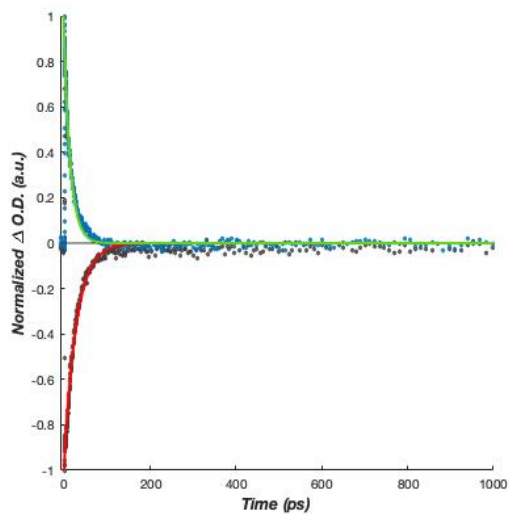


Figure S51. Exponential decay fits for the ESA and GSB of **Fe-phen** excited at 290 nm. **ESA:** 588 nm / 17,000 cm^{-1} , **GSB:** 370 nm / 27,000 cm^{-1} .

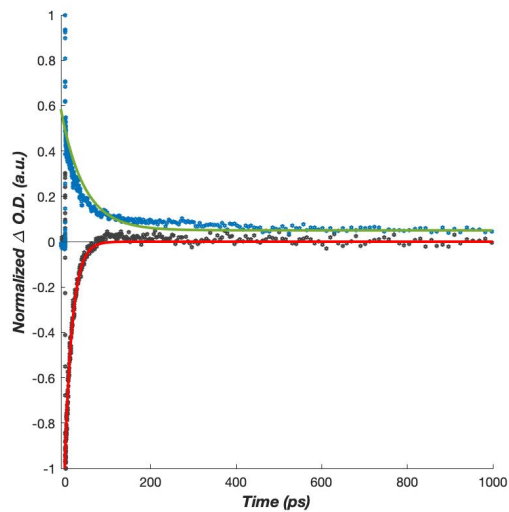


Figure S52. Exponential decay fits for the ESA and GSB of **Fe-phen-BPh₃** excited at 290 nm. **ESA:** 500 nm / 20,000 cm^{-1} , **GSB:** 435 nm / 23,000 cm^{-1} .

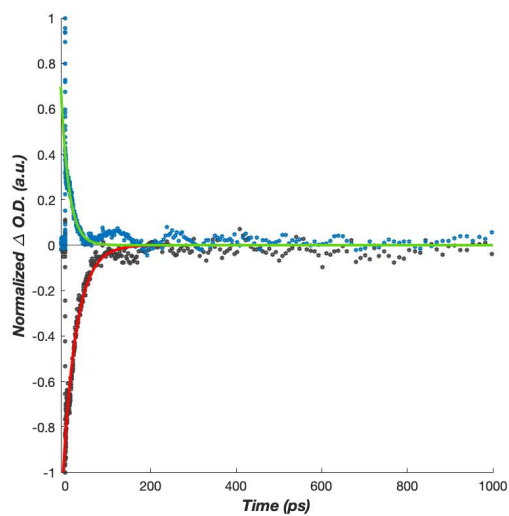


Figure S53. Exponential decay fits for the ESA and GSB of **Fe-phen-BCF** excited at 290 nm. **ESA:** 477 nm / 21,000 cm^{-1} , **GSB:** 400 nm / 25,000 cm^{-1} .

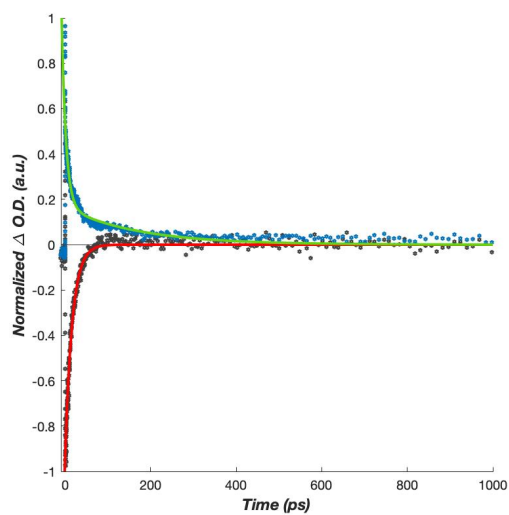


Figure S54. Exponential decay fits for the ESA and GSB of **Fe-bpy-BPh₃** excited at 290 nm. **ESA:** 515 nm / 19,500 cm^{-1} , **GSB:** 435 nm / 23,000 cm^{-1} .

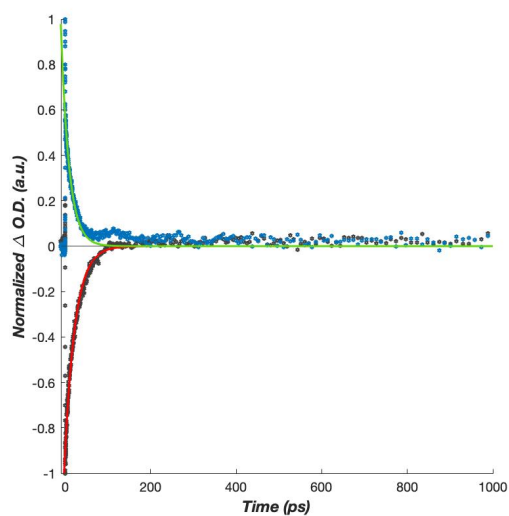


Figure S55. Exponential decay fits for the ESA and GSB of **Fe-bpy-BCF** excited at 290 nm. **ESA:** 477 nm / 21,000 cm^{-1} , **GSB:** 417 nm / 24,000 cm^{-1} .

S.4. Additional Electrochemistry Data

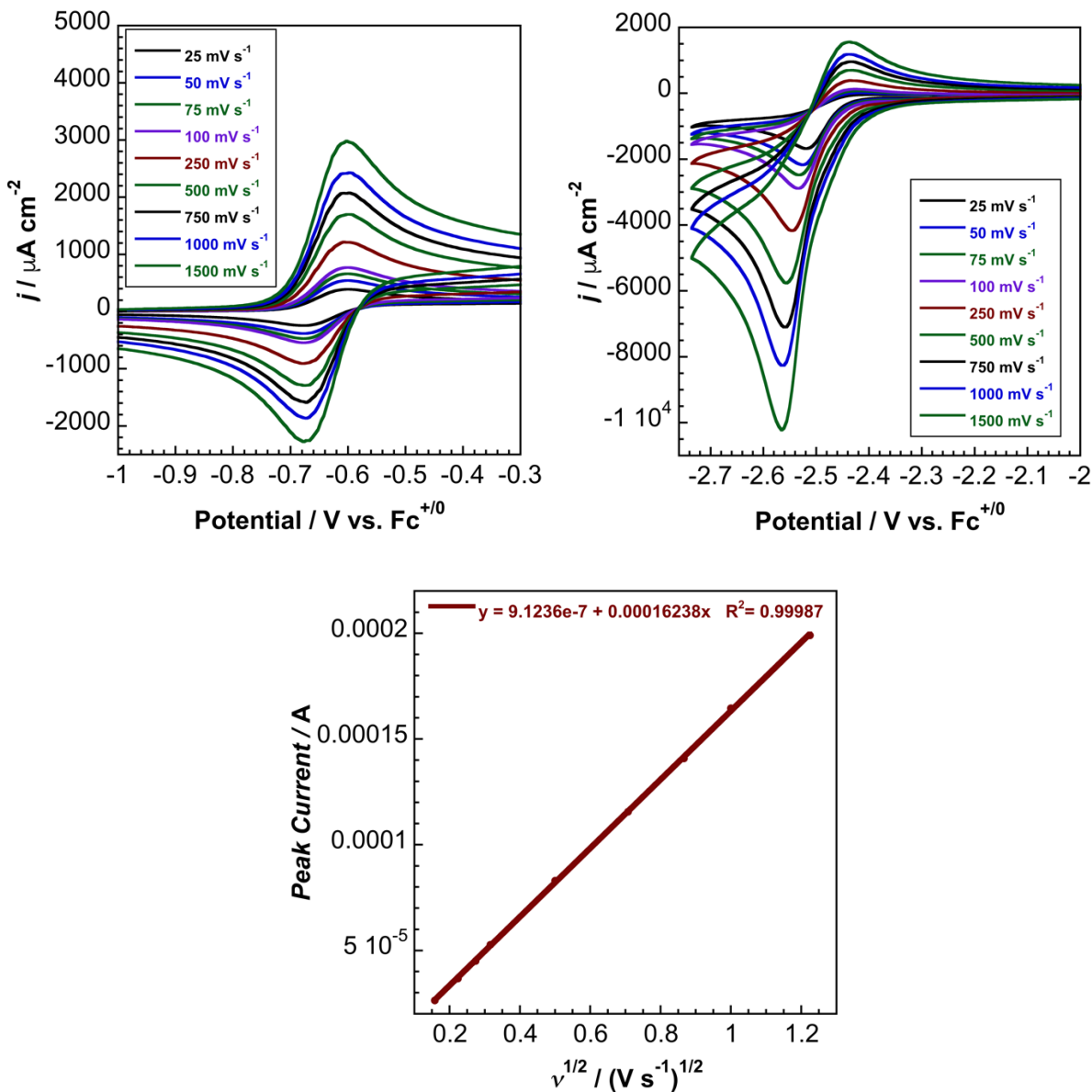


Figure S56. Scan rate dependence and oxidation Randles-Ševčík plot for 3.5 mM $(\text{PPN})_2[\text{Fe}(\text{bpy})(\text{CN})_4]$ (**Fe-bpy**) in MeCN with 0.2 M TBAPF_6 electrolyte.

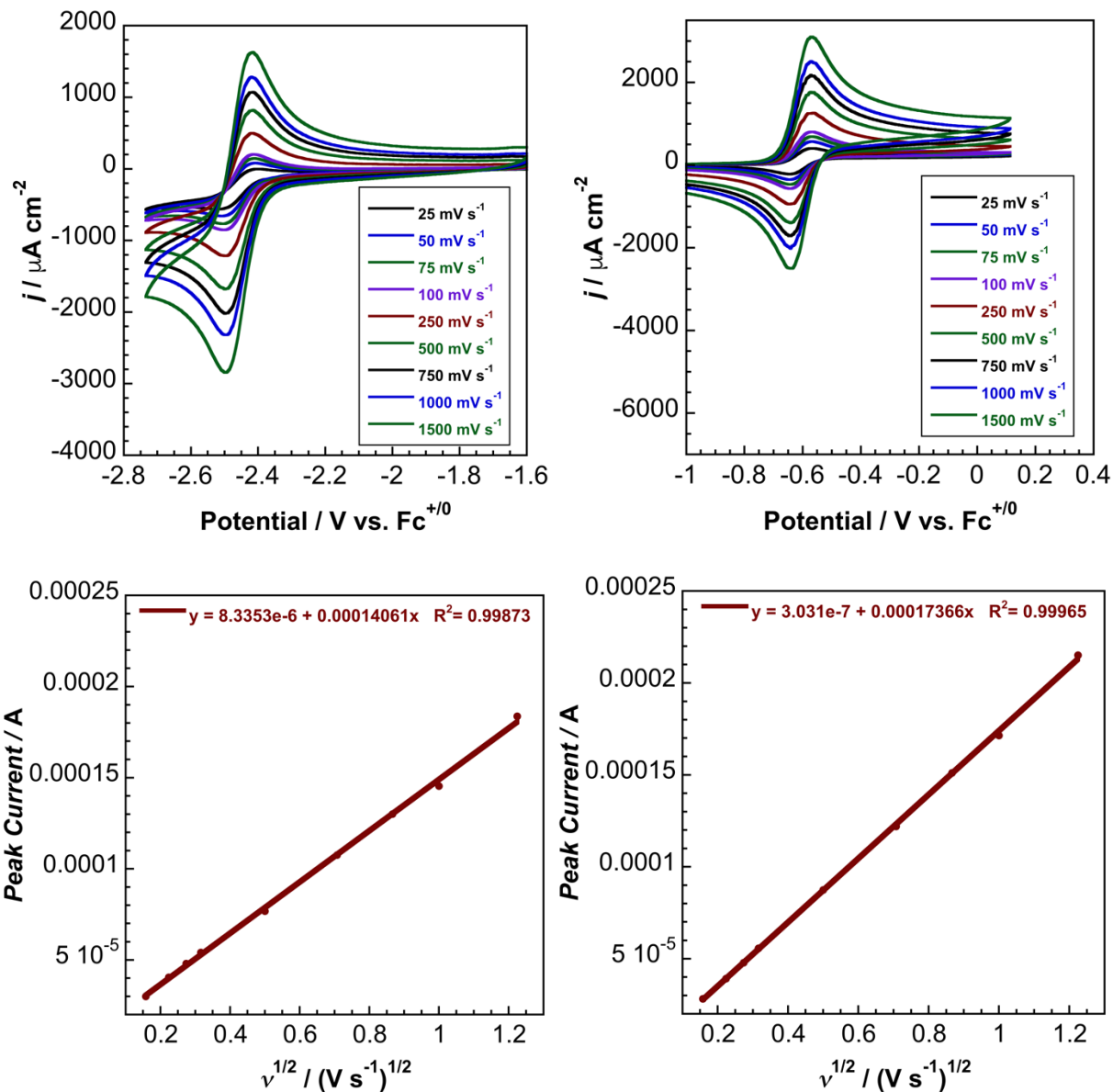


Figure S57. Scan rate dependence and Randles-Ševčík plots for 3.1(reduction)/3.2(oxidation) mM $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN})_4]$ (**Fe-phen**) in MeCN with 0.2 M TBAPF₆ electrolyte.

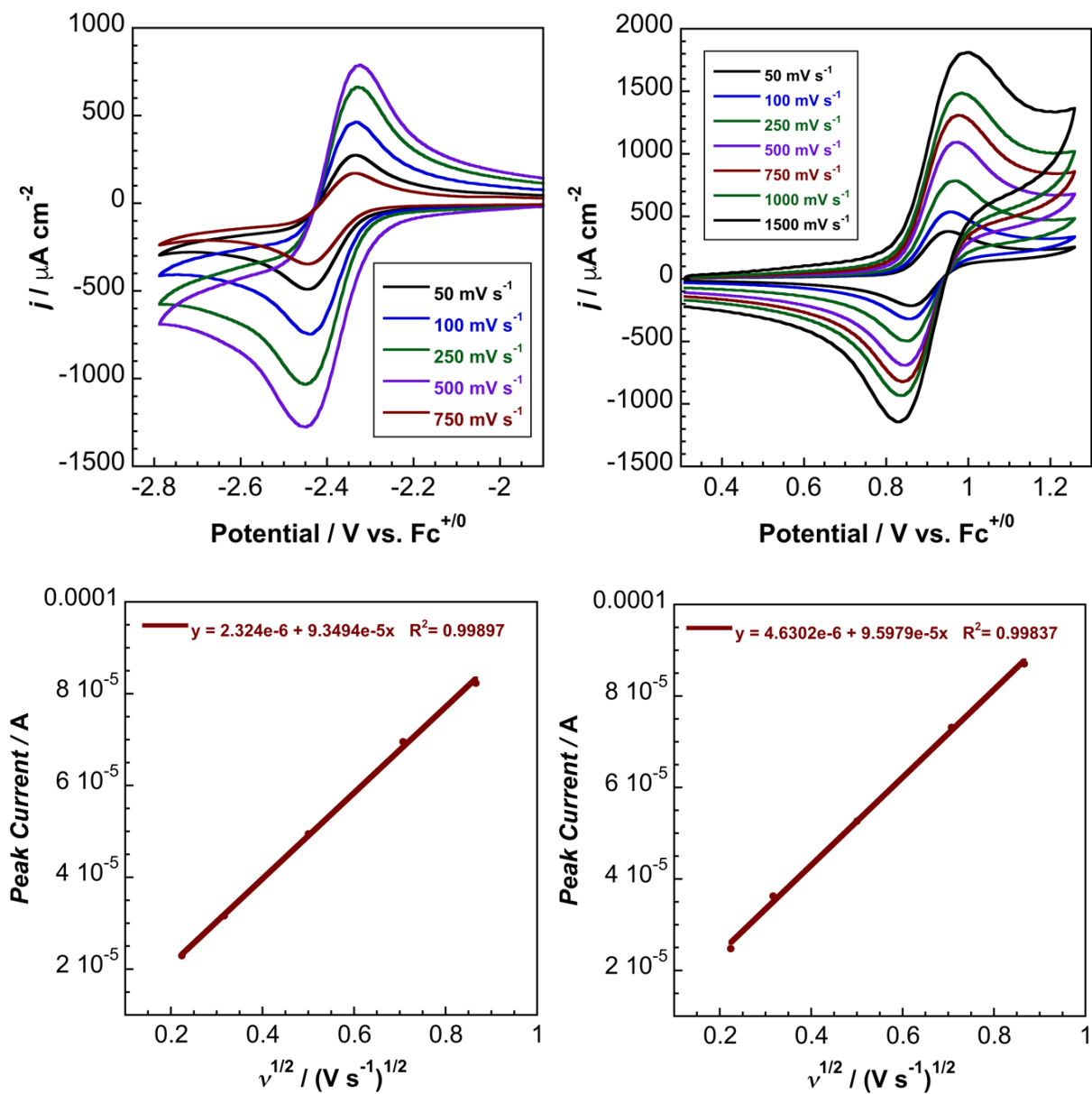


Figure S58. Scan rate dependence and Randles-Ševčík plots for 2.9 mM (TBA)₂[Fe(bpy)(CN-B(C₆F₅)₃)₄] (**Fe-bpy-BCF**) in THF with 0.2 M TBAPF₆ electrolyte.

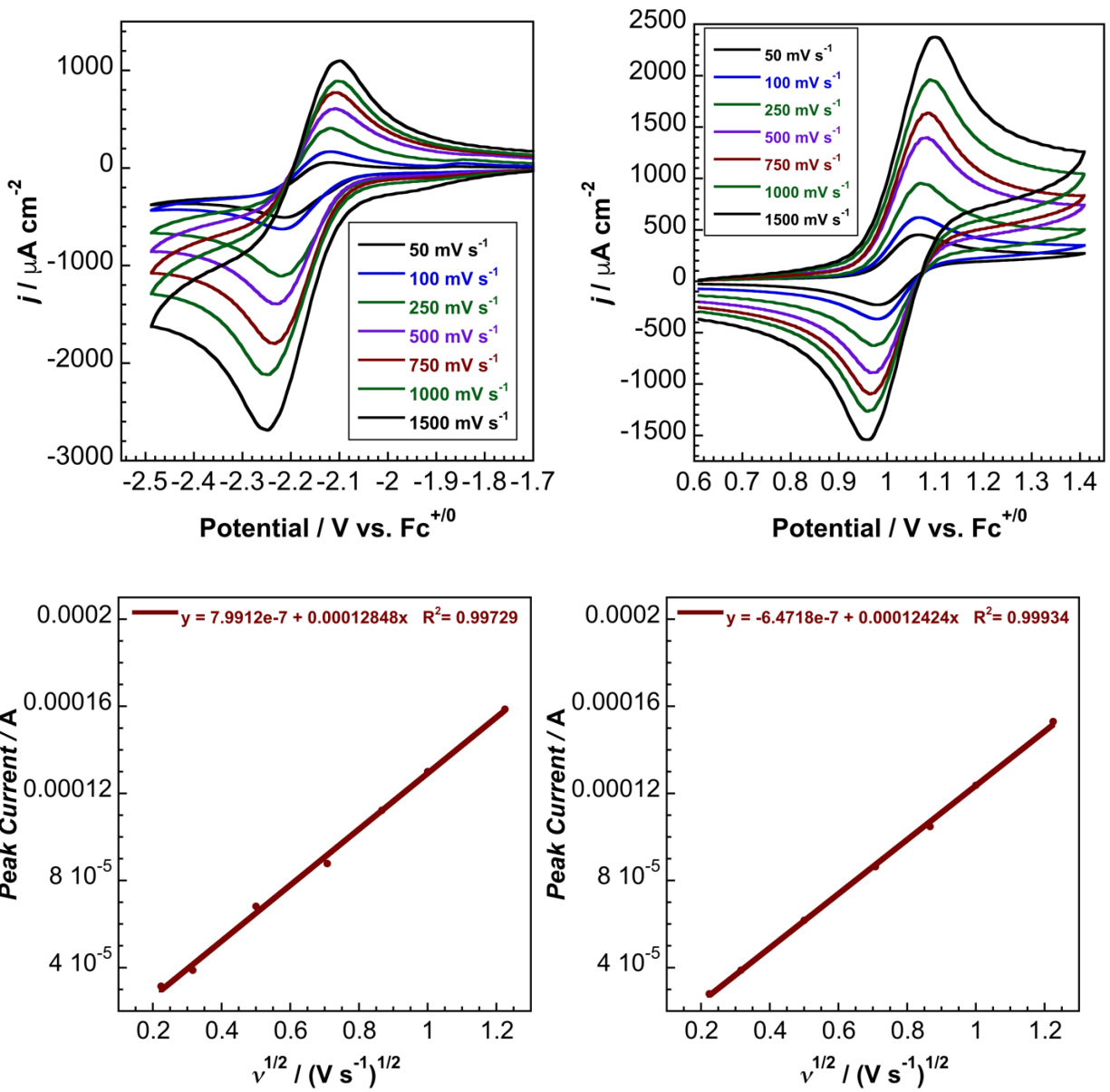


Figure S59. Scan rate dependence and Randles-Ševčík plots for 3.0 mM (TBA)₂[Fe(phen)(CN-B(C₆F₅)₃)₄] (**Fe-phen-BCF**) in MeCN with 0.1 M TBAPF₆ electrolyte.

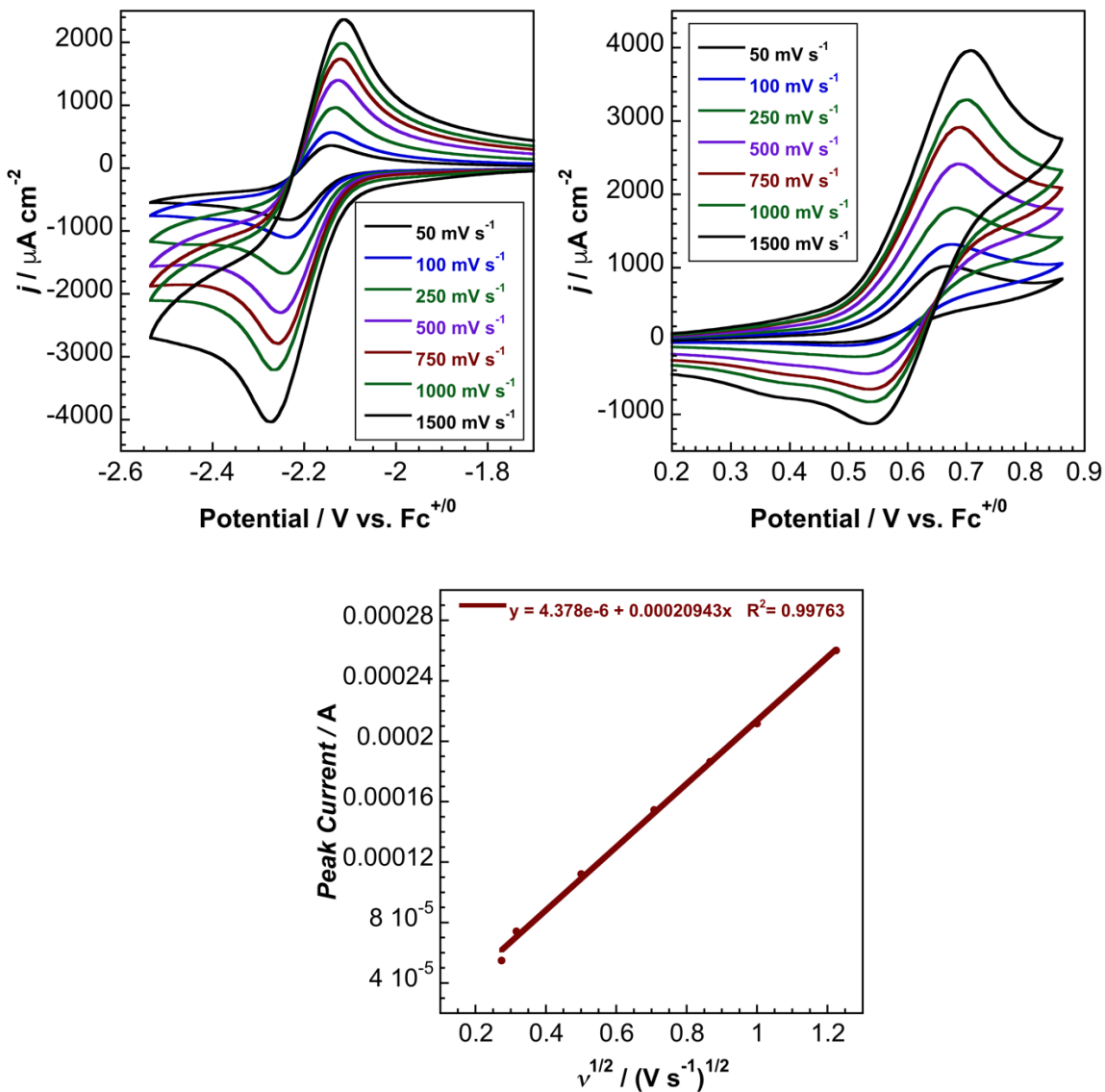


Figure S60. Scan rate dependence and reduction Randles-Ševčík plot for 5.0 mM $(\text{TBA})_2[\text{Fe}(\text{bpy})(\text{CN-BPh}_3)_4]$ (**Fe-bpy-BPh₃**) in MeCN with 0.1 M TBAPF₆ electrolyte.

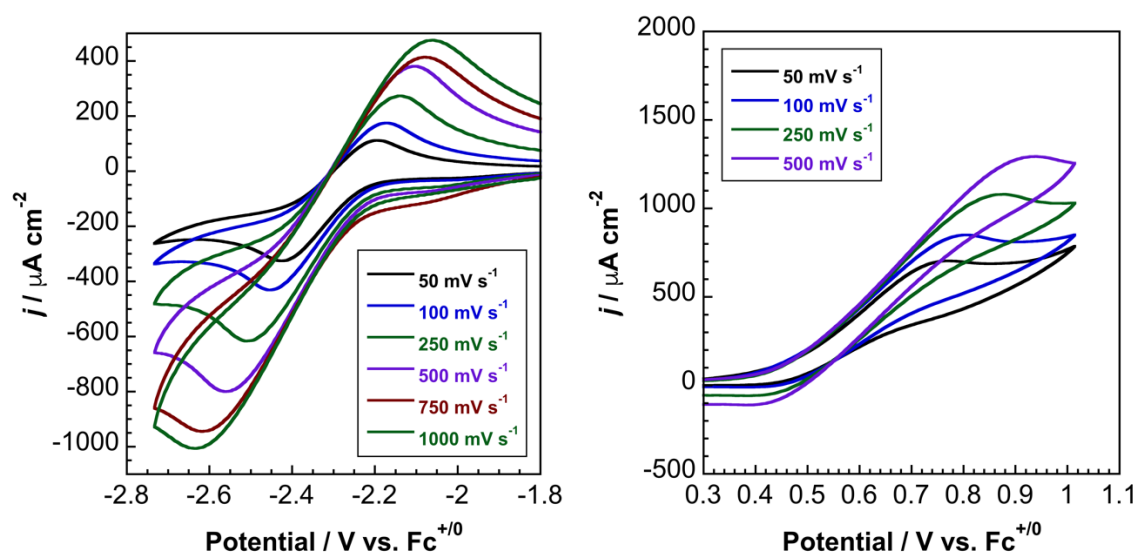


Figure S61. Scan rate dependence for 3.9 mM $(\text{TBA})_2[\text{Fe}(\text{phen})(\text{CN-BPh}_3)_4]$ (**Fe-phen-BPh₃**) in MeCN with 0.1 M TBAPF₆ electrolyte.

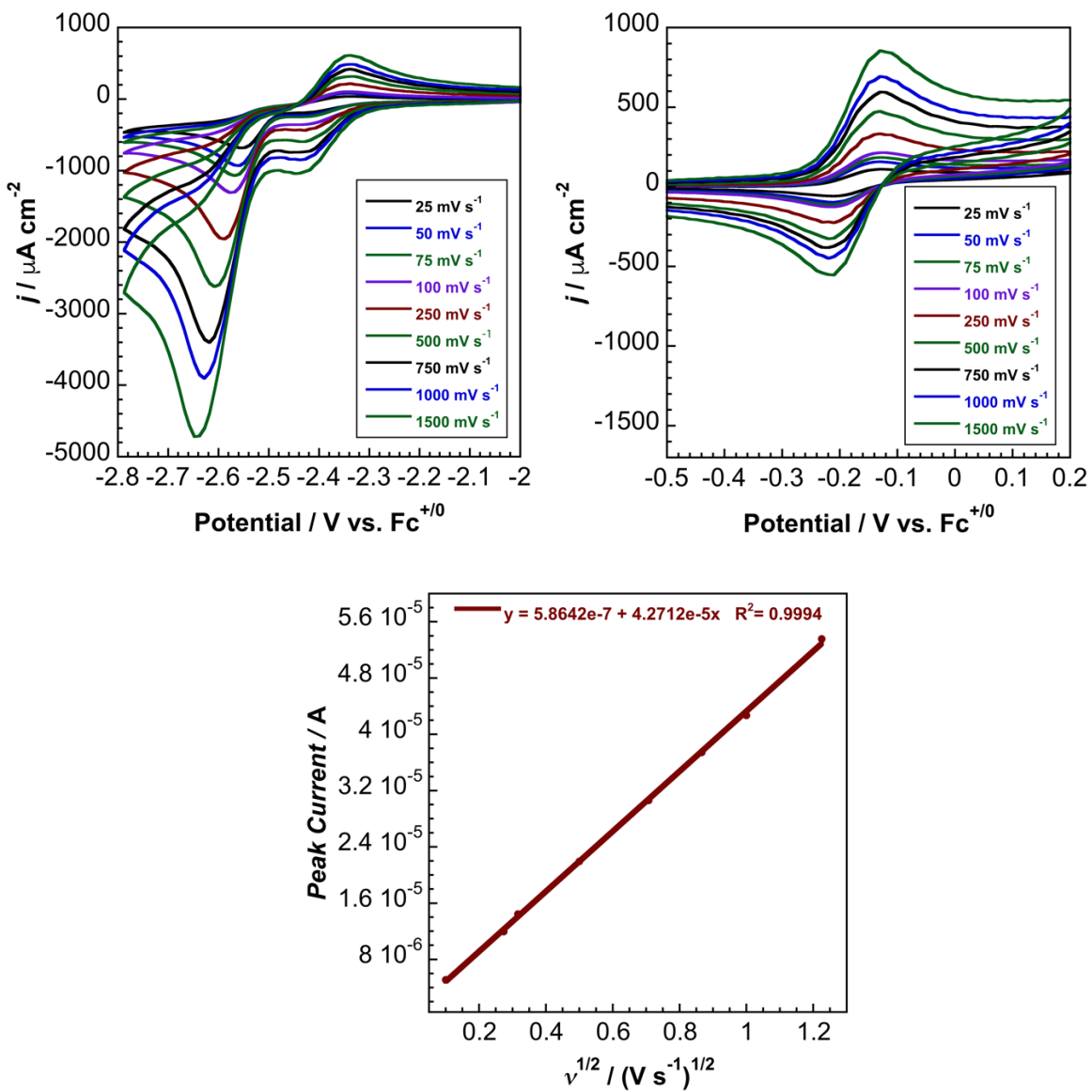


Figure S62. Scan rate dependence and oxidation Randles-Ševčík plot for 1.4 mM $(\text{PPN})_2[\text{Ru}(\text{bpy})(\text{CN})_4]$ (**Ru-bpy**) in MeCN with 0.1 M TBAPF₆ electrolyte.

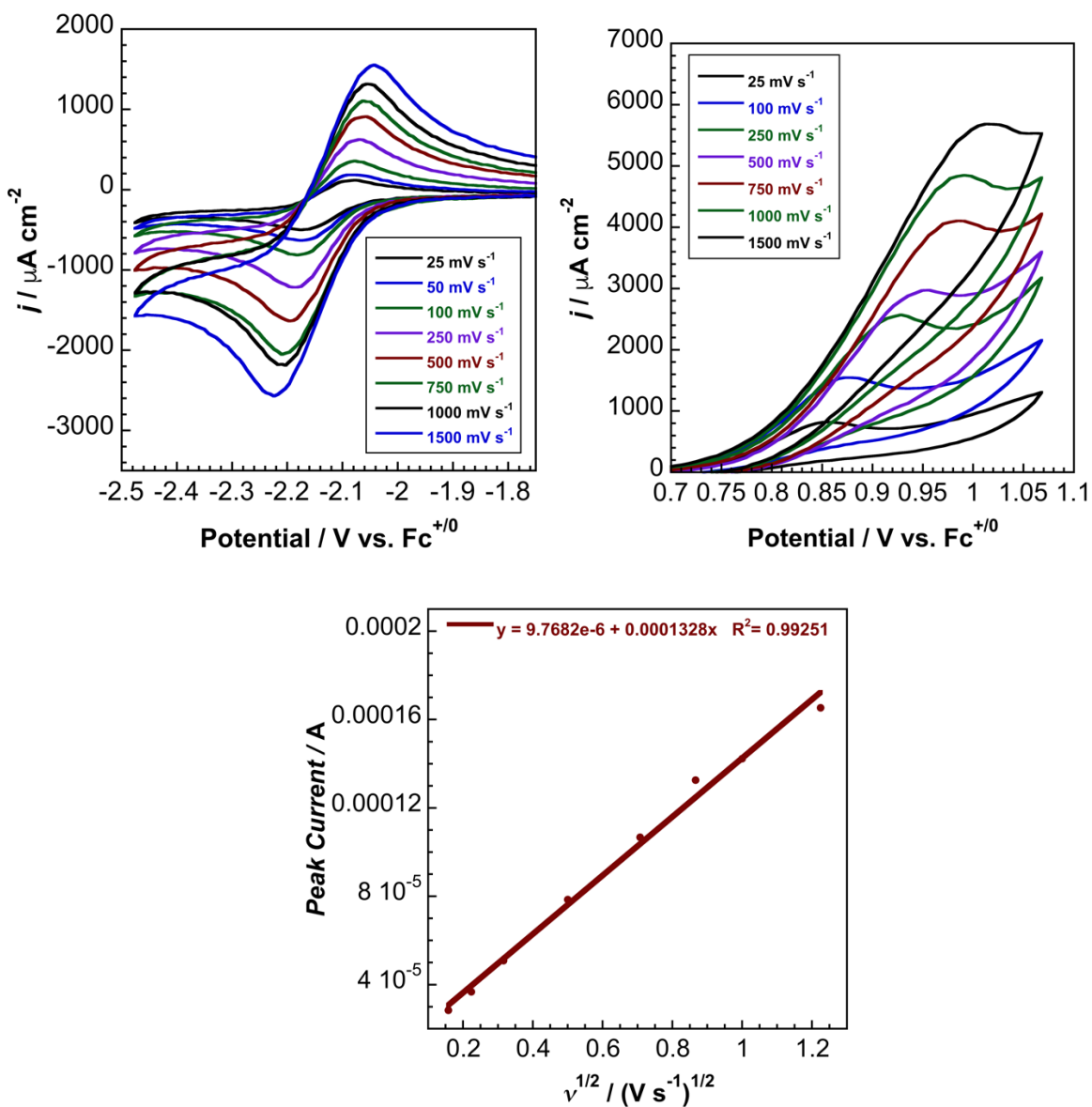


Figure S63. Scan rate dependence and reduction Randles-Ševčík plot for 4.8 mM $(\text{PPN})_2[\text{Ru}(\text{bpy})(\text{CN-BPh}_3)_4]$ (**Ru-bpy-BPh₃**) in MeCN with 0.1 M TBAPF₆ electrolyte.

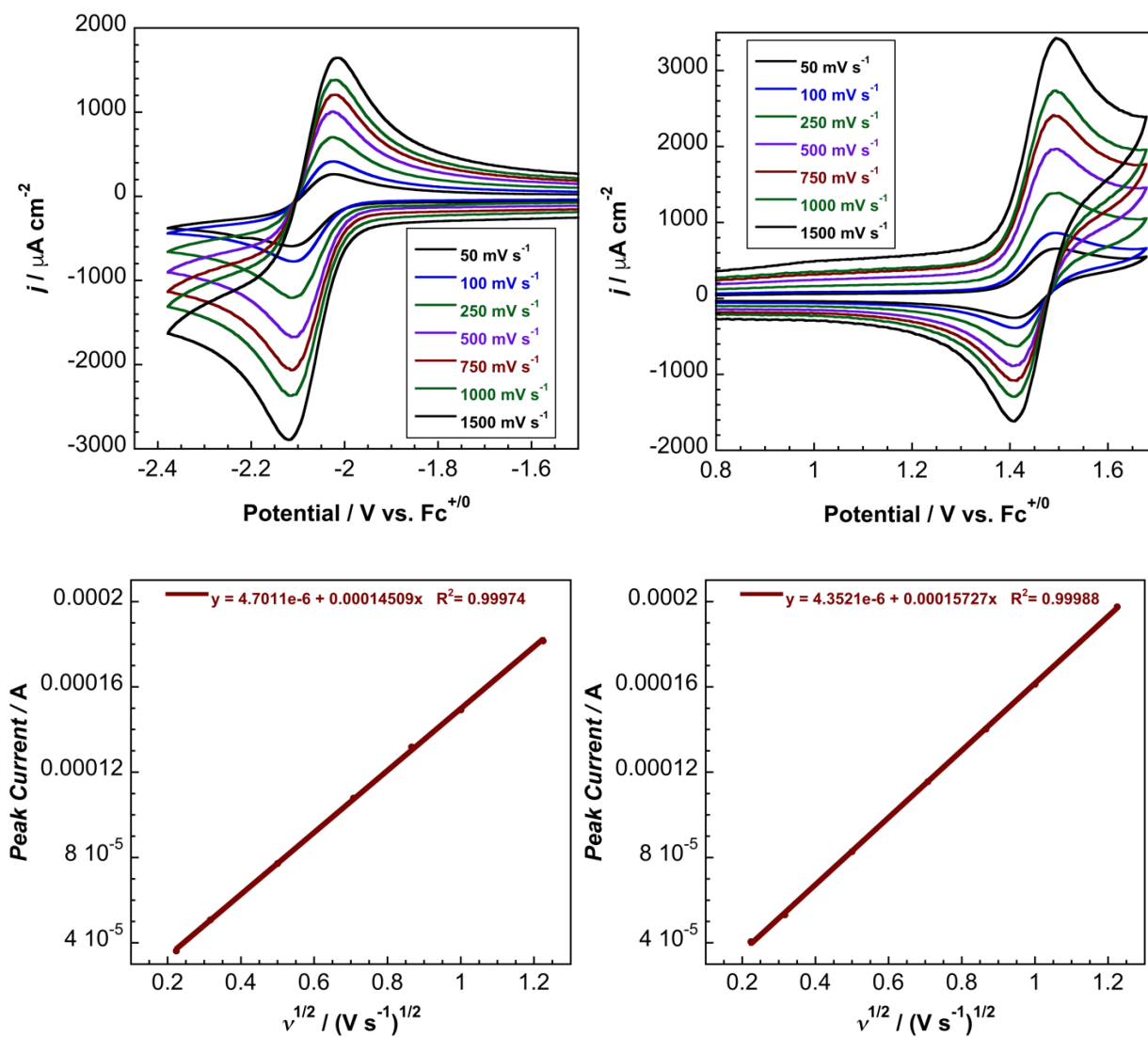


Figure S64. Scan rate dependence and Randles-Ševčík plots for 3.7 mM (TBA)₂[Ru(bpy)(CN-B(C₆F₅)₃)₄] (**Ru-bpy-BCF**) in MeCN with 0.2 M TBAPF₆ electrolyte.

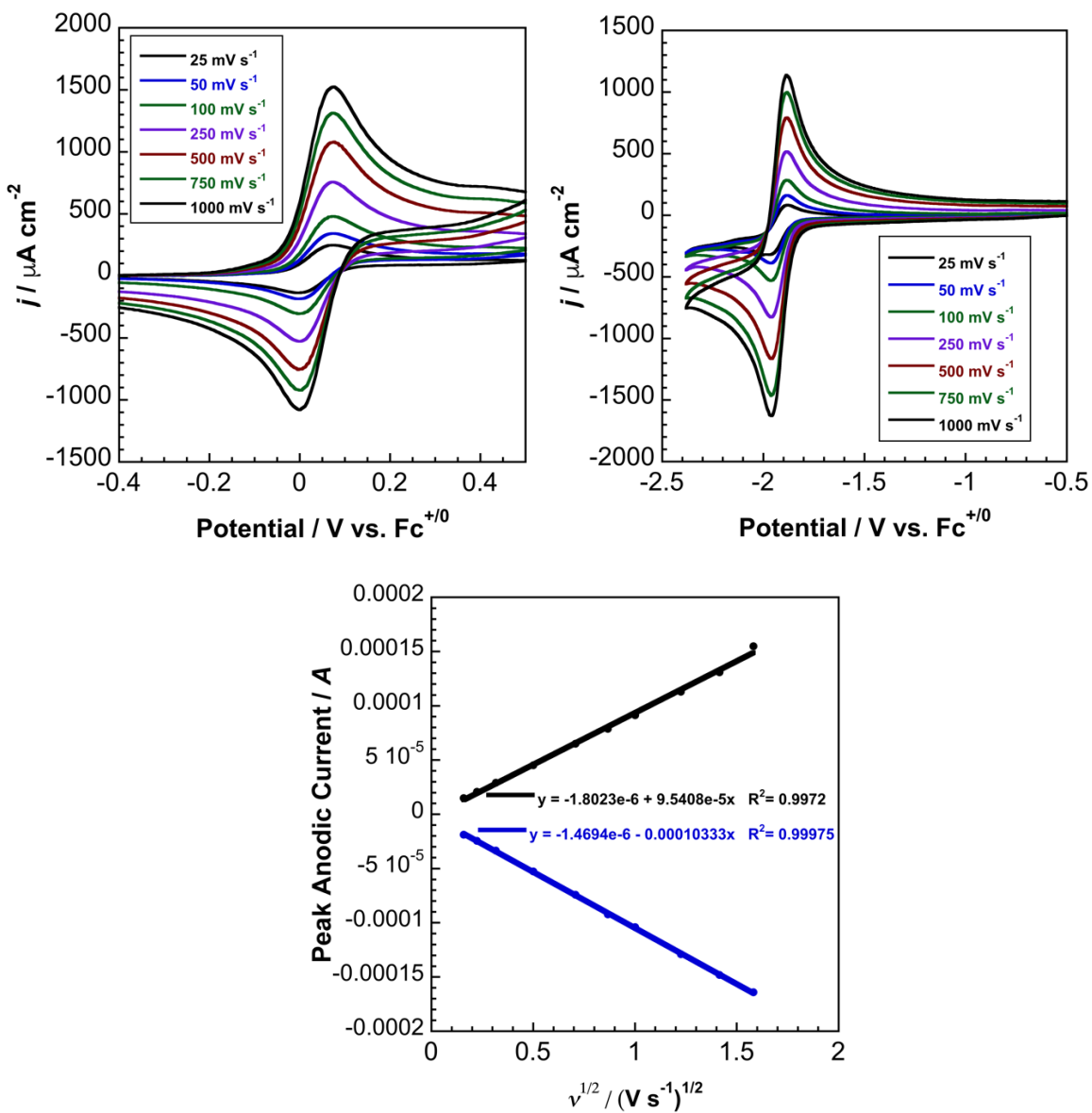


Figure S65. Scan rate dependence and Randles-Ševčík plots for 2.3 mM (left) and 2.2 mM (right) $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN})_4]$ (**Ru-flpy**) in MeCN with 0.2 M TBAPF₆ electrolyte.

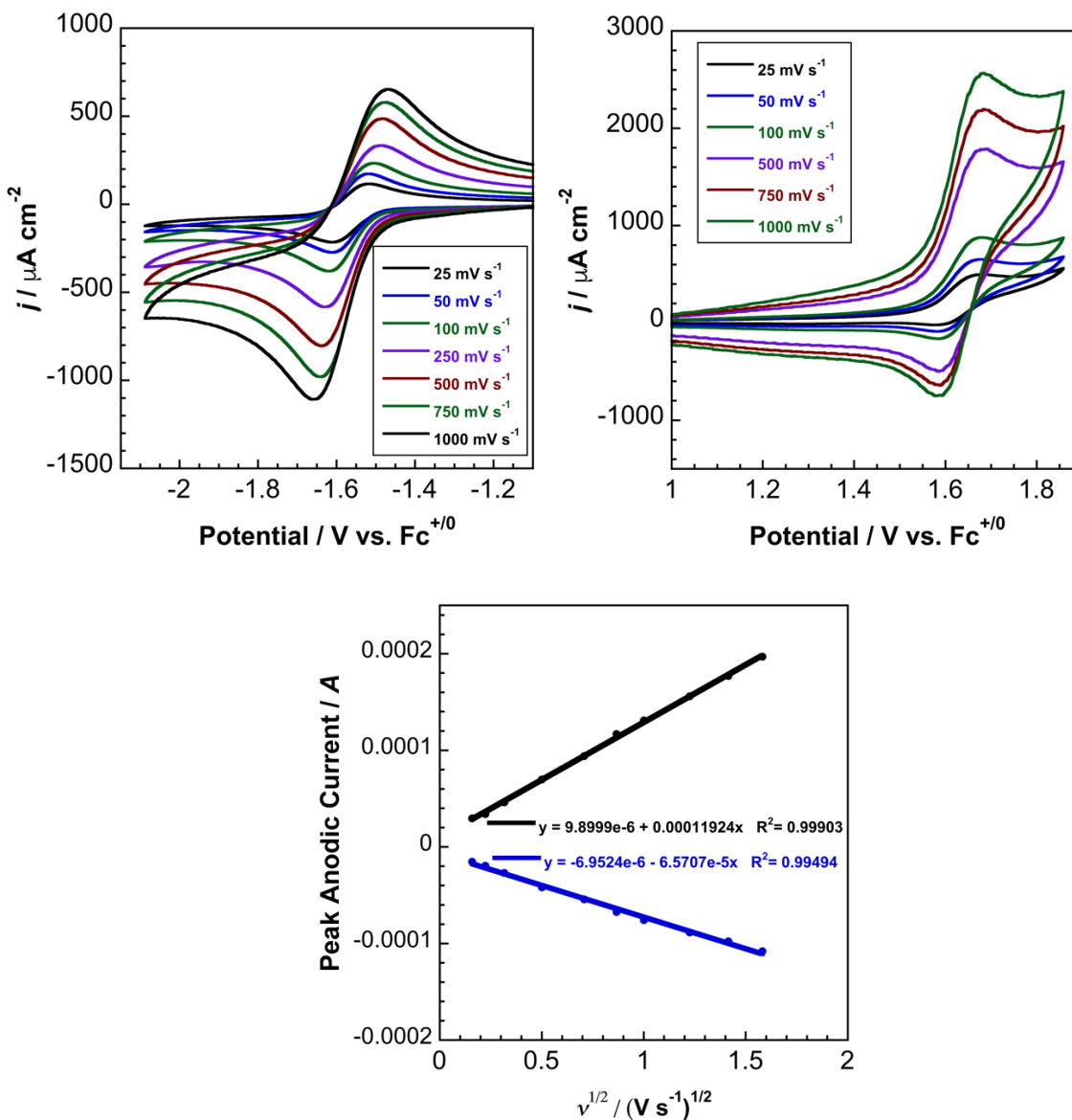


Figure S66. Scan rate dependence and Randles-Ševčík plots for 2.2 mM (PPN)₂[Ru(flpy)(CN-B(C₆F₅)₃)₄] (**Ru-flpy-BCF**) in MeCN with 0.2 M TBAPF₆ electrolyte.

S.5. X-Ray Crystallographic Data

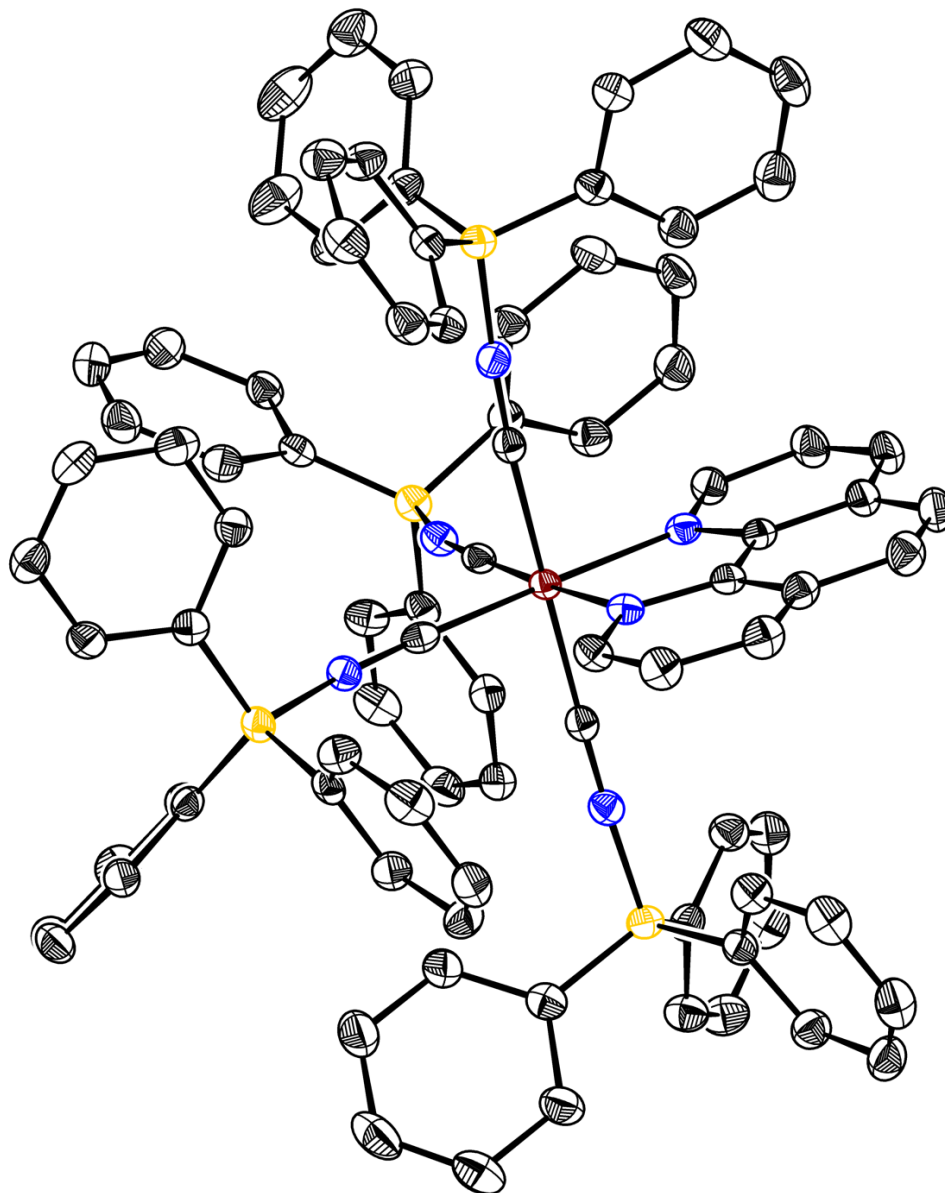


Figure S67. Crystal structure of $(\text{PPN})_2[\text{Fe}(\text{phen})(\text{CN-BPh}_3)_4]$ (solvent, protons, and cations are omitted for clarity). Thermal ellipsoids set at 50% probability.

Table S2. Crystal data and structure refinement for **(PPN)₂[Fe(phen)(CN-BPh₃)₄]**.

Empirical formula	C161 H130 B4 Cl2 Fe N8 P4
Formula weight	2470.59
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 21.782(2) Å a = 90°. b = 17.4783(19) Å b = 94.841(7)°. c = 35.354(5) Å g = 90°.
Volume	13412(3) Å ³
Z	4
Density (calculated)	1.224 Mg/m ³
Absorption coefficient	2.151 mm ⁻¹
F(000)	5168
Crystal size	0.300 x 0.200 x 0.050 mm ³
Theta range for data collection	3.246 to 74.772°.
Index ranges	-27 ≤ h ≤ 26, -21 ≤ k ≤ 21, -44 ≤ l ≤ 43
Reflections collected	112475
Independent reflections	13749 [R(int) = 0.0780]
Completeness to theta = 67.679°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.7510
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	13749 / 1 / 836
Goodness-of-fit on F ²	1.021
Final R indices [I > 2σ(I)]	R1 = 0.0558, wR2 = 0.1393
R indices (all data)	R1 = 0.0695, wR2 = 0.1502
Extinction coefficient	n/a
Largest diff. peak and hole	1.411 and -0.708 e.Å ⁻³

Table S3. Bond lengths [Å] and angles [°] for **(PPN)₂[Fe(phen)(CN-BPh₃)₄]**. Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Fe(1)-C(2)	1.857(2)	C(31)-C(36)	1.393(4)
Fe(1)-C(2)#1	1.857(2)	C(31)-C(32)	1.402(3)
Fe(1)-C(1)#1	1.913(2)	C(32)-C(33)	1.395(4)
Fe(1)-C(1)	1.913(2)	C(32)-H(32A)	0.9500
Fe(1)-N(3)	1.9918(19)	C(33)-C(34)	1.384(5)
Fe(1)-N(3)#1	1.9918(19)	C(33)-H(33A)	0.9500
C(1)-N(1)	1.142(3)	C(34)-C(35)	1.378(5)
N(1)-B(1)	1.568(3)	C(34)-H(34A)	0.9500
B(1)-C(11)	1.630(3)	C(35)-C(36)	1.395(4)
B(1)-C(31)	1.636(4)	C(35)-H(35A)	0.9500
B(1)-C(21)	1.641(3)	C(36)-H(36A)	0.9500
C(11)-C(12)	1.398(3)	C(2)-N(2)	1.160(3)
C(11)-C(16)	1.399(3)	N(2)-B(2)	1.563(3)
C(12)-C(13)	1.389(4)	B(2)-C(51)	1.622(3)
C(12)-H(12A)	0.9500	B(2)-C(61)	1.635(3)
C(13)-C(14)	1.378(4)	B(2)-C(41)	1.640(3)
C(13)-H(13A)	0.9500	C(41)-C(46)	1.396(3)
C(14)-C(15)	1.392(4)	C(41)-C(42)	1.402(3)
C(14)-H(14A)	0.9500	C(42)-C(43)	1.393(3)
C(15)-C(16)	1.390(4)	C(42)-H(42A)	0.9500
C(15)-H(15A)	0.9500	C(43)-C(44)	1.391(4)
C(16)-H(16A)	0.9500	C(43)-H(43A)	0.9500
C(21)-C(26)	1.392(3)	C(44)-C(45)	1.377(4)
C(21)-C(22)	1.404(3)	C(44)-H(44A)	0.9500
C(22)-C(23)	1.393(4)	C(45)-C(46)	1.388(4)
C(22)-H(22A)	0.9500	C(45)-H(45A)	0.9500
C(23)-C(24)	1.380(4)	C(46)-H(46A)	0.9500
C(23)-H(23A)	0.9500	C(51)-C(56)	1.402(3)
C(24)-C(25)	1.385(4)	C(51)-C(52)	1.403(3)
C(24)-H(24A)	0.9500	C(52)-C(53)	1.395(4)
C(25)-C(26)	1.392(4)	C(52)-H(52A)	0.9500
C(25)-H(25A)	0.9500	C(53)-C(54)	1.382(4)
C(26)-H(26A)	0.9500	C(53)-H(53A)	0.9500

C(54)-C(55)	1.388(4)	C(112)-C(113)	1.398(4)
C(54)-H(54A)	0.9500	C(112)-H(11A)	0.9500
C(55)-C(56)	1.387(4)	C(113)-C(114)	1.367(6)
C(55)-H(55A)	0.9500	C(113)-H(11B)	0.9500
C(56)-H(56A)	0.9500	C(114)-C(115)	1.356(6)
C(61)-C(62)	1.396(3)	C(114)-H(11C)	0.9500
C(61)-C(66)	1.401(3)	C(115)-C(116)	1.384(4)
C(62)-C(63)	1.394(4)	C(115)-H(11D)	0.9500
C(62)-H(62A)	0.9500	C(116)-H(11E)	0.9500
C(63)-C(64)	1.384(4)	C(121)-C(126)	1.389(4)
C(63)-H(63A)	0.9500	C(121)-C(122)	1.392(4)
C(64)-C(65)	1.383(4)	C(122)-C(123)	1.394(4)
C(64)-H(64A)	0.9500	C(122)-H(12B)	0.9500
C(65)-C(66)	1.395(3)	C(123)-C(124)	1.385(5)
C(65)-H(65A)	0.9500	C(123)-H(12C)	0.9500
C(66)-H(66A)	0.9500	C(124)-C(125)	1.374(4)
N(3)-C(71)	1.330(3)	C(124)-H(12D)	0.9500
N(3)-C(75)	1.364(3)	C(125)-C(126)	1.384(4)
C(71)-C(72)	1.401(3)	C(125)-H(12E)	0.9500
C(71)-H(71A)	0.9500	C(126)-H(12F)	0.9500
C(72)-C(73)	1.365(4)	C(131)-C(136)	1.390(3)
C(72)-H(72A)	0.9500	C(131)-C(132)	1.403(3)
C(73)-C(74)	1.408(3)	C(132)-C(133)	1.382(4)
C(73)-H(73A)	0.9500	C(132)-H(13B)	0.9500
C(74)-C(75)	1.409(3)	C(133)-C(134)	1.387(4)
C(74)-C(76)	1.434(4)	C(133)-H(13C)	0.9500
C(75)-C(75)#1	1.419(4)	C(134)-C(135)	1.383(4)
C(76)-C(76)#1	1.358(5)	C(134)-H(13D)	0.9500
C(76)-H(76A)	0.9500	C(135)-C(136)	1.386(4)
N(4)-P(1)	1.578(2)	C(135)-H(13E)	0.9500
N(4)-P(2)	1.580(2)	C(136)-H(13F)	0.9500
P(1)-C(131)	1.785(2)	P(2)-C(211)	1.799(2)
P(1)-C(121)	1.801(3)	P(2)-C(221)	1.801(3)
P(1)-C(111)	1.805(3)	P(2)-C(231)	1.802(3)
C(111)-C(112)	1.375(4)	C(211)-C(216)	1.393(3)
C(111)-C(116)	1.387(4)	C(211)-C(212)	1.400(3)

C(212)-C(213)	1.387(4)	C(2)-Fe(1)-C(2)#1	89.57(13)
C(212)-H(21A)	0.9500	C(2)-Fe(1)-C(1)#1	88.66(9)
C(213)-C(214)	1.386(4)	C(2)#1-Fe(1)-C(1)#1	91.67(9)
C(213)-H(21B)	0.9500	C(2)-Fe(1)-C(1)	91.67(9)
C(214)-C(215)	1.380(4)	C(2)#1-Fe(1)-C(1)	88.66(9)
C(214)-H(21C)	0.9500	C(1)#1-Fe(1)-C(1)	179.54(14)
C(215)-C(216)	1.389(4)	C(2)-Fe(1)-N(3)	176.10(9)
C(215)-H(21D)	0.9500	C(2)#1-Fe(1)-N(3)	94.33(9)
C(216)-H(21E)	0.9500	C(1)#1-Fe(1)-N(3)	91.46(8)
C(221)-C(226)	1.391(3)	C(1)-Fe(1)-N(3)	88.19(8)
C(221)-C(222)	1.396(4)	C(2)-Fe(1)-N(3)#1	94.32(9)
C(222)-C(223)	1.387(4)	C(2)#1-Fe(1)-N(3)#1	176.10(9)
C(222)-H(22B)	0.9500	C(1)#1-Fe(1)-N(3)#1	88.20(8)
C(223)-C(224)	1.384(5)	C(1)-Fe(1)-N(3)#1	91.46(8)
C(223)-H(22C)	0.9500	N(3)-Fe(1)-N(3)#1	81.78(11)
C(224)-C(225)	1.382(4)	N(1)-C(1)-Fe(1)	175.8(2)
C(224)-H(22D)	0.9500	C(1)-N(1)-B(1)	176.8(2)
C(225)-C(226)	1.388(4)	N(1)-B(1)-C(11)	107.17(19)
C(225)-H(22E)	0.9500	N(1)-B(1)-C(31)	107.29(19)
C(226)-H(22F)	0.9500	C(11)-B(1)-C(31)	109.76(19)
C(231)-C(236)	1.389(3)	N(1)-B(1)-C(21)	106.35(18)
C(231)-C(232)	1.392(3)	C(11)-B(1)-C(21)	111.52(19)
C(232)-C(233)	1.388(4)	C(31)-B(1)-C(21)	114.4(2)
C(232)-H(23B)	0.9500	C(12)-C(11)-C(16)	115.7(2)
C(233)-C(234)	1.377(4)	C(12)-C(11)-B(1)	122.8(2)
C(233)-H(23C)	0.9500	C(16)-C(11)-B(1)	121.4(2)
C(234)-C(235)	1.386(4)	C(13)-C(12)-C(11)	122.3(2)
C(234)-H(23D)	0.9500	C(13)-C(12)-H(12A)	118.8
C(235)-C(236)	1.383(4)	C(11)-C(12)-H(12A)	118.8
C(235)-H(23E)	0.9500	C(14)-C(13)-C(12)	120.6(3)
C(236)-H(23F)	0.9500	C(14)-C(13)-H(13A)	119.7
C(1S)-Cl(1S)	1.645(8)	C(12)-C(13)-H(13A)	119.7
C(1S)-Cl(2S)	1.650(10)	C(13)-C(14)-C(15)	118.8(2)
C(1S)-H(1S1)	0.9900	C(13)-C(14)-H(14A)	120.6
C(1S)-H(1S2)	0.9900	C(15)-C(14)-H(14A)	120.6
		C(16)-C(15)-C(14)	120.0(3)

C(16)-C(15)-H(15A)	120.0	C(34)-C(35)-H(35A)	120.0
C(14)-C(15)-H(15A)	120.0	C(36)-C(35)-H(35A)	120.0
C(15)-C(16)-C(11)	122.6(2)	C(31)-C(36)-C(35)	122.5(3)
C(15)-C(16)-H(16A)	118.7	C(31)-C(36)-H(36A)	118.7
C(11)-C(16)-H(16A)	118.7	C(35)-C(36)-H(36A)	118.7
C(26)-C(21)-C(22)	116.0(2)	N(2)-C(2)-Fe(1)	177.7(2)
C(26)-C(21)-B(1)	121.9(2)	C(2)-N(2)-B(2)	166.0(2)
C(22)-C(21)-B(1)	122.1(2)	N(2)-B(2)-C(51)	108.93(18)
C(23)-C(22)-C(21)	122.2(2)	N(2)-B(2)-C(61)	102.56(18)
C(23)-C(22)-H(22A)	118.9	C(51)-B(2)-C(61)	112.26(18)
C(21)-C(22)-H(22A)	118.9	N(2)-B(2)-C(41)	106.44(18)
C(24)-C(23)-C(22)	120.2(2)	C(51)-B(2)-C(41)	113.34(19)
C(24)-C(23)-H(23A)	119.9	C(61)-B(2)-C(41)	112.49(19)
C(22)-C(23)-H(23A)	119.9	C(46)-C(41)-C(42)	115.7(2)
C(23)-C(24)-C(25)	119.0(2)	C(46)-C(41)-B(2)	121.7(2)
C(23)-C(24)-H(24A)	120.5	C(42)-C(41)-B(2)	122.5(2)
C(25)-C(24)-H(24A)	120.5	C(43)-C(42)-C(41)	122.4(2)
C(24)-C(25)-C(26)	120.3(2)	C(43)-C(42)-H(42A)	118.8
C(24)-C(25)-H(25A)	119.8	C(41)-C(42)-H(42A)	118.8
C(26)-C(25)-H(25A)	119.8	C(44)-C(43)-C(42)	119.9(2)
C(21)-C(26)-C(25)	122.3(2)	C(44)-C(43)-H(43A)	120.1
C(21)-C(26)-H(26A)	118.9	C(42)-C(43)-H(43A)	120.1
C(25)-C(26)-H(26A)	118.9	C(45)-C(44)-C(43)	119.0(2)
C(36)-C(31)-C(32)	115.8(2)	C(45)-C(44)-H(44A)	120.5
C(36)-C(31)-B(1)	122.4(2)	C(43)-C(44)-H(44A)	120.5
C(32)-C(31)-B(1)	121.7(2)	C(44)-C(45)-C(46)	120.4(2)
C(33)-C(32)-C(31)	122.3(3)	C(44)-C(45)-H(45A)	119.8
C(33)-C(32)-H(32A)	118.8	C(46)-C(45)-H(45A)	119.8
C(31)-C(32)-H(32A)	118.8	C(45)-C(46)-C(41)	122.5(2)
C(34)-C(33)-C(32)	119.9(3)	C(45)-C(46)-H(46A)	118.7
C(34)-C(33)-H(33A)	120.1	C(41)-C(46)-H(46A)	118.7
C(32)-C(33)-H(33A)	120.1	C(56)-C(51)-C(52)	115.6(2)
C(35)-C(34)-C(33)	119.4(3)	C(56)-C(51)-B(2)	120.5(2)
C(35)-C(34)-H(34A)	120.3	C(52)-C(51)-B(2)	123.9(2)
C(33)-C(34)-H(34A)	120.3	C(53)-C(52)-C(51)	122.2(2)
C(34)-C(35)-C(36)	120.1(3)	C(53)-C(52)-H(52A)	118.9

C(51)-C(52)-H(52A)	118.9	C(72)-C(71)-H(71A)	118.8
C(54)-C(53)-C(52)	120.3(2)	C(73)-C(72)-C(71)	120.3(2)
C(54)-C(53)-H(53A)	119.8	C(73)-C(72)-H(72A)	119.8
C(52)-C(53)-H(53A)	119.8	C(71)-C(72)-H(72A)	119.8
C(53)-C(54)-C(55)	119.0(2)	C(72)-C(73)-C(74)	119.2(2)
C(53)-C(54)-H(54A)	120.5	C(72)-C(73)-H(73A)	120.4
C(55)-C(54)-H(54A)	120.5	C(74)-C(73)-H(73A)	120.4
C(56)-C(55)-C(54)	120.2(2)	C(73)-C(74)-C(75)	116.9(2)
C(56)-C(55)-H(55A)	119.9	C(73)-C(74)-C(76)	125.2(2)
C(54)-C(55)-H(55A)	119.9	C(75)-C(74)-C(76)	117.8(2)
C(55)-C(56)-C(51)	122.7(2)	N(3)-C(75)-C(74)	123.5(2)
C(55)-C(56)-H(56A)	118.7	N(3)-C(75)-C(75)#1	115.83(12)
C(51)-C(56)-H(56A)	118.7	C(74)-C(75)-C(75)#1	120.65(13)
C(62)-C(61)-C(66)	116.4(2)	C(76)#1-C(76)-C(74)	121.49(14)
C(62)-C(61)-B(2)	124.0(2)	C(76)#1-C(76)-H(76A)	119.3
C(66)-C(61)-B(2)	119.2(2)	C(74)-C(76)-H(76A)	119.3
C(63)-C(62)-C(61)	122.2(2)	P(1)-N(4)-P(2)	141.38(14)
C(63)-C(62)-H(62A)	118.9	N(4)-P(1)-C(131)	114.85(11)
C(61)-C(62)-H(62A)	118.9	N(4)-P(1)-C(121)	108.17(12)
C(64)-C(63)-C(62)	120.0(2)	C(131)-P(1)-C(121)	108.96(11)
C(64)-C(63)-H(63A)	120.0	N(4)-P(1)-C(111)	110.48(12)
C(62)-C(63)-H(63A)	120.0	C(131)-P(1)-C(111)	107.73(12)
C(65)-C(64)-C(63)	119.4(2)	C(121)-P(1)-C(111)	106.31(11)
C(65)-C(64)-H(64A)	120.3	C(112)-C(111)-C(116)	119.2(3)
C(63)-C(64)-H(64A)	120.3	C(112)-C(111)-P(1)	120.7(2)
C(64)-C(65)-C(66)	120.1(3)	C(116)-C(111)-P(1)	120.0(2)
C(64)-C(65)-H(65A)	120.0	C(111)-C(112)-C(113)	119.4(4)
C(66)-C(65)-H(65A)	120.0	C(111)-C(112)-H(11A)	120.3
C(65)-C(66)-C(61)	121.9(2)	C(113)-C(112)-H(11A)	120.3
C(65)-C(66)-H(66A)	119.0	C(114)-C(113)-C(112)	120.8(4)
C(61)-C(66)-H(66A)	119.0	C(114)-C(113)-H(11B)	119.6
C(71)-N(3)-C(75)	117.7(2)	C(112)-C(113)-H(11B)	119.6
C(71)-N(3)-Fe(1)	129.01(16)	C(115)-C(114)-C(113)	119.9(3)
C(75)-N(3)-Fe(1)	113.27(14)	C(115)-C(114)-H(11C)	120.1
N(3)-C(71)-C(72)	122.3(2)	C(113)-C(114)-H(11C)	120.1
N(3)-C(71)-H(71A)	118.8	C(114)-C(115)-C(116)	120.4(4)

C(114)-C(115)-H(11D)	119.8	C(134)-C(135)-H(13E)	120.0
C(116)-C(115)-H(11D)	119.8	C(136)-C(135)-H(13E)	120.0
C(115)-C(116)-C(111)	120.4(3)	C(135)-C(136)-C(131)	120.1(2)
C(115)-C(116)-H(11E)	119.8	C(135)-C(136)-H(13F)	120.0
C(111)-C(116)-H(11E)	119.8	C(131)-C(136)-H(13F)	120.0
C(126)-C(121)-C(122)	119.8(2)	N(4)-P(2)-C(211)	106.95(11)
C(126)-C(121)-P(1)	118.57(19)	N(4)-P(2)-C(221)	111.83(11)
C(122)-C(121)-P(1)	121.6(2)	C(211)-P(2)-C(221)	109.17(11)
C(121)-C(122)-C(123)	119.7(3)	N(4)-P(2)-C(231)	115.20(11)
C(121)-C(122)-H(12B)	120.2	C(211)-P(2)-C(231)	107.38(11)
C(123)-C(122)-H(12B)	120.2	C(221)-P(2)-C(231)	106.13(11)
C(124)-C(123)-C(122)	119.9(3)	C(216)-C(211)-C(212)	119.6(2)
C(124)-C(123)-H(12C)	120.1	C(216)-C(211)-P(2)	122.28(19)
C(122)-C(123)-H(12C)	120.1	C(212)-C(211)-P(2)	118.10(19)
C(125)-C(124)-C(123)	120.3(3)	C(213)-C(212)-C(211)	119.8(2)
C(125)-C(124)-H(12D)	119.8	C(213)-C(212)-H(21A)	120.1
C(123)-C(124)-H(12D)	119.8	C(211)-C(212)-H(21A)	120.1
C(124)-C(125)-C(126)	120.3(3)	C(214)-C(213)-C(212)	120.2(3)
C(124)-C(125)-H(12E)	119.8	C(214)-C(213)-H(21B)	119.9
C(126)-C(125)-H(12E)	119.8	C(212)-C(213)-H(21B)	119.9
C(125)-C(126)-C(121)	120.0(3)	C(215)-C(214)-C(213)	120.2(2)
C(125)-C(126)-H(12F)	120.0	C(215)-C(214)-H(21C)	119.9
C(121)-C(126)-H(12F)	120.0	C(213)-C(214)-H(21C)	119.9
C(136)-C(131)-C(132)	119.5(2)	C(214)-C(215)-C(216)	120.3(3)
C(136)-C(131)-P(1)	121.00(18)	C(214)-C(215)-H(21D)	119.9
C(132)-C(131)-P(1)	119.06(19)	C(216)-C(215)-H(21D)	119.9
C(133)-C(132)-C(131)	120.0(2)	C(215)-C(216)-C(211)	119.9(2)
C(133)-C(132)-H(13B)	120.0	C(215)-C(216)-H(21E)	120.0
C(131)-C(132)-H(13B)	120.0	C(211)-C(216)-H(21E)	120.0
C(132)-C(133)-C(134)	119.9(2)	C(226)-C(221)-C(222)	119.1(2)
C(132)-C(133)-H(13C)	120.1	C(226)-C(221)-P(2)	120.9(2)
C(134)-C(133)-H(13C)	120.1	C(222)-C(221)-P(2)	120.0(2)
C(135)-C(134)-C(133)	120.5(2)	C(223)-C(222)-C(221)	120.3(3)
C(135)-C(134)-H(13D)	119.8	C(223)-C(222)-H(22B)	119.9
C(133)-C(134)-H(13D)	119.8	C(221)-C(222)-H(22B)	119.9
C(134)-C(135)-C(136)	120.0(3)	C(224)-C(223)-C(222)	120.2(3)

C(224)-C(223)-H(22C)	119.9	C(234)-C(233)-H(23C)	119.7
C(222)-C(223)-H(22C)	119.9	C(232)-C(233)-H(23C)	119.7
C(225)-C(224)-C(223)	119.9(3)	C(233)-C(234)-C(235)	120.0(3)
C(225)-C(224)-H(22D)	120.1	C(233)-C(234)-H(23D)	120.0
C(223)-C(224)-H(22D)	120.1	C(235)-C(234)-H(23D)	120.0
C(224)-C(225)-C(226)	120.3(3)	C(236)-C(235)-C(234)	120.1(3)
C(224)-C(225)-H(22E)	119.9	C(236)-C(235)-H(23E)	120.0
C(226)-C(225)-H(22E)	119.9	C(234)-C(235)-H(23E)	120.0
C(225)-C(226)-C(221)	120.3(3)	C(235)-C(236)-C(231)	120.0(2)
C(225)-C(226)-H(22F)	119.8	C(235)-C(236)-H(23F)	120.0
C(221)-C(226)-H(22F)	119.8	C(231)-C(236)-H(23F)	120.0
C(236)-C(231)-C(232)	119.9(2)	Cl(1S)-C(1S)-Cl(2S)	122.2(7)
C(236)-C(231)-P(2)	118.92(18)	Cl(1S)-C(1S)-H(1S1)	106.8
C(232)-C(231)-P(2)	120.95(19)	Cl(2S)-C(1S)-H(1S1)	106.8
C(233)-C(232)-C(231)	119.4(3)	Cl(1S)-C(1S)-H(1S2)	106.8
C(233)-C(232)-H(23B)	120.3	Cl(2S)-C(1S)-H(1S2)	106.8
C(231)-C(232)-H(23B)	120.3	H(1S1)-C(1S)-H(1S2)	106.6
C(234)-C(233)-C(232)	120.6(3)		

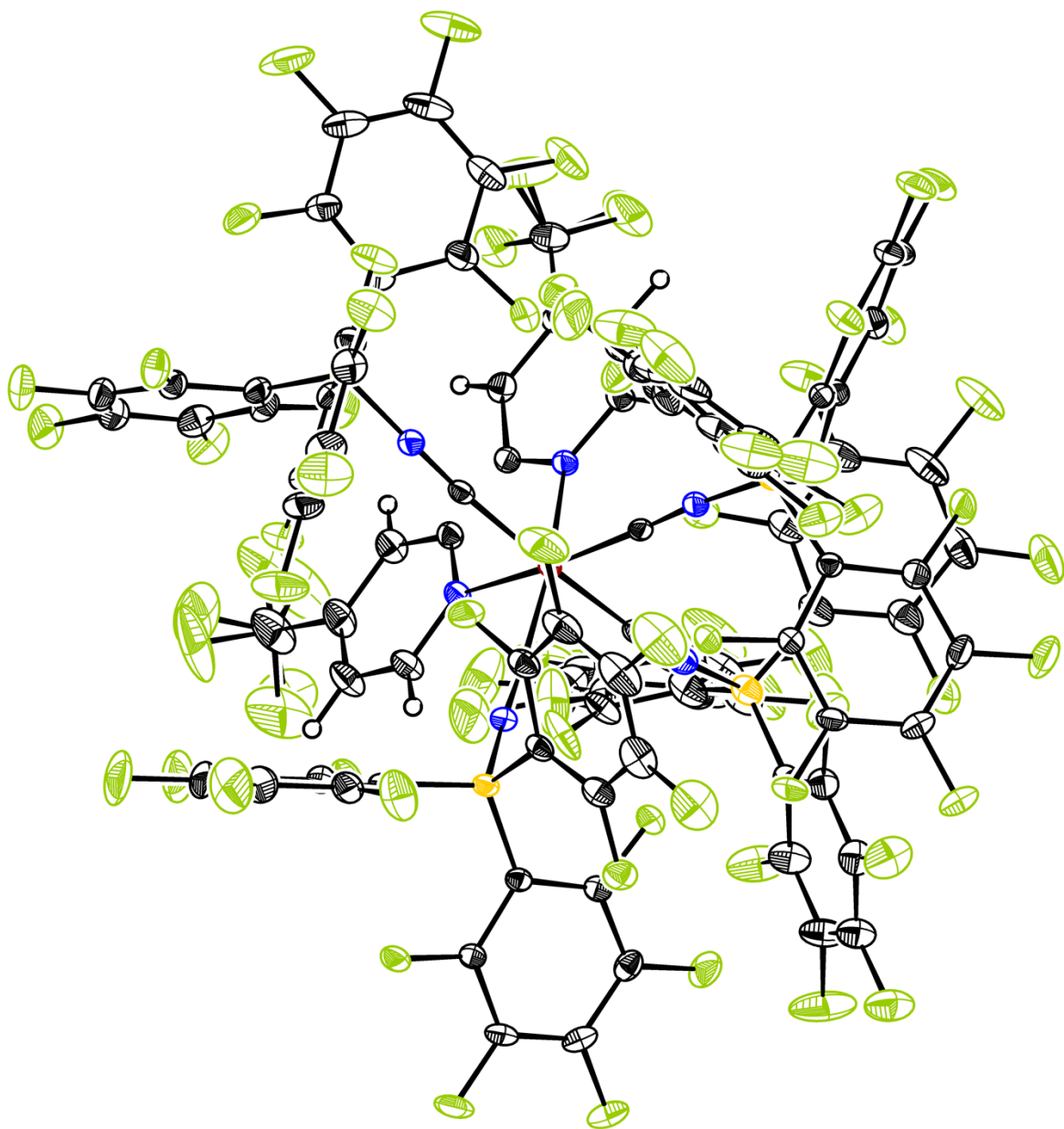


Figure S68. Crystal structure of $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN-B}(\text{C}_6\text{F}_5)_3)_4]$ (solvent and cations are omitted for clarity). Thermal ellipsoids set at 50% probability.

Table S4. Crystal data and structure refinement for **(PPN)₂[Ru(flpy)(CN-B(C₆F₅)₃)₄]**.

Empirical formula	C161 H69 B4 F66 N8 O0.50 P4 Ru	
Formula weight	3645.43	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.024(6) Å	a = 73.248(14)°.
	b = 21.220(6) Å	b = 76.541(18)°.
	c = 23.585(10) Å	g = 79.114(12)°.
Volume	7404(5) Å ³	
Z	2	
Density (calculated)	1.635 Mg/m ³	
Absorption coefficient	0.291 mm ⁻¹	
F(000)	3626	
Crystal size	0.300 x 0.250 x 0.150 mm ³	
Theta range for data collection	1.523 to 30.508°.	
Index ranges	-22 ≤ h ≤ 22, -29 ≤ k ≤ 30, -33 ≤ l ≤ 33	
Reflections collected	246908	
Independent reflections	44916 [R(int) = 0.0493]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.9509	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	44916 / 2373 / 2588	
Goodness-of-fit on F ²	1.011	
Final R indices [I > 2σ(I)]	R1 = 0.0395, wR2 = 0.0858	
R indices (all data)	R1 = 0.0588, wR2 = 0.0936	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.577 and -0.980 e.Å ⁻³	

Table S5. Bond lengths [Å] and angles [°] for (PPN)₂[Ru(flpy)(CN-B(C₆F₅)₃)₄].

N(7)-P(1)	1.5762(14)	C(163)-H(163)	0.9500
N(7)-P(2)	1.5819(14)	C(164)-C(165)	1.378(3)
P(1)-C(51B)	1.763(11)	C(164)-H(164)	0.9500
P(1)-C(161)	1.7931(19)	C(165)-C(166)	1.391(3)
P(1)-C(171)	1.7932(18)	C(165)-H(165)	0.9500
P(1)-C(151)	1.819(5)	C(166)-H(166)	0.9500
C(151)-C(156)	1.384(5)	C(171)-C(176)	1.387(2)
C(151)-C(152)	1.405(5)	C(171)-C(172)	1.389(3)
C(152)-C(153)	1.391(5)	C(172)-C(173)	1.384(3)
C(152)-H(152)	0.9500	C(172)-H(172)	0.9500
C(153)-C(154)	1.378(7)	C(173)-C(174)	1.376(4)
C(153)-H(153)	0.9500	C(173)-H(173)	0.9500
C(154)-C(155)	1.396(7)	C(174)-C(175)	1.377(3)
C(154)-H(154)	0.9500	C(174)-H(174)	0.9500
C(155)-C(156)	1.391(5)	C(175)-C(176)	1.386(2)
C(155)-H(155)	0.9500	C(175)-H(175)	0.9500
C(156)-H(156)	0.9500	C(176)-H(176)	0.9500
C(51B)-C(56B)	1.377(11)	P(2)-C(201)	1.7936(16)
C(51B)-C(52B)	1.383(11)	P(2)-C(191)	1.7960(16)
C(52B)-C(53B)	1.385(9)	P(2)-C(181)	1.7975(17)
C(52B)-H(52B)	0.9500	C(181)-C(182)	1.392(2)
C(53B)-C(54B)	1.370(11)	C(181)-C(186)	1.395(2)
C(53B)-H(53B)	0.9500	C(182)-C(183)	1.386(2)
C(54B)-C(55B)	1.425(11)	C(182)-H(182)	0.9500
C(54B)-H(54B)	0.9500	C(183)-C(184)	1.378(3)
C(55B)-C(56B)	1.398(10)	C(183)-H(183)	0.9500
C(55B)-H(55B)	0.9500	C(184)-C(185)	1.385(3)
C(56B)-H(56B)	0.9500	C(184)-H(184)	0.9500
C(161)-C(166)	1.383(3)	C(185)-C(186)	1.384(2)
C(161)-C(162)	1.394(3)	C(185)-H(185)	0.9500
C(162)-C(163)	1.379(3)	C(186)-H(186)	0.9500
C(162)-H(162)	0.9500	C(191)-C(196)	1.395(2)
C(163)-C(164)	1.373(3)	C(191)-C(192)	1.395(2)

C(192)-C(193)	1.387(2)	C(221)-C(222)	1.389(3)
C(192)-H(192)	0.9500	C(221)-C(226)	1.391(2)
C(193)-C(194)	1.380(3)	C(222)-C(223)	1.391(3)
C(193)-H(193)	0.9500	C(222)-H(222)	0.9500
C(194)-C(195)	1.386(3)	C(223)-C(224)	1.380(3)
C(194)-H(194)	0.9500	C(223)-H(223)	0.9500
C(195)-C(196)	1.388(2)	C(224)-C(225)	1.384(3)
C(195)-H(195)	0.9500	C(224)-H(224)	0.9500
C(196)-H(196)	0.9500	C(225)-C(226)	1.382(3)
C(201)-C(206)	1.392(2)	C(225)-H(225)	0.9500
C(201)-C(202)	1.392(2)	C(226)-H(226)	0.9500
C(202)-C(203)	1.388(2)	C(231)-C(232)	1.392(3)
C(202)-H(202)	0.9500	C(231)-C(236)	1.395(3)
C(203)-C(204)	1.385(3)	C(232)-C(233)	1.392(3)
C(203)-H(203)	0.9500	C(232)-H(232)	0.9500
C(204)-C(205)	1.380(3)	C(233)-C(234)	1.381(4)
C(204)-H(204)	0.9500	C(233)-H(233)	0.9500
C(205)-C(206)	1.391(2)	C(234)-C(235)	1.375(4)
C(205)-H(205)	0.9500	C(234)-H(234)	0.9500
C(206)-H(206)	0.9500	C(235)-C(236)	1.397(3)
N(8)-P(4)	1.5745(17)	C(235)-H(235)	0.9500
N(8)-P(3)	1.5754(17)	C(236)-H(236)	0.9500
P(3)-C(221)	1.7919(18)	P(4)-C(251)	1.799(2)
P(3)-C(231)	1.795(2)	P(4)-C(261)	1.7992(18)
P(3)-C(211)	1.7964(18)	P(4)-C(241)	1.8007(17)
C(211)-C(216)	1.384(3)	C(241)-C(242)	1.390(3)
C(211)-C(212)	1.387(3)	C(241)-C(246)	1.395(3)
C(212)-C(213)	1.391(3)	C(242)-C(243)	1.389(3)
C(212)-H(212)	0.9500	C(242)-H(242)	0.9500
C(213)-C(214)	1.379(4)	C(243)-C(244)	1.374(3)
C(213)-H(213)	0.9500	C(243)-H(243)	0.9500
C(214)-C(215)	1.369(4)	C(244)-C(245)	1.381(3)
C(214)-H(214)	0.9500	C(244)-H(244)	0.9500
C(215)-C(216)	1.389(3)	C(245)-C(246)	1.388(3)
C(215)-H(215)	0.9500	C(245)-H(245)	0.9500
C(216)-H(216)	0.9500	C(246)-H(246)	0.9500

C(251)-C(252)	1.386(3)	C(12)-C(13)	1.377(2)
C(251)-C(256)	1.394(3)	C(13)-F(13)	1.346(2)
C(252)-C(253)	1.389(3)	C(13)-C(14)	1.374(3)
C(252)-H(252)	0.9500	C(14)-F(14)	1.3406(19)
C(253)-C(254)	1.386(4)	C(14)-C(15)	1.373(3)
C(253)-H(253)	0.9500	C(15)-F(15)	1.3411(19)
C(254)-C(255)	1.358(4)	C(15)-C(16)	1.384(2)
C(254)-H(254)	0.9500	C(16)-F(16)	1.3459(19)
C(255)-C(256)	1.395(3)	C(21)-C(26)	1.386(2)
C(255)-H(255)	0.9500	C(21)-C(22)	1.390(2)
C(256)-H(256)	0.9500	C(22)-F(22)	1.347(2)
C(261)-C(262)	1.395(2)	C(22)-C(23)	1.380(2)
C(261)-C(266)	1.395(2)	C(23)-F(23)	1.343(2)
C(262)-C(263)	1.382(3)	C(23)-C(24)	1.375(3)
C(262)-H(262)	0.9500	C(24)-F(24)	1.339(2)
C(263)-C(264)	1.381(3)	C(24)-C(25)	1.367(3)
C(263)-H(263)	0.9500	C(25)-F(25)	1.344(2)
C(264)-C(265)	1.383(3)	C(25)-C(26)	1.389(3)
C(264)-H(264)	0.9500	C(26)-F(26)	1.342(2)
C(265)-C(266)	1.386(3)	C(31)-C(32)	1.383(2)
C(265)-H(265)	0.9500	C(31)-C(36)	1.387(2)
C(266)-H(266)	0.9500	C(32)-F(32)	1.3508(19)
Ru(1)-C(3)	1.9640(16)	C(32)-C(33)	1.381(2)
Ru(1)-C(2)	1.9687(16)	C(33)-F(33)	1.344(2)
Ru(1)-C(4)	2.0137(16)	C(33)-C(34)	1.371(3)
Ru(1)-C(1)	2.0167(16)	C(34)-F(34)	1.343(2)
Ru(1)-N(6)	2.1043(14)	C(34)-C(35)	1.374(3)
Ru(1)-N(5)	2.1052(14)	C(35)-F(35)	1.342(2)
C(1)-N(1)	1.1494(19)	C(35)-C(36)	1.378(2)
N(1)-B(1)	1.550(2)	C(36)-F(36)	1.3531(19)
B(1)-C(31)	1.634(2)	C(2)-N(2)	1.155(2)
B(1)-C(11)	1.643(2)	N(2)-B(2)	1.554(2)
B(1)-C(21)	1.643(2)	B(2)-C(51)	1.636(2)
C(11)-C(12)	1.387(2)	B(2)-C(61)	1.639(2)
C(11)-C(16)	1.387(2)	B(2)-C(41)	1.640(2)
C(12)-F(12)	1.3546(19)	C(41)-C(46)	1.389(2)

C(41)-C(42)	1.389(2)	B(3)-C(71A)	1.644(12)
C(42)-F(42)	1.3511(18)	B(3)-C(81)	1.652(2)
C(42)-C(43)	1.380(2)	C(71)-C(76)	1.380(3)
C(43)-F(43)	1.3442(18)	C(71)-C(72)	1.395(3)
C(43)-C(44)	1.374(2)	C(72)-F(72)	1.349(3)
C(44)-F(44)	1.3416(17)	C(72)-C(73)	1.380(3)
C(44)-C(45)	1.373(2)	C(73)-F(73)	1.349(3)
C(45)-F(45)	1.3463(18)	C(73)-C(74)	1.369(4)
C(45)-C(46)	1.385(2)	C(74)-F(74)	1.343(3)
C(46)-F(46)	1.3475(18)	C(74)-C(75)	1.367(4)
C(51)-C(52)	1.384(2)	C(75)-F(75)	1.343(3)
C(51)-C(56)	1.388(2)	C(75)-C(76)	1.388(4)
C(52)-F(52)	1.353(2)	C(76)-F(76)	1.350(3)
C(52)-C(53)	1.383(2)	C(71A)-C(72A)	1.375(12)
C(53)-F(53)	1.344(2)	C(71A)-C(76A)	1.381(11)
C(53)-C(54)	1.369(3)	C(72A)-F(72A)	1.334(11)
C(54)-F(54)	1.341(2)	C(72A)-C(73A)	1.399(11)
C(54)-C(55)	1.359(3)	C(73A)-F(73A)	1.327(11)
C(55)-F(55)	1.342(2)	C(73A)-C(74A)	1.342(11)
C(55)-C(56)	1.381(3)	C(74A)-C(75A)	1.351(11)
C(56)-F(56)	1.348(2)	C(74A)-F(74A)	1.353(11)
C(61)-C(66)	1.383(2)	C(75A)-F(75A)	1.353(11)
C(61)-C(62)	1.393(2)	C(75A)-C(76A)	1.391(11)
C(62)-F(62)	1.349(2)	C(76A)-F(76A)	1.338(11)
C(62)-C(63)	1.375(2)	C(81)-C(82)	1.389(2)
C(63)-F(63)	1.347(2)	C(81)-C(86)	1.389(2)
C(63)-C(64)	1.375(3)	C(82)-F(82)	1.3501(19)
C(64)-F(64)	1.348(2)	C(82)-C(83)	1.385(2)
C(64)-C(65)	1.372(3)	C(83)-F(83)	1.3454(19)
C(65)-F(65)	1.344(2)	C(83)-C(84)	1.372(2)
C(65)-C(66)	1.384(2)	C(84)-F(84)	1.3402(18)
C(66)-F(66)	1.3536(19)	C(84)-C(85)	1.376(2)
C(3)-N(3)	1.1553(19)	C(85)-F(85)	1.3430(19)
N(3)-B(3)	1.551(2)	C(85)-C(86)	1.384(2)
B(3)-C(91)	1.634(2)	C(86)-F(86)	1.3542(18)
B(3)-C(71)	1.638(3)	C(91)-C(92)	1.385(2)

C(91)-C(96)	1.385(2)	C(05B)-C(06B)	1.355(10)
C(92)-F(92)	1.3453(19)	C(06B)-F(06B)	1.336(9)
C(92)-C(93)	1.389(2)	C(111)-C(116)	1.385(3)
C(93)-F(93)	1.3465(19)	C(111)-C(112)	1.390(3)
C(93)-C(94)	1.366(2)	C(112)-F(112)	1.356(2)
C(94)-F(94)	1.3410(17)	C(112)-C(113)	1.378(3)
C(94)-C(95)	1.374(2)	C(113)-F(113)	1.343(2)
C(95)-F(95)	1.3447(19)	C(113)-C(114)	1.372(3)
C(95)-C(96)	1.378(2)	C(114)-F(114)	1.347(2)
C(96)-F(96)	1.3464(18)	C(114)-C(115)	1.372(3)
C(4)-N(4)	1.150(2)	C(115)-F(115)	1.345(2)
N(4)-B(4)	1.556(2)	C(115)-C(116)	1.388(3)
B(4)-C(01B)	1.612(10)	C(116)-F(116)	1.350(2)
B(4)-C(121)	1.625(2)	C(121)-C(126)	1.383(2)
B(4)-C(111)	1.652(2)	C(121)-C(122)	1.390(2)
B(4)-C(101)	1.656(5)	C(122)-F(122)	1.3520(19)
C(101)-C(102)	1.383(5)	C(122)-C(123)	1.375(2)
C(101)-C(106)	1.393(6)	C(123)-F(123)	1.3401(19)
C(102)-F(102)	1.346(4)	C(123)-C(124)	1.381(2)
C(102)-C(103)	1.382(5)	C(124)-F(124)	1.340(2)
C(103)-F(103)	1.348(4)	C(124)-C(125)	1.369(3)
C(103)-C(104)	1.376(6)	C(125)-F(125)	1.348(2)
C(104)-F(104)	1.339(5)	C(125)-C(126)	1.378(3)
C(104)-C(105)	1.360(6)	C(126)-F(126)	1.351(2)
C(105)-F(105)	1.350(5)	N(5)-C(131)	1.338(2)
C(105)-C(106)	1.395(6)	N(5)-C(135)	1.3511(19)
C(106)-F(106)	1.357(5)	C(131)-C(132)	1.384(2)
C(01B)-C(06B)	1.360(11)	C(131)-H(131)	0.9500
C(01B)-C(02B)	1.405(10)	C(132)-C(133)	1.382(2)
C(02B)-F(02B)	1.338(8)	C(132)-H(132)	0.9500
C(02B)-C(03B)	1.402(8)	C(133)-C(134)	1.381(2)
C(03B)-F(03B)	1.340(7)	C(133)-C(141)	1.505(2)
C(03B)-C(04B)	1.344(9)	C(141)-F(131)	1.318(7)
C(04B)-F(04B)	1.348(9)	C(141)-F(33B)	1.325(9)
C(04B)-C(05B)	1.354(9)	C(141)-F(132)	1.329(7)
C(05B)-F(05B)	1.336(10)	C(141)-F(32B)	1.345(10)

C(141)-F(31B)	1.346(8)	C(22S)-H(22C)	0.9800
C(141)-F(133)	1.355(8)	O(3S)-C(31S)	1.32(3)
C(134)-C(135)	1.391(2)	O(3S)-H(3S)	0.8400
C(134)-H(134)	0.9500	C(31S)-C(32S)	1.536(17)
C(135)-C(136)	1.477(2)	C(31S)-H(31A)	0.9900
C(136)-N(6)	1.3534(19)	C(31S)-H(31B)	0.9900
C(136)-C(137)	1.390(2)	C(32S)-H(32A)	0.9800
C(137)-C(138)	1.379(2)	C(32S)-H(32B)	0.9800
C(137)-H(137)	0.9500	C(32S)-H(32C)	0.9800
C(138)-C(139)	1.383(3)		
C(138)-C(142)	1.507(2)	P(1)-N(7)-P(2)	140.07(9)
C(142)-F(34B)	1.270(9)	N(7)-P(1)-C(51B)	117.5(4)
C(142)-F(135)	1.287(7)	N(7)-P(1)-C(161)	114.94(8)
C(142)-F(36B)	1.331(7)	C(51B)-P(1)-C(161)	106.7(3)
C(142)-F(35B)	1.335(10)	N(7)-P(1)-C(171)	106.50(8)
C(142)-F(136)	1.336(4)	C(51B)-P(1)-C(171)	102.7(3)
C(142)-F(134)	1.342(6)	C(161)-P(1)-C(171)	107.36(8)
C(139)-C(140)	1.380(2)	N(7)-P(1)-C(151)	111.45(16)
C(139)-H(139)	0.9500	C(161)-P(1)-C(151)	107.53(16)
C(140)-N(6)	1.344(2)	C(171)-P(1)-C(151)	108.86(16)
C(140)-H(140)	0.9500	C(156)-C(151)-C(152)	119.3(4)
O(1S)-C(11S)	1.311(17)	C(156)-C(151)-P(1)	120.3(3)
O(1S)-H(1S)	0.8400	C(152)-C(151)-P(1)	120.4(3)
C(11S)-C(12S)	1.585(16)	C(153)-C(152)-C(151)	119.6(4)
C(11S)-H(11A)	0.9900	C(153)-C(152)-H(152)	120.2
C(11S)-H(11B)	0.9900	C(151)-C(152)-H(152)	120.2
C(12S)-H(12A)	0.9800	C(154)-C(153)-C(152)	120.7(4)
C(12S)-H(12B)	0.9800	C(154)-C(153)-H(153)	119.7
C(12S)-H(12C)	0.9800	C(152)-C(153)-H(153)	119.7
O(2S)-C(21S)	1.472(18)	C(153)-C(154)-C(155)	119.8(5)
O(2S)-H(2S)	0.8400	C(153)-C(154)-H(154)	120.1
C(21S)-C(22S)	1.520(17)	C(155)-C(154)-H(154)	120.1
C(21S)-H(21A)	0.9900	C(156)-C(155)-C(154)	119.5(4)
C(21S)-H(21B)	0.9900	C(156)-C(155)-H(155)	120.3
C(22S)-H(22A)	0.9800	C(154)-C(155)-H(155)	120.3
C(22S)-H(22B)	0.9800	C(151)-C(156)-C(155)	120.7(4)

C(151)-C(156)-H(156)	119.6	C(161)-C(166)-H(166)	120.1
C(155)-C(156)-H(156)	119.6	C(165)-C(166)-H(166)	120.1
C(56B)-C(51B)-C(52B)	121.7(10)	C(176)-C(171)-C(172)	119.92(17)
C(56B)-C(51B)-P(1)	117.5(8)	C(176)-C(171)-P(1)	119.60(13)
C(52B)-C(51B)-P(1)	120.8(8)	C(172)-C(171)-P(1)	120.43(16)
C(51B)-C(52B)-C(53B)	119.1(8)	C(173)-C(172)-C(171)	119.6(2)
C(51B)-C(52B)-H(52B)	120.4	C(173)-C(172)-H(172)	120.2
C(53B)-C(52B)-H(52B)	120.4	C(171)-C(172)-H(172)	120.2
C(54B)-C(53B)-C(52B)	119.5(8)	C(174)-C(173)-C(172)	120.2(2)
C(54B)-C(53B)-H(53B)	120.3	C(174)-C(173)-H(173)	119.9
C(52B)-C(53B)-H(53B)	120.3	C(172)-C(173)-H(173)	119.9
C(53B)-C(54B)-C(55B)	122.0(10)	C(173)-C(174)-C(175)	120.48(19)
C(53B)-C(54B)-H(54B)	119.0	C(173)-C(174)-H(174)	119.8
C(55B)-C(54B)-H(54B)	119.0	C(175)-C(174)-H(174)	119.8
C(56B)-C(55B)-C(54B)	116.0(9)	C(174)-C(175)-C(176)	119.78(19)
C(56B)-C(55B)-H(55B)	122.0	C(174)-C(175)-H(175)	120.1
C(54B)-C(55B)-H(55B)	122.0	C(176)-C(175)-H(175)	120.1
C(51B)-C(56B)-C(55B)	120.5(9)	C(175)-C(176)-C(171)	119.99(17)
C(51B)-C(56B)-H(56B)	119.8	C(175)-C(176)-H(176)	120.0
C(55B)-C(56B)-H(56B)	119.8	C(171)-C(176)-H(176)	120.0
C(166)-C(161)-C(162)	120.03(17)	N(7)-P(2)-C(201)	115.59(7)
C(166)-C(161)-P(1)	120.38(13)	N(7)-P(2)-C(191)	109.14(8)
C(162)-C(161)-P(1)	119.44(15)	C(201)-P(2)-C(191)	108.21(7)
C(163)-C(162)-C(161)	119.5(2)	N(7)-P(2)-C(181)	109.29(7)
C(163)-C(162)-H(162)	120.2	C(201)-P(2)-C(181)	106.93(7)
C(161)-C(162)-H(162)	120.2	C(191)-P(2)-C(181)	107.38(7)
C(164)-C(163)-C(162)	120.30(19)	C(182)-C(181)-C(186)	119.55(14)
C(164)-C(163)-H(163)	119.8	C(182)-C(181)-P(2)	120.57(12)
C(162)-C(163)-H(163)	119.8	C(186)-C(181)-P(2)	119.86(11)
C(163)-C(164)-C(165)	120.70(19)	C(183)-C(182)-C(181)	119.82(16)
C(163)-C(164)-H(164)	119.6	C(183)-C(182)-H(182)	120.1
C(165)-C(164)-H(164)	119.6	C(181)-C(182)-H(182)	120.1
C(164)-C(165)-C(166)	119.6(2)	C(184)-C(183)-C(182)	120.34(16)
C(164)-C(165)-H(165)	120.2	C(184)-C(183)-H(183)	119.8
C(166)-C(165)-H(165)	120.2	C(182)-C(183)-H(183)	119.8
C(161)-C(166)-C(165)	119.82(19)	C(183)-C(184)-C(185)	120.28(16)

C(183)-C(184)-H(184)	119.9	C(205)-C(204)-H(204)	120.0
C(185)-C(184)-H(184)	119.9	C(203)-C(204)-H(204)	120.0
C(186)-C(185)-C(184)	119.89(16)	C(204)-C(205)-C(206)	120.14(17)
C(186)-C(185)-H(185)	120.1	C(204)-C(205)-H(205)	119.9
C(184)-C(185)-H(185)	120.1	C(206)-C(205)-H(205)	119.9
C(185)-C(186)-C(181)	120.12(15)	C(205)-C(206)-C(201)	119.95(16)
C(185)-C(186)-H(186)	119.9	C(205)-C(206)-H(206)	120.0
C(181)-C(186)-H(186)	119.9	C(201)-C(206)-H(206)	120.0
C(196)-C(191)-C(192)	119.89(14)	P(4)-N(8)-P(3)	142.43(10)
C(196)-C(191)-P(2)	121.64(12)	N(8)-P(3)-C(221)	113.61(8)
C(192)-C(191)-P(2)	118.41(12)	N(8)-P(3)-C(231)	106.67(9)
C(193)-C(192)-C(191)	119.80(16)	C(221)-P(3)-C(231)	107.66(9)
C(193)-C(192)-H(192)	120.1	N(8)-P(3)-C(211)	113.00(9)
C(191)-C(192)-H(192)	120.1	C(221)-P(3)-C(211)	107.92(8)
C(194)-C(193)-C(192)	120.10(16)	C(231)-P(3)-C(211)	107.71(8)
C(194)-C(193)-H(193)	119.9	C(216)-C(211)-C(212)	119.73(17)
C(192)-C(193)-H(193)	119.9	C(216)-C(211)-P(3)	120.89(14)
C(193)-C(194)-C(195)	120.51(16)	C(212)-C(211)-P(3)	119.38(14)
C(193)-C(194)-H(194)	119.7	C(211)-C(212)-C(213)	119.9(2)
C(195)-C(194)-H(194)	119.7	C(211)-C(212)-H(212)	120.1
C(194)-C(195)-C(196)	119.95(17)	C(213)-C(212)-H(212)	120.1
C(194)-C(195)-H(195)	120.0	C(214)-C(213)-C(212)	119.9(2)
C(196)-C(195)-H(195)	120.0	C(214)-C(213)-H(213)	120.0
C(195)-C(196)-C(191)	119.74(16)	C(212)-C(213)-H(213)	120.0
C(195)-C(196)-H(196)	120.1	C(215)-C(214)-C(213)	120.28(18)
C(191)-C(196)-H(196)	120.1	C(215)-C(214)-H(214)	119.9
C(206)-C(201)-C(202)	119.74(14)	C(213)-C(214)-H(214)	119.9
C(206)-C(201)-P(2)	120.25(12)	C(214)-C(215)-C(216)	120.3(2)
C(202)-C(201)-P(2)	119.90(13)	C(214)-C(215)-H(215)	119.8
C(203)-C(202)-C(201)	119.76(17)	C(216)-C(215)-H(215)	119.8
C(203)-C(202)-H(202)	120.1	C(211)-C(216)-C(215)	119.9(2)
C(201)-C(202)-H(202)	120.1	C(211)-C(216)-H(216)	120.1
C(204)-C(203)-C(202)	120.32(17)	C(215)-C(216)-H(216)	120.1
C(204)-C(203)-H(203)	119.8	C(222)-C(221)-C(226)	119.77(17)
C(202)-C(203)-H(203)	119.8	C(222)-C(221)-P(3)	123.18(14)
C(205)-C(204)-C(203)	120.07(16)	C(226)-C(221)-P(3)	117.06(13)

C(221)-C(222)-C(223)	119.89(18)	N(8)-P(4)-C(241)	107.25(8)
C(221)-C(222)-H(222)	120.1	C(251)-P(4)-C(241)	110.30(9)
C(223)-C(222)-H(222)	120.1	C(261)-P(4)-C(241)	106.70(8)
C(224)-C(223)-C(222)	119.9(2)	C(242)-C(241)-C(246)	119.73(16)
C(224)-C(223)-H(223)	120.0	C(242)-C(241)-P(4)	118.90(13)
C(222)-C(223)-H(223)	120.0	C(246)-C(241)-P(4)	121.37(14)
C(223)-C(224)-C(225)	120.25(18)	C(243)-C(242)-C(241)	120.00(18)
C(223)-C(224)-H(224)	119.9	C(243)-C(242)-H(242)	120.0
C(225)-C(224)-H(224)	119.9	C(241)-C(242)-H(242)	120.0
C(226)-C(225)-C(224)	120.14(17)	C(244)-C(243)-C(242)	120.16(19)
C(226)-C(225)-H(225)	119.9	C(244)-C(243)-H(243)	119.9
C(224)-C(225)-H(225)	119.9	C(242)-C(243)-H(243)	119.9
C(225)-C(226)-C(221)	119.95(17)	C(243)-C(244)-C(245)	120.19(17)
C(225)-C(226)-H(226)	120.0	C(243)-C(244)-H(244)	119.9
C(221)-C(226)-H(226)	120.0	C(245)-C(244)-H(244)	119.9
C(232)-C(231)-C(236)	120.26(18)	C(244)-C(245)-C(246)	120.48(18)
C(232)-C(231)-P(3)	120.65(14)	C(244)-C(245)-H(245)	119.8
C(236)-C(231)-P(3)	119.05(16)	C(246)-C(245)-H(245)	119.8
C(233)-C(232)-C(231)	119.7(2)	C(245)-C(246)-C(241)	119.43(18)
C(233)-C(232)-H(232)	120.1	C(245)-C(246)-H(246)	120.3
C(231)-C(232)-H(232)	120.1	C(241)-C(246)-H(246)	120.3
C(234)-C(233)-C(232)	119.9(2)	C(252)-C(251)-C(256)	119.86(19)
C(234)-C(233)-H(233)	120.1	C(252)-C(251)-P(4)	121.13(15)
C(232)-C(233)-H(233)	120.1	C(256)-C(251)-P(4)	118.91(17)
C(235)-C(234)-C(233)	120.8(2)	C(251)-C(252)-C(253)	119.9(2)
C(235)-C(234)-H(234)	119.6	C(251)-C(252)-H(252)	120.0
C(233)-C(234)-H(234)	119.6	C(253)-C(252)-H(252)	120.0
C(234)-C(235)-C(236)	120.2(2)	C(254)-C(253)-C(252)	119.6(2)
C(234)-C(235)-H(235)	119.9	C(254)-C(253)-H(253)	120.2
C(236)-C(235)-H(235)	119.9	C(252)-C(253)-H(253)	120.2
C(231)-C(236)-C(235)	119.2(2)	C(255)-C(254)-C(253)	121.0(2)
C(231)-C(236)-H(236)	120.4	C(255)-C(254)-H(254)	119.5
C(235)-C(236)-H(236)	120.4	C(253)-C(254)-H(254)	119.5
N(8)-P(4)-C(251)	110.02(9)	C(254)-C(255)-C(256)	120.2(2)
N(8)-P(4)-C(261)	116.07(8)	C(254)-C(255)-H(255)	119.9
C(251)-P(4)-C(261)	106.42(8)	C(256)-C(255)-H(255)	119.9

C(251)-C(256)-C(255)	119.5(2)	N(1)-C(1)-Ru(1)	170.03(13)
C(251)-C(256)-H(256)	120.3	C(1)-N(1)-B(1)	178.37(15)
C(255)-C(256)-H(256)	120.3	N(1)-B(1)-C(31)	102.99(12)
C(262)-C(261)-C(266)	119.35(16)	N(1)-B(1)-C(11)	106.78(12)
C(262)-C(261)-P(4)	121.52(13)	C(31)-B(1)-C(11)	114.19(13)
C(266)-C(261)-P(4)	119.02(13)	N(1)-B(1)-C(21)	109.46(13)
C(263)-C(262)-C(261)	119.86(17)	C(31)-B(1)-C(21)	116.03(13)
C(263)-C(262)-H(262)	120.1	C(11)-B(1)-C(21)	106.93(12)
C(261)-C(262)-H(262)	120.1	C(12)-C(11)-C(16)	113.69(14)
C(264)-C(263)-C(262)	120.53(18)	C(12)-C(11)-B(1)	120.88(14)
C(264)-C(263)-H(263)	119.7	C(16)-C(11)-B(1)	125.36(14)
C(262)-C(263)-H(263)	119.7	F(12)-C(12)-C(13)	115.56(14)
C(263)-C(264)-C(265)	120.09(18)	F(12)-C(12)-C(11)	119.88(14)
C(263)-C(264)-H(264)	120.0	C(13)-C(12)-C(11)	124.55(15)
C(265)-C(264)-H(264)	120.0	F(13)-C(13)-C(14)	119.89(15)
C(264)-C(265)-C(266)	119.93(17)	F(13)-C(13)-C(12)	121.08(16)
C(264)-C(265)-H(265)	120.0	C(14)-C(13)-C(12)	119.02(15)
C(266)-C(265)-H(265)	120.0	F(14)-C(14)-C(15)	120.79(16)
C(265)-C(266)-C(261)	120.21(17)	F(14)-C(14)-C(13)	119.86(16)
C(265)-C(266)-H(266)	119.9	C(15)-C(14)-C(13)	119.34(15)
C(261)-C(266)-H(266)	119.9	F(15)-C(15)-C(14)	119.71(15)
C(3)-Ru(1)-C(2)	89.82(6)	F(15)-C(15)-C(16)	120.67(15)
C(3)-Ru(1)-C(4)	90.89(6)	C(14)-C(15)-C(16)	119.59(15)
C(2)-Ru(1)-C(4)	95.16(6)	F(16)-C(16)-C(15)	115.76(14)
C(3)-Ru(1)-C(1)	91.81(6)	F(16)-C(16)-C(11)	120.55(14)
C(2)-Ru(1)-C(1)	91.23(6)	C(15)-C(16)-C(11)	123.68(15)
C(4)-Ru(1)-C(1)	173.07(6)	C(26)-C(21)-C(22)	113.12(15)
C(3)-Ru(1)-N(6)	173.07(5)	C(26)-C(21)-B(1)	126.92(14)
C(2)-Ru(1)-N(6)	97.09(6)	C(22)-C(21)-B(1)	119.87(14)
C(4)-Ru(1)-N(6)	87.97(6)	F(22)-C(22)-C(23)	115.97(15)
C(1)-Ru(1)-N(6)	88.57(6)	F(22)-C(22)-C(21)	119.40(15)
C(3)-Ru(1)-N(5)	95.39(6)	C(23)-C(22)-C(21)	124.62(17)
C(2)-Ru(1)-N(5)	173.98(5)	F(23)-C(23)-C(24)	120.04(17)
C(4)-Ru(1)-N(5)	87.79(6)	F(23)-C(23)-C(22)	120.39(19)
C(1)-Ru(1)-N(5)	85.60(6)	C(24)-C(23)-C(22)	119.58(17)
N(6)-Ru(1)-N(5)	77.74(5)	F(24)-C(24)-C(25)	120.98(19)

F(24)-C(24)-C(23)	120.39(19)	C(42)-C(41)-B(2)	121.00(13)
C(25)-C(24)-C(23)	118.63(16)	F(42)-C(42)-C(43)	116.20(14)
F(25)-C(25)-C(24)	120.01(17)	F(42)-C(42)-C(41)	119.79(13)
F(25)-C(25)-C(26)	119.97(18)	C(43)-C(42)-C(41)	124.00(14)
C(24)-C(25)-C(26)	120.02(17)	F(43)-C(43)-C(44)	119.42(14)
F(26)-C(26)-C(21)	121.21(15)	F(43)-C(43)-C(42)	120.99(15)
F(26)-C(26)-C(25)	114.77(16)	C(44)-C(43)-C(42)	119.60(14)
C(21)-C(26)-C(25)	124.01(16)	F(44)-C(44)-C(45)	120.26(15)
C(32)-C(31)-C(36)	113.95(14)	F(44)-C(44)-C(43)	120.71(15)
C(32)-C(31)-B(1)	125.82(14)	C(45)-C(44)-C(43)	119.03(14)
C(36)-C(31)-B(1)	119.75(13)	F(45)-C(45)-C(44)	119.66(13)
F(32)-C(32)-C(33)	115.56(14)	F(45)-C(45)-C(46)	120.56(14)
F(32)-C(32)-C(31)	120.42(14)	C(44)-C(45)-C(46)	119.77(14)
C(33)-C(32)-C(31)	124.02(15)	F(46)-C(46)-C(45)	115.10(13)
F(33)-C(33)-C(34)	119.99(16)	F(46)-C(46)-C(41)	121.27(13)
F(33)-C(33)-C(32)	120.75(16)	C(45)-C(46)-C(41)	123.62(14)
C(34)-C(33)-C(32)	119.26(16)	C(52)-C(51)-C(56)	113.64(15)
F(34)-C(34)-C(33)	119.91(17)	C(52)-C(51)-B(2)	122.03(14)
F(34)-C(34)-C(35)	120.60(17)	C(56)-C(51)-B(2)	124.32(14)
C(33)-C(34)-C(35)	119.49(16)	F(52)-C(52)-C(53)	116.23(16)
F(35)-C(35)-C(34)	119.82(16)	F(52)-C(52)-C(51)	119.84(14)
F(35)-C(35)-C(36)	120.95(16)	C(53)-C(52)-C(51)	123.88(17)
C(34)-C(35)-C(36)	119.24(16)	F(53)-C(53)-C(54)	120.45(17)
F(36)-C(36)-C(35)	116.39(15)	F(53)-C(53)-C(52)	120.03(19)
F(36)-C(36)-C(31)	119.59(14)	C(54)-C(53)-C(52)	119.50(18)
C(35)-C(36)-C(31)	124.01(15)	F(54)-C(54)-C(55)	120.4(2)
N(2)-C(2)-Ru(1)	176.87(13)	F(54)-C(54)-C(53)	120.2(2)
C(2)-N(2)-B(2)	171.18(14)	C(55)-C(54)-C(53)	119.38(17)
N(2)-B(2)-C(51)	108.03(12)	F(55)-C(55)-C(54)	119.72(18)
N(2)-B(2)-C(61)	104.28(12)	F(55)-C(55)-C(56)	120.6(2)
C(51)-B(2)-C(61)	109.69(12)	C(54)-C(55)-C(56)	119.64(18)
N(2)-B(2)-C(41)	107.00(12)	F(56)-C(56)-C(55)	114.93(16)
C(51)-B(2)-C(41)	112.71(12)	F(56)-C(56)-C(51)	121.15(15)
C(61)-B(2)-C(41)	114.55(12)	C(55)-C(56)-C(51)	123.93(18)
C(46)-C(41)-C(42)	113.96(13)	C(66)-C(61)-C(62)	114.07(14)
C(46)-C(41)-B(2)	125.04(13)	C(66)-C(61)-B(2)	126.81(13)

C(62)-C(61)-B(2)	119.05(14)	F(74)-C(74)-C(75)	120.5(3)
F(62)-C(62)-C(63)	115.98(15)	F(74)-C(74)-C(73)	120.1(3)
F(62)-C(62)-C(61)	119.90(14)	C(75)-C(74)-C(73)	119.3(2)
C(63)-C(62)-C(61)	124.10(17)	F(75)-C(75)-C(74)	120.9(3)
F(63)-C(63)-C(64)	120.14(16)	F(75)-C(75)-C(76)	119.9(3)
F(63)-C(63)-C(62)	120.59(18)	C(74)-C(75)-C(76)	119.2(2)
C(64)-C(63)-C(62)	119.27(17)	F(76)-C(76)-C(71)	120.3(2)
F(64)-C(64)-C(65)	120.4(2)	F(76)-C(76)-C(75)	115.4(2)
F(64)-C(64)-C(63)	120.30(19)	C(71)-C(76)-C(75)	124.3(3)
C(65)-C(64)-C(63)	119.33(16)	C(72A)-C(71A)-C(76A)	114.7(10)
F(65)-C(65)-C(64)	120.30(16)	C(72A)-C(71A)-B(3)	121.9(9)
F(65)-C(65)-C(66)	120.03(17)	C(76A)-C(71A)-B(3)	123.3(9)
C(64)-C(65)-C(66)	119.67(18)	F(72A)-C(72A)-C(71A)	120.0(11)
F(66)-C(66)-C(61)	121.12(14)	F(72A)-C(72A)-C(73A)	115.3(10)
F(66)-C(66)-C(65)	115.31(15)	C(71A)-C(72A)-C(73A)	124.6(10)
C(61)-C(66)-C(65)	123.56(16)	F(73A)-C(73A)-C(74A)	123.0(10)
N(3)-C(3)-Ru(1)	175.87(13)	F(73A)-C(73A)-C(72A)	120.0(10)
C(3)-N(3)-B(3)	175.27(14)	C(74A)-C(73A)-C(72A)	117.0(9)
N(3)-B(3)-C(91)	104.58(12)	C(73A)-C(74A)-C(75A)	121.8(9)
N(3)-B(3)-C(71)	105.47(15)	C(73A)-C(74A)-F(74A)	119.2(10)
C(91)-B(3)-C(71)	115.06(15)	C(75A)-C(74A)-F(74A)	119.0(10)
N(3)-B(3)-C(71A)	114.3(4)	C(74A)-C(75A)-F(75A)	121.8(9)
C(91)-B(3)-C(71A)	109.1(4)	C(74A)-C(75A)-C(76A)	119.8(9)
N(3)-B(3)-C(81)	107.77(12)	F(75A)-C(75A)-C(76A)	118.4(9)
C(91)-B(3)-C(81)	114.15(12)	F(76A)-C(76A)-C(71A)	120.6(9)
C(71)-B(3)-C(81)	109.10(14)	F(76A)-C(76A)-C(75A)	117.2(9)
C(71A)-B(3)-C(81)	107.1(3)	C(71A)-C(76A)-C(75A)	121.9(10)
C(76)-C(71)-C(72)	113.7(2)	C(82)-C(81)-C(86)	113.42(14)
C(76)-C(71)-B(3)	125.9(2)	C(82)-C(81)-B(3)	124.96(13)
C(72)-C(71)-B(3)	120.0(2)	C(86)-C(81)-B(3)	121.61(13)
F(72)-C(72)-C(73)	116.1(2)	F(82)-C(82)-C(83)	114.76(13)
F(72)-C(72)-C(71)	120.2(2)	F(82)-C(82)-C(81)	121.16(14)
C(73)-C(72)-C(71)	123.6(3)	C(83)-C(82)-C(81)	124.08(15)
F(73)-C(73)-C(74)	119.7(2)	F(83)-C(83)-C(84)	120.11(14)
F(73)-C(73)-C(72)	120.5(3)	F(83)-C(83)-C(82)	120.05(15)
C(74)-C(73)-C(72)	119.8(2)	C(84)-C(83)-C(82)	119.84(14)

F(84)-C(84)-C(83)	120.94(15)	C(121)-B(4)-C(101)	115.49(17)
F(84)-C(84)-C(85)	120.31(16)	C(111)-B(4)-C(101)	106.10(19)
C(83)-C(84)-C(85)	118.75(14)	C(102)-C(101)-C(106)	113.2(4)
F(85)-C(85)-C(84)	119.69(14)	C(102)-C(101)-B(4)	121.0(4)
F(85)-C(85)-C(86)	120.65(14)	C(106)-C(101)-B(4)	125.5(4)
C(84)-C(85)-C(86)	119.65(15)	F(102)-C(102)-C(103)	116.8(3)
F(86)-C(86)-C(85)	115.79(14)	F(102)-C(102)-C(101)	119.2(3)
F(86)-C(86)-C(81)	120.00(13)	C(103)-C(102)-C(101)	124.0(4)
C(85)-C(86)-C(81)	124.19(14)	F(103)-C(103)-C(104)	119.8(3)
C(92)-C(91)-C(96)	113.74(13)	F(103)-C(103)-C(102)	120.3(4)
C(92)-C(91)-B(3)	127.37(13)	C(104)-C(103)-C(102)	119.9(3)
C(96)-C(91)-B(3)	118.83(13)	F(104)-C(104)-C(105)	120.2(4)
F(92)-C(92)-C(91)	120.79(14)	F(104)-C(104)-C(103)	120.6(4)
F(92)-C(92)-C(93)	115.95(14)	C(105)-C(104)-C(103)	119.1(4)
C(91)-C(92)-C(93)	123.26(15)	F(105)-C(105)-C(104)	120.9(4)
F(93)-C(93)-C(94)	119.36(14)	F(105)-C(105)-C(106)	119.8(5)
F(93)-C(93)-C(92)	120.43(15)	C(104)-C(105)-C(106)	119.3(4)
C(94)-C(93)-C(92)	120.21(15)	F(106)-C(106)-C(101)	121.4(5)
F(94)-C(94)-C(93)	120.54(15)	F(106)-C(106)-C(105)	114.4(4)
F(94)-C(94)-C(95)	120.51(15)	C(101)-C(106)-C(105)	124.2(5)
C(93)-C(94)-C(95)	118.95(14)	C(06B)-C(01B)-C(02B)	113.4(8)
F(95)-C(95)-C(94)	120.36(13)	C(06B)-C(01B)-B(4)	126.2(8)
F(95)-C(95)-C(96)	120.49(14)	C(02B)-C(01B)-B(4)	120.4(7)
C(94)-C(95)-C(96)	119.14(14)	F(02B)-C(02B)-C(03B)	116.3(6)
F(96)-C(96)-C(95)	116.13(13)	F(02B)-C(02B)-C(01B)	120.8(7)
F(96)-C(96)-C(91)	119.18(13)	C(03B)-C(02B)-C(01B)	122.9(7)
C(95)-C(96)-C(91)	124.68(14)	F(03B)-C(03B)-C(04B)	121.5(7)
N(4)-C(4)-Ru(1)	169.58(13)	F(03B)-C(03B)-C(02B)	119.5(7)
C(4)-N(4)-B(4)	174.77(15)	C(04B)-C(03B)-C(02B)	119.0(6)
N(4)-B(4)-C(01B)	102.8(4)	C(03B)-C(04B)-F(04B)	118.7(8)
N(4)-B(4)-C(121)	105.41(13)	C(03B)-C(04B)-C(05B)	119.1(8)
C(01B)-B(4)-C(121)	120.6(2)	F(04B)-C(04B)-C(05B)	122.1(8)
N(4)-B(4)-C(111)	104.52(12)	F(05B)-C(05B)-C(04B)	118.9(8)
C(01B)-B(4)-C(111)	107.0(3)	F(05B)-C(05B)-C(06B)	119.9(8)
C(121)-B(4)-C(111)	114.61(14)	C(04B)-C(05B)-C(06B)	121.1(9)
N(4)-B(4)-C(101)	110.2(2)	F(06B)-C(06B)-C(05B)	117.5(8)

F(06B)-C(06B)-C(01B)	118.4(8)	F(126)-C(126)-C(121)	120.33(16)
C(05B)-C(06B)-C(01B)	124.0(9)	C(125)-C(126)-C(121)	123.98(16)
C(116)-C(111)-C(112)	114.04(16)	C(131)-N(5)-C(135)	119.33(13)
C(116)-C(111)-B(4)	126.00(16)	C(131)-N(5)-Ru(1)	125.08(10)
C(112)-C(111)-B(4)	119.89(15)	C(135)-N(5)-Ru(1)	115.28(10)
F(112)-C(112)-C(113)	115.80(16)	N(5)-C(131)-C(132)	122.61(15)
F(112)-C(112)-C(111)	119.80(15)	N(5)-C(131)-H(131)	118.7
C(113)-C(112)-C(111)	124.39(18)	C(132)-C(131)-H(131)	118.7
F(113)-C(113)-C(114)	120.41(17)	C(133)-C(132)-C(131)	117.97(15)
F(113)-C(113)-C(112)	120.65(18)	C(133)-C(132)-H(132)	121.0
C(114)-C(113)-C(112)	118.94(18)	C(131)-C(132)-H(132)	121.0
F(114)-C(114)-C(115)	119.94(19)	C(134)-C(133)-C(132)	120.04(14)
F(114)-C(114)-C(113)	120.46(19)	C(134)-C(133)-C(141)	120.95(15)
C(115)-C(114)-C(113)	119.60(17)	C(132)-C(133)-C(141)	118.97(15)
F(115)-C(115)-C(114)	120.01(17)	F(131)-C(141)-F(132)	111.0(9)
F(115)-C(115)-C(116)	120.36(19)	F(33B)-C(141)-F(32B)	104.5(9)
C(114)-C(115)-C(116)	119.62(18)	F(33B)-C(141)-F(31B)	109.4(8)
F(116)-C(116)-C(111)	120.92(16)	F(32B)-C(141)-F(31B)	102.6(9)
F(116)-C(116)-C(115)	115.69(17)	F(131)-C(141)-F(133)	104.4(9)
C(111)-C(116)-C(115)	123.39(18)	F(132)-C(141)-F(133)	108.5(7)
C(126)-C(121)-C(122)	113.71(15)	F(131)-C(141)-C(133)	111.7(6)
C(126)-C(121)-B(4)	126.08(14)	F(33B)-C(141)-C(133)	116.7(9)
C(122)-C(121)-B(4)	120.16(14)	F(132)-C(141)-C(133)	113.1(5)
F(122)-C(122)-C(123)	116.36(14)	F(32B)-C(141)-C(133)	111.9(7)
F(122)-C(122)-C(121)	119.46(15)	F(31B)-C(141)-C(133)	110.7(7)
C(123)-C(122)-C(121)	124.16(15)	F(133)-C(141)-C(133)	107.7(8)
F(123)-C(123)-C(122)	121.33(15)	C(133)-C(134)-C(135)	118.96(14)
F(123)-C(123)-C(124)	119.25(16)	C(133)-C(134)-H(134)	120.5
C(122)-C(123)-C(124)	119.42(15)	C(135)-C(134)-H(134)	120.5
F(124)-C(124)-C(125)	121.22(16)	N(5)-C(135)-C(134)	120.94(14)
F(124)-C(124)-C(123)	119.99(16)	N(5)-C(135)-C(136)	115.63(13)
C(125)-C(124)-C(123)	118.78(16)	C(134)-C(135)-C(136)	123.39(14)
F(125)-C(125)-C(124)	119.53(17)	N(6)-C(136)-C(137)	121.34(14)
F(125)-C(125)-C(126)	120.54(17)	N(6)-C(136)-C(135)	115.23(13)
C(124)-C(125)-C(126)	119.93(16)	C(137)-C(136)-C(135)	123.43(14)
F(126)-C(126)-C(125)	115.69(15)	C(138)-C(137)-C(136)	119.03(15)

C(138)-C(137)-H(137)	120.5	C(11S)-C(12S)-H(12A)	109.5
C(136)-C(137)-H(137)	120.5	C(11S)-C(12S)-H(12B)	109.5
C(137)-C(138)-C(139)	119.70(15)	H(12A)-C(12S)-H(12B)	109.5
C(137)-C(138)-C(142)	120.70(16)	C(11S)-C(12S)-H(12C)	109.5
C(139)-C(138)-C(142)	119.59(17)	H(12A)-C(12S)-H(12C)	109.5
F(34B)-C(142)-F(36B)	113.8(7)	H(12B)-C(12S)-H(12C)	109.5
F(34B)-C(142)-F(35B)	109.6(10)	C(21S)-O(2S)-H(2S)	109.5
F(36B)-C(142)-F(35B)	101.9(8)	O(2S)-C(21S)-C(22S)	108.2(16)
F(135)-C(142)-F(136)	109.4(5)	O(2S)-C(21S)-H(21A)	110.1
F(135)-C(142)-F(134)	105.3(7)	C(22S)-C(21S)-H(21A)	110.1
F(136)-C(142)-F(134)	102.9(4)	O(2S)-C(21S)-H(21B)	110.1
F(34B)-C(142)-C(138)	113.8(6)	C(22S)-C(21S)-H(21B)	110.1
F(135)-C(142)-C(138)	115.1(5)	H(21A)-C(21S)-H(21B)	108.4
F(36B)-C(142)-C(138)	109.2(4)	C(21S)-C(22S)-H(22A)	109.5
F(35B)-C(142)-C(138)	107.8(7)	C(21S)-C(22S)-H(22B)	109.5
F(136)-C(142)-C(138)	113.0(3)	H(22A)-C(22S)-H(22B)	109.5
F(134)-C(142)-C(138)	110.3(4)	C(21S)-C(22S)-H(22C)	109.5
C(140)-C(139)-C(138)	118.56(16)	H(22A)-C(22S)-H(22C)	109.5
C(140)-C(139)-H(139)	120.7	H(22B)-C(22S)-H(22C)	109.5
C(138)-C(139)-H(139)	120.7	C(31S)-O(3S)-H(3S)	109.5
N(6)-C(140)-C(139)	122.45(15)	O(3S)-C(31S)-C(32S)	111.4(19)
N(6)-C(140)-H(140)	118.8	O(3S)-C(31S)-H(31A)	109.4
C(139)-C(140)-H(140)	118.8	C(32S)-C(31S)-H(31A)	109.4
C(140)-N(6)-C(136)	118.91(13)	O(3S)-C(31S)-H(31B)	109.4
C(140)-N(6)-Ru(1)	125.46(10)	C(32S)-C(31S)-H(31B)	109.4
C(136)-N(6)-Ru(1)	115.64(10)	H(31A)-C(31S)-H(31B)	108.0
C(11S)-O(1S)-H(1S)	109.5	C(31S)-C(32S)-H(32A)	109.5
O(1S)-C(11S)-C(12S)	109.5(16)	C(31S)-C(32S)-H(32B)	109.5
O(1S)-C(11S)-H(11A)	109.8	H(32A)-C(32S)-H(32B)	109.5
C(12S)-C(11S)-H(11A)	109.8	C(31S)-C(32S)-H(32C)	109.5
O(1S)-C(11S)-H(11B)	109.8	H(32A)-C(32S)-H(32C)	109.5
C(12S)-C(11S)-H(11B)	109.8	H(32B)-C(32S)-H(32C)	109.5
H(11A)-C(11S)-H(11B)	108.2		

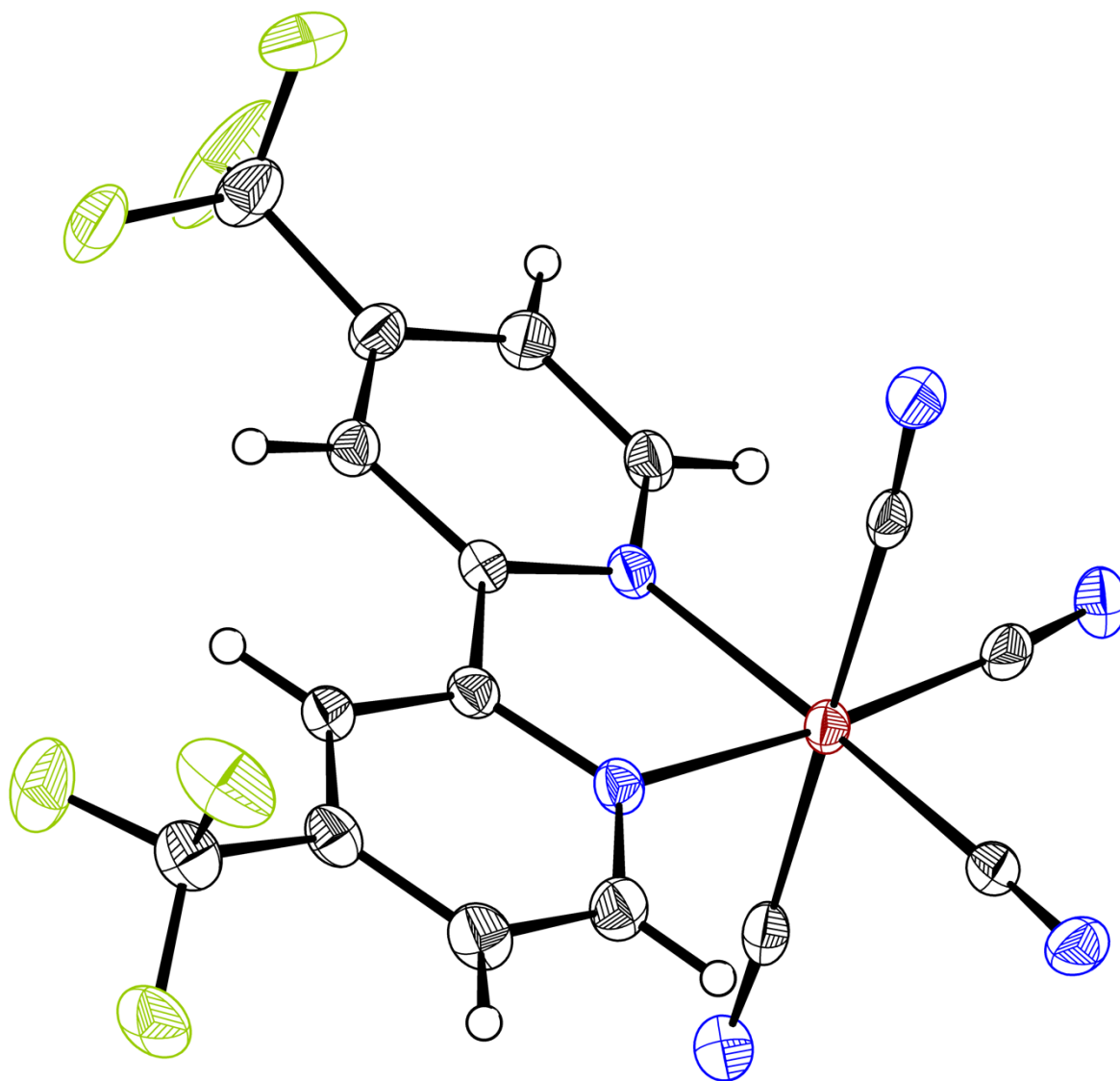


Figure S69. Crystal structure of $(\text{PPN})_2[\text{Ru}(\text{flpy})(\text{CN})_4]$ (solvent and cations are omitted for clarity). Thermal ellipsoids set at 50% probability.

Table S6. Crystal data and structure refinement for **(PPN)₂[Ru(flpy)(CN)₄]**.

Empirical formula	C _{90.22} H _{70.45} Cl _{4.45} F ₆ N ₈ P ₄ Ru	
Formula weight	1763.39	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1 (# 2)	
Unit cell dimensions	a = 14.4673(16) Å	a = 104.706(6)°
	b = 14.6282(16) Å	b = 101.091(7)°
	c = 21.314(2) Å	g = 105.094(6)°
Volume	4047.9(8) Å ³	
Z	2	
Density (calculated)	1.447 g/cm ³	
Absorption coefficient	4.215 mm ⁻¹	
F(000)	1803	
Crystal size	0.07 x 0.23 x 0.26 mm ³	
Theta range for data collection	3.29 to 79.44°	
Index ranges	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -27 ≤ l ≤ 25	
Reflections collected	196088	
Independent reflections	16799 [R(int) = 0.0435]	
Completeness to theta = 67.679°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.6999	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	16799 / 3 / 1075	
Goodness-of-fit on F ²	1.082	
Final R indices [I > 2σ(I)]	R1 = 0.0339, wR2 = 0.0783	
R indices (all data)	R1 = 0.0373, wR2 = 0.0816	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.74 and -0.94 e.Å ⁻³	

Table S7. Bond lengths [Å] and angles [°] for (PPN)₂[Ru(flpy)(CN)₄].

Ru(1)-N(1)	2.0880(15)	C(8)-C(12)	1.493(3)
Ru(1)-N(2)	2.0816(16)	C(9)-H(9)	0.9500
Ru(1)-C(13)	2.0090(19)	C(9)-C(10)	1.376(3)
Ru(1)-C(14)	2.017(2)	C(10)-H(10)	0.9500
Ru(1)-C(15)	2.059(2)	P(1)-N(7)	1.5759(16)
Ru(1)-C(16)	2.063(2)	P(1)-C(17)	1.797(2)
F(1)-C(11)	1.337(3)	P(1)-C(23)	1.804(2)
F(2)-C(11)	1.330(3)	P(1)-C(29)	1.8058(19)
F(3)-C(11)	1.317(3)	P(2)-N(7)	1.5748(17)
F(4)-C(12)	1.346(3)	P(2)-C(35)	1.796(2)
F(5)-C(12)	1.330(3)	P(2)-C(41)	1.798(2)
F(6)-C(12)	1.343(2)	P(2)-C(47)	1.7969(19)
N(1)-C(1)	1.351(2)	C(17)-C(18)	1.396(3)
N(1)-C(5)	1.359(2)	C(17)-C(22)	1.397(3)
N(2)-C(6)	1.361(2)	C(18)-H(18)	0.9500
N(2)-C(10)	1.350(2)	C(18)-C(19)	1.390(3)
N(3)-C(13)	1.160(3)	C(19)-H(19)	0.9500
N(4)-C(14)	1.161(3)	C(19)-C(20)	1.387(3)
N(5)-C(15)	1.158(3)	C(20)-H(20)	0.9500
N(6)-C(16)	1.162(3)	C(20)-C(21)	1.383(4)
C(1)-H(1)	0.9500	C(21)-H(21)	0.9500
C(1)-C(2)	1.375(3)	C(21)-C(22)	1.390(3)
C(2)-H(2)	0.9500	C(22)-H(22)	0.9500
C(2)-C(3)	1.390(3)	C(23)-C(24)	1.398(3)
C(3)-C(4)	1.383(3)	C(23)-C(28)	1.394(3)
C(3)-C(11)	1.497(3)	C(24)-H(24)	0.9500
C(4)-H(4)	0.9500	C(24)-C(25)	1.388(3)
C(4)-C(5)	1.393(3)	C(25)-H(25)	0.9500
C(5)-C(6)	1.467(2)	C(25)-C(26)	1.385(3)
C(6)-C(7)	1.394(3)	C(26)-H(26)	0.9500
C(7)-H(7)	0.9500	C(26)-C(27)	1.390(3)
C(7)-C(8)	1.386(3)	C(27)-H(27)	0.9500
C(8)-C(9)	1.389(3)	C(27)-C(28)	1.395(3)

C(28)-H(28)	0.9500	C(48)-H(48)	0.9500
C(29)-C(30)	1.393(3)	C(48)-C(49)	1.393(3)
C(29)-C(34)	1.396(3)	C(49)-H(49)	0.9500
C(30)-H(30)	0.9500	C(49)-C(50)	1.377(4)
C(30)-C(31)	1.391(3)	C(50)-H(50)	0.9500
C(31)-H(31)	0.9500	C(50)-C(51)	1.388(4)
C(31)-C(32)	1.380(4)	C(51)-H(51)	0.9500
C(32)-H(32)	0.9500	C(51)-C(52)	1.386(3)
C(32)-C(33)	1.388(3)	C(52)-H(52)	0.9500
C(33)-H(33)	0.9500	P(3)-N(8)	1.5718(19)
C(33)-C(34)	1.388(3)	P(3)-C(53)	1.794(2)
C(34)-H(34)	0.9500	P(3)-C(59)	1.804(2)
C(35)-C(36)	1.401(3)	P(3)-C(65)	1.798(2)
C(35)-C(40)	1.393(3)	P(4)-N(8)	1.5645(19)
C(36)-H(36)	0.9500	P(4)-C(71)	1.792(2)
C(36)-C(37)	1.381(3)	P(4)-C(77)	1.815(2)
C(37)-H(37)	0.9500	P(4)-C(83)	1.804(2)
C(37)-C(38)	1.391(3)	C(53)-C(54)	1.393(3)
C(38)-H(38)	0.9500	C(53)-C(58)	1.397(3)
C(38)-C(39)	1.384(3)	C(54)-H(54)	0.9500
C(39)-H(39)	0.9500	C(54)-C(55)	1.390(3)
C(39)-C(40)	1.399(3)	C(55)-H(55)	0.9500
C(40)-H(40)	0.9500	C(55)-C(56)	1.389(3)
C(41)-C(42)	1.397(3)	C(56)-H(56)	0.9500
C(41)-C(46)	1.386(3)	C(56)-C(57)	1.383(3)
C(42)-H(42)	0.9500	C(57)-H(57)	0.9500
C(42)-C(43)	1.392(3)	C(57)-C(58)	1.389(3)
C(43)-H(43)	0.9500	C(58)-H(58)	0.9500
C(43)-C(44)	1.376(3)	C(59)-C(60)	1.385(4)
C(44)-H(44)	0.9500	C(59)-C(64)	1.392(3)
C(44)-C(45)	1.380(4)	C(60)-H(60)	0.9500
C(45)-H(45)	0.9500	C(60)-C(61)	1.387(4)
C(45)-C(46)	1.391(3)	C(61)-H(61)	0.9500
C(46)-H(46)	0.9500	C(61)-C(62)	1.378(4)
C(47)-C(48)	1.392(3)	C(62)-H(62)	0.9500
C(47)-C(52)	1.394(3)	C(62)-C(63)	1.372(4)

C(63)-H(63)	0.9500	C(83)-C(84)	1.393(3)
C(63)-C(64)	1.386(4)	C(83)-C(88)	1.396(3)
C(64)-H(64)	0.9500	C(84)-H(84)	0.9500
C(65)-C(66)	1.393(3)	C(84)-C(85)	1.394(3)
C(65)-C(70)	1.398(3)	C(85)-H(85)	0.9500
C(66)-H(66)	0.9500	C(85)-C(86)	1.387(3)
C(66)-C(67)	1.395(3)	C(86)-H(86)	0.9500
C(67)-H(67)	0.9500	C(86)-C(87)	1.383(3)
C(67)-C(68)	1.388(3)	C(87)-H(87)	0.9500
C(68)-H(68)	0.9500	C(87)-C(88)	1.387(3)
C(68)-C(69)	1.384(3)	C(88)-H(88)	0.9500
C(69)-H(69)	0.9500	Cl(1)-C(89)	1.778(2)
C(69)-C(70)	1.392(3)	Cl(2)-C(89)	1.765(3)
C(70)-H(70)	0.9500	C(89)-H(89A)	0.9900
C(71)-C(72)	1.395(3)	C(89)-H(89B)	0.9900
C(71)-C(76)	1.397(3)	Cl(3)-C(90)	1.713(15)
C(72)-H(72)	0.9500	Cl(4)-C(90)	1.683(15)
C(72)-C(73)	1.387(3)	C(90)-H(90A)	0.9900
C(73)-H(73)	0.9500	C(90)-H(90B)	0.9900
C(73)-C(74)	1.388(4)	Cl(5)-C(91)	1.729(6)
C(74)-H(74)	0.9500	Cl(6)-C(91)	1.773(5)
C(74)-C(75)	1.383(4)	C(91)-H(91A)	0.9900
C(75)-H(75)	0.9500	C(91)-H(91B)	0.9900
C(75)-C(76)	1.392(3)	Cl(7)-C(92)	1.741(9)
C(76)-H(76)	0.9500	Cl(8)-C(92)	1.752(10)
C(77)-C(78)	1.401(3)	C(92)-H(92A)	0.9900
C(77)-C(82)	1.395(3)	C(92)-H(92B)	0.9900
C(78)-H(78)	0.9500		
C(78)-C(79)	1.394(3)	N(2)-Ru(1)-N(1)	77.39(6)
C(79)-H(79)	0.9500	C(13)-Ru(1)-N(1)	169.05(7)
C(79)-C(80)	1.387(3)	C(13)-Ru(1)-N(2)	93.38(7)
C(80)-H(80)	0.9500	C(13)-Ru(1)-C(14)	94.04(8)
C(80)-C(81)	1.390(3)	C(13)-Ru(1)-C(15)	88.33(7)
C(81)-H(81)	0.9500	C(13)-Ru(1)-C(16)	92.08(7)
C(81)-C(82)	1.393(3)	C(14)-Ru(1)-N(1)	95.26(7)
C(82)-H(82)	0.9500	C(14)-Ru(1)-N(2)	172.57(7)

C(14)-Ru(1)-C(15)	89.52(7)	C(9)-C(8)-C(12)	118.98(18)
C(14)-Ru(1)-C(16)	89.83(7)	C(8)-C(9)-H(9)	120.6
C(15)-Ru(1)-N(1)	86.00(6)	C(10)-C(9)-C(8)	118.81(18)
C(15)-Ru(1)-N(2)	91.03(7)	C(10)-C(9)-H(9)	120.6
C(15)-Ru(1)-C(16)	179.25(7)	N(2)-C(10)-C(9)	122.61(18)
C(16)-Ru(1)-N(1)	93.70(7)	N(2)-C(10)-H(10)	118.7
C(16)-Ru(1)-N(2)	89.57(7)	C(9)-C(10)-H(10)	118.7
C(1)-N(1)-Ru(1)	125.27(12)	F(1)-C(11)-C(3)	111.25(19)
C(1)-N(1)-C(5)	118.10(16)	F(2)-C(11)-F(1)	105.0(2)
C(5)-N(1)-Ru(1)	115.99(12)	F(2)-C(11)-C(3)	111.78(18)
C(6)-N(2)-Ru(1)	116.38(12)	F(3)-C(11)-F(1)	107.55(19)
C(10)-N(2)-Ru(1)	125.26(13)	F(3)-C(11)-F(2)	107.0(2)
C(10)-N(2)-C(6)	118.36(16)	F(3)-C(11)-C(3)	113.81(17)
N(1)-C(1)-H(1)	118.6	F(4)-C(12)-C(8)	111.08(17)
N(1)-C(1)-C(2)	122.72(17)	F(5)-C(12)-F(4)	107.17(19)
C(2)-C(1)-H(1)	118.6	F(5)-C(12)-F(6)	106.96(17)
C(1)-C(2)-H(2)	120.6	F(5)-C(12)-C(8)	113.35(17)
C(1)-C(2)-C(3)	118.79(18)	F(6)-C(12)-F(4)	105.45(16)
C(3)-C(2)-H(2)	120.6	F(6)-C(12)-C(8)	112.36(18)
C(2)-C(3)-C(11)	119.93(18)	N(3)-C(13)-Ru(1)	172.28(18)
C(4)-C(3)-C(2)	119.77(17)	N(4)-C(14)-Ru(1)	175.08(17)
C(4)-C(3)-C(11)	120.21(18)	N(5)-C(15)-Ru(1)	176.21(16)
C(3)-C(4)-H(4)	120.8	N(6)-C(16)-Ru(1)	177.03(17)
C(3)-C(4)-C(5)	118.35(17)	N(7)-P(1)-C(17)	116.71(9)
C(5)-C(4)-H(4)	120.8	N(7)-P(1)-C(23)	107.02(9)
N(1)-C(5)-C(4)	122.21(17)	N(7)-P(1)-C(29)	110.15(9)
N(1)-C(5)-C(6)	114.73(16)	C(17)-P(1)-C(23)	107.30(9)
C(4)-C(5)-C(6)	123.05(17)	C(17)-P(1)-C(29)	106.52(9)
N(2)-C(6)-C(5)	114.71(16)	C(23)-P(1)-C(29)	108.92(9)
N(2)-C(6)-C(7)	121.96(17)	N(7)-P(2)-C(35)	114.43(9)
C(7)-C(6)-C(5)	123.32(17)	N(7)-P(2)-C(41)	109.28(9)
C(6)-C(7)-H(7)	120.8	N(7)-P(2)-C(47)	109.10(9)
C(8)-C(7)-C(6)	118.38(17)	C(35)-P(2)-C(41)	107.80(9)
C(8)-C(7)-H(7)	120.8	C(35)-P(2)-C(47)	107.44(9)
C(7)-C(8)-C(9)	119.79(18)	C(47)-P(2)-C(41)	108.64(9)
C(7)-C(8)-C(12)	121.15(18)	P(2)-N(7)-P(1)	146.59(12)

C(18)-C(17)-P(1)	118.42(15)	C(30)-C(29)-P(1)	119.63(15)
C(18)-C(17)-C(22)	119.84(19)	C(30)-C(29)-C(34)	119.68(18)
C(22)-C(17)-P(1)	121.69(16)	C(34)-C(29)-P(1)	120.68(15)
C(17)-C(18)-H(18)	119.8	C(29)-C(30)-H(30)	120.0
C(19)-C(18)-C(17)	120.4(2)	C(31)-C(30)-C(29)	120.0(2)
C(19)-C(18)-H(18)	119.8	C(31)-C(30)-H(30)	120.0
C(18)-C(19)-H(19)	120.3	C(30)-C(31)-H(31)	119.9
C(20)-C(19)-C(18)	119.4(2)	C(32)-C(31)-C(30)	120.2(2)
C(20)-C(19)-H(19)	120.3	C(32)-C(31)-H(31)	119.9
C(19)-C(20)-H(20)	119.8	C(31)-C(32)-H(32)	120.0
C(21)-C(20)-C(19)	120.5(2)	C(31)-C(32)-C(33)	120.0(2)
C(21)-C(20)-H(20)	119.8	C(33)-C(32)-H(32)	120.0
C(20)-C(21)-H(21)	119.7	C(32)-C(33)-H(33)	119.8
C(20)-C(21)-C(22)	120.6(2)	C(32)-C(33)-C(34)	120.4(2)
C(22)-C(21)-H(21)	119.7	C(34)-C(33)-H(33)	119.8
C(17)-C(22)-H(22)	120.4	C(29)-C(34)-H(34)	120.1
C(21)-C(22)-C(17)	119.2(2)	C(33)-C(34)-C(29)	119.71(19)
C(21)-C(22)-H(22)	120.4	C(33)-C(34)-H(34)	120.1
C(24)-C(23)-P(1)	121.06(15)	C(36)-C(35)-P(2)	117.88(15)
C(28)-C(23)-P(1)	119.39(15)	C(40)-C(35)-P(2)	122.39(15)
C(28)-C(23)-C(24)	119.54(18)	C(40)-C(35)-C(36)	119.59(19)
C(23)-C(24)-H(24)	120.0	C(35)-C(36)-H(36)	119.7
C(25)-C(24)-C(23)	120.08(19)	C(37)-C(36)-C(35)	120.68(19)
C(25)-C(24)-H(24)	120.0	C(37)-C(36)-H(36)	119.7
C(24)-C(25)-H(25)	119.9	C(36)-C(37)-H(37)	120.2
C(26)-C(25)-C(24)	120.2(2)	C(36)-C(37)-C(38)	119.6(2)
C(26)-C(25)-H(25)	119.9	C(38)-C(37)-H(37)	120.2
C(25)-C(26)-H(26)	119.9	C(37)-C(38)-H(38)	119.8
C(25)-C(26)-C(27)	120.1(2)	C(39)-C(38)-C(37)	120.3(2)
C(27)-C(26)-H(26)	119.9	C(39)-C(38)-H(38)	119.8
C(26)-C(27)-H(27)	120.0	C(38)-C(39)-H(39)	119.8
C(26)-C(27)-C(28)	119.9(2)	C(38)-C(39)-C(40)	120.4(2)
C(28)-C(27)-H(27)	120.0	C(40)-C(39)-H(39)	119.8
C(23)-C(28)-C(27)	120.0(2)	C(35)-C(40)-C(39)	119.38(19)
C(23)-C(28)-H(28)	120.0	C(35)-C(40)-H(40)	120.3
C(27)-C(28)-H(28)	120.0	C(39)-C(40)-H(40)	120.3

C(42)-C(41)-P(2)	118.55(15)	N(8)-P(3)-C(53)	109.51(9)
C(46)-C(41)-P(2)	121.74(16)	N(8)-P(3)-C(59)	110.66(10)
C(46)-C(41)-C(42)	119.60(19)	N(8)-P(3)-C(65)	116.31(10)
C(41)-C(42)-H(42)	119.9	C(53)-P(3)-C(59)	105.67(10)
C(43)-C(42)-C(41)	120.12(19)	C(53)-P(3)-C(65)	106.69(9)
C(43)-C(42)-H(42)	119.9	C(65)-P(3)-C(59)	107.40(10)
C(42)-C(43)-H(43)	120.1	N(8)-P(4)-C(71)	110.15(10)
C(44)-C(43)-C(42)	119.9(2)	N(8)-P(4)-C(77)	111.03(10)
C(44)-C(43)-H(43)	120.1	N(8)-P(4)-C(83)	114.13(10)
C(43)-C(44)-H(44)	119.9	C(71)-P(4)-C(77)	108.34(9)
C(43)-C(44)-C(45)	120.2(2)	C(71)-P(4)-C(83)	107.58(10)
C(45)-C(44)-H(44)	119.9	C(83)-P(4)-C(77)	105.33(9)
C(44)-C(45)-H(45)	119.7	P(4)-N(8)-P(3)	151.96(12)
C(44)-C(45)-C(46)	120.6(2)	C(54)-C(53)-P(3)	121.17(15)
C(46)-C(45)-H(45)	119.7	C(54)-C(53)-C(58)	120.01(19)
C(41)-C(46)-C(45)	119.6(2)	C(58)-C(53)-P(3)	118.43(15)
C(41)-C(46)-H(46)	120.2	C(53)-C(54)-H(54)	120.0
C(45)-C(46)-H(46)	120.2	C(55)-C(54)-C(53)	119.95(19)
C(48)-C(47)-P(2)	121.22(15)	C(55)-C(54)-H(54)	120.0
C(48)-C(47)-C(52)	119.56(18)	C(54)-C(55)-H(55)	120.1
C(52)-C(47)-P(2)	119.22(15)	C(56)-C(55)-C(54)	119.8(2)
C(47)-C(48)-H(48)	120.1	C(56)-C(55)-H(55)	120.1
C(47)-C(48)-C(49)	119.8(2)	C(55)-C(56)-H(56)	119.9
C(49)-C(48)-H(48)	120.1	C(57)-C(56)-C(55)	120.3(2)
C(48)-C(49)-H(49)	119.7	C(57)-C(56)-H(56)	119.9
C(50)-C(49)-C(48)	120.5(2)	C(56)-C(57)-H(57)	119.8
C(50)-C(49)-H(49)	119.7	C(56)-C(57)-C(58)	120.4(2)
C(49)-C(50)-H(50)	120.1	C(58)-C(57)-H(57)	119.8
C(49)-C(50)-C(51)	119.8(2)	C(53)-C(58)-H(58)	120.2
C(51)-C(50)-H(50)	120.1	C(57)-C(58)-C(53)	119.54(19)
C(50)-C(51)-H(51)	119.8	C(57)-C(58)-H(58)	120.2
C(52)-C(51)-C(50)	120.3(2)	C(60)-C(59)-P(3)	120.71(18)
C(52)-C(51)-H(51)	119.8	C(60)-C(59)-C(64)	119.1(2)
C(47)-C(52)-H(52)	120.0	C(64)-C(59)-P(3)	120.16(19)
C(51)-C(52)-C(47)	120.0(2)	C(59)-C(60)-H(60)	119.8
C(51)-C(52)-H(52)	120.0	C(59)-C(60)-C(61)	120.3(3)

C(61)-C(60)-H(60)	119.8	C(73)-C(72)-H(72)	120.1
C(60)-C(61)-H(61)	120.0	C(72)-C(73)-H(73)	119.9
C(62)-C(61)-C(60)	120.0(3)	C(72)-C(73)-C(74)	120.2(2)
C(62)-C(61)-H(61)	120.0	C(74)-C(73)-H(73)	119.9
C(61)-C(62)-H(62)	119.9	C(73)-C(74)-H(74)	119.9
C(63)-C(62)-C(61)	120.2(3)	C(75)-C(74)-C(73)	120.1(2)
C(63)-C(62)-H(62)	119.9	C(75)-C(74)-H(74)	119.9
C(62)-C(63)-H(63)	119.9	C(74)-C(75)-H(75)	119.8
C(62)-C(63)-C(64)	120.1(2)	C(74)-C(75)-C(76)	120.4(2)
C(64)-C(63)-H(63)	119.9	C(76)-C(75)-H(75)	119.8
C(59)-C(64)-H(64)	119.9	C(71)-C(76)-H(76)	120.2
C(63)-C(64)-C(59)	120.2(3)	C(75)-C(76)-C(71)	119.5(2)
C(63)-C(64)-H(64)	119.9	C(75)-C(76)-H(76)	120.2
C(66)-C(65)-P(3)	118.89(16)	C(78)-C(77)-P(4)	118.24(15)
C(66)-C(65)-C(70)	119.98(19)	C(82)-C(77)-P(4)	122.04(15)
C(70)-C(65)-P(3)	121.11(16)	C(82)-C(77)-C(78)	119.63(19)
C(65)-C(66)-H(66)	120.2	C(77)-C(78)-H(78)	119.9
C(65)-C(66)-C(67)	119.7(2)	C(79)-C(78)-C(77)	120.2(2)
C(67)-C(66)-H(66)	120.2	C(79)-C(78)-H(78)	119.9
C(66)-C(67)-H(67)	119.9	C(78)-C(79)-H(79)	120.2
C(68)-C(67)-C(66)	120.2(2)	C(80)-C(79)-C(78)	119.7(2)
C(68)-C(67)-H(67)	119.9	C(80)-C(79)-H(79)	120.2
C(67)-C(68)-H(68)	119.9	C(79)-C(80)-H(80)	119.8
C(69)-C(68)-C(67)	120.14(19)	C(79)-C(80)-C(81)	120.5(2)
C(69)-C(68)-H(68)	119.9	C(81)-C(80)-H(80)	119.8
C(68)-C(69)-H(69)	119.9	C(80)-C(81)-H(81)	120.0
C(68)-C(69)-C(70)	120.2(2)	C(80)-C(81)-C(82)	120.1(2)
C(70)-C(69)-H(69)	119.9	C(82)-C(81)-H(81)	120.0
C(65)-C(70)-H(70)	120.1	C(77)-C(82)-H(82)	120.1
C(69)-C(70)-C(65)	119.7(2)	C(81)-C(82)-C(77)	119.90(19)
C(69)-C(70)-H(70)	120.1	C(81)-C(82)-H(82)	120.1
C(72)-C(71)-P(4)	120.57(16)	C(84)-C(83)-P(4)	121.78(16)
C(72)-C(71)-C(76)	119.9(2)	C(84)-C(83)-C(88)	119.75(19)
C(76)-C(71)-P(4)	119.31(17)	C(88)-C(83)-P(4)	118.41(16)
C(71)-C(72)-H(72)	120.1	C(83)-C(84)-H(84)	120.1
C(73)-C(72)-C(71)	119.9(2)	C(83)-C(84)-C(85)	119.9(2)

C(85)-C(84)-H(84)	120.1	Cl(3)-C(90)-H(90A)	108.0
C(84)-C(85)-H(85)	120.1	Cl(3)-C(90)-H(90B)	108.0
C(86)-C(85)-C(84)	119.9(2)	Cl(4)-C(90)-Cl(3)	117.3(8)
C(86)-C(85)-H(85)	120.1	Cl(4)-C(90)-H(90A)	108.0
C(85)-C(86)-H(86)	119.8	Cl(4)-C(90)-H(90B)	108.0
C(87)-C(86)-C(85)	120.4(2)	H(90A)-C(90)-H(90B)	107.2
C(87)-C(86)-H(86)	119.8	Cl(5)-C(91)-Cl(6)	113.0(3)
C(86)-C(87)-H(87)	120.0	Cl(5)-C(91)-H(91A)	109.0
C(86)-C(87)-C(88)	120.1(2)	Cl(5)-C(91)-H(91B)	109.0
C(88)-C(87)-H(87)	120.0	Cl(6)-C(91)-H(91A)	109.0
C(83)-C(88)-H(88)	120.0	Cl(6)-C(91)-H(91B)	109.0
C(87)-C(88)-C(83)	120.0(2)	H(91A)-C(91)-H(91B)	107.8
C(87)-C(88)-H(88)	120.0	Cl(7)-C(92)-Cl(8)	111.3(5)
Cl(1)-C(89)-H(89A)	109.5	Cl(7)-C(92)-H(92A)	109.4
Cl(1)-C(89)-H(89B)	109.5	Cl(7)-C(92)-H(92B)	109.4
Cl(2)-C(89)-Cl(1)	110.80(13)	Cl(8)-C(92)-H(92A)	109.4
Cl(2)-C(89)-H(89A)	109.5	Cl(8)-C(92)-H(92B)	109.4
Cl(2)-C(89)-H(89B)	109.5	H(92A)-C(92)-H(92B)	108.0
H(89A)-C(89)-H(89B)	108.1		

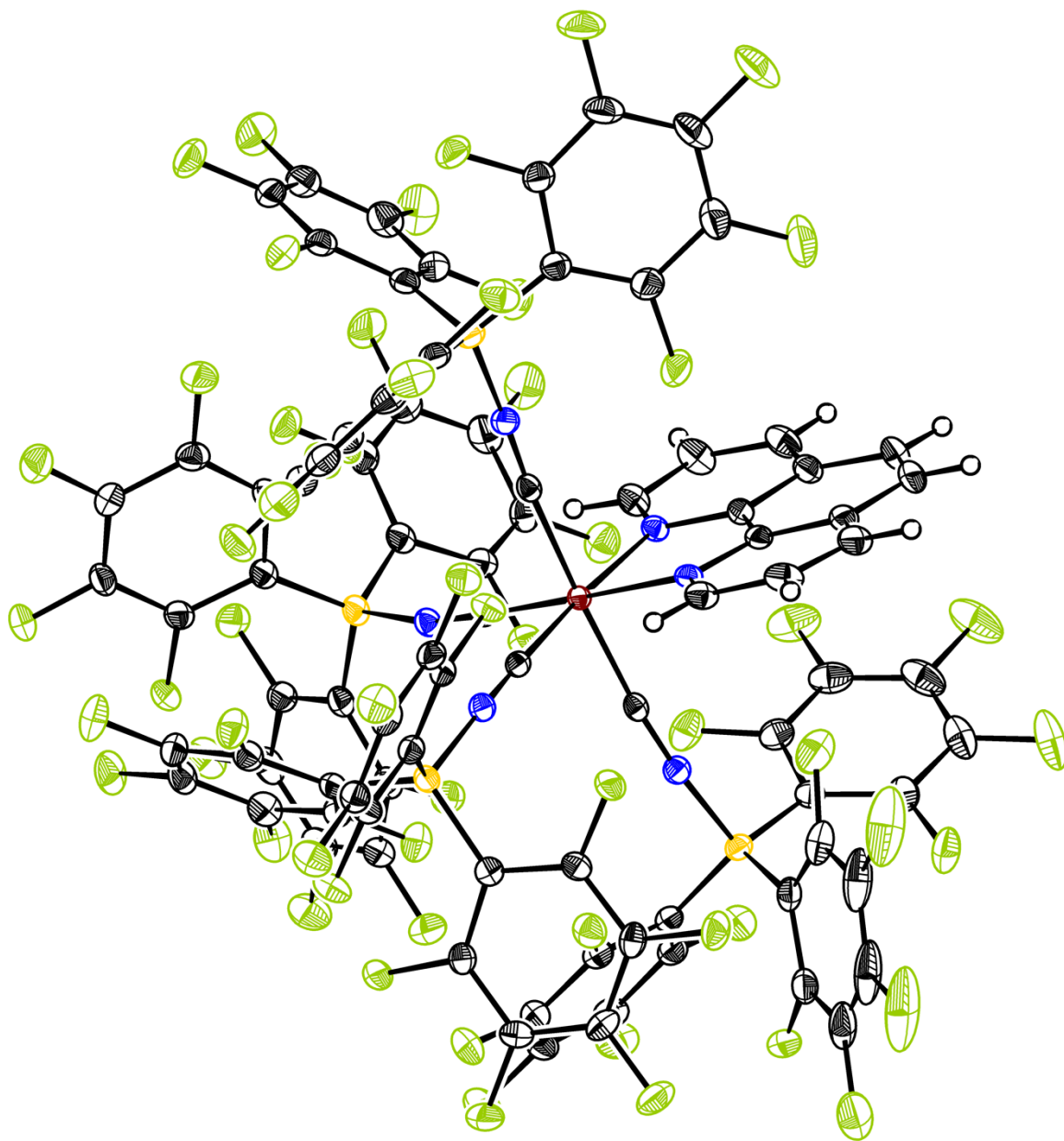


Figure S70. Crystal structure of $(\text{TBA})(\text{Ph}_4\text{As})[\text{Fe}(\text{phen})(\text{CN}-\text{B}(\text{C}_6\text{F}_5)_3)_4]$ (solvent and cations are omitted for clarity). Thermal ellipsoids set at 50% probability.

Table S8. Crystal data and structure refinement for **(TBA)(Ph₄As)[Fe(phen)(CN-B(C₆F₅)₃)₄]**.

Empirical formula	C128 H64 As B4 F60 Fe N7	
Formula weight	3013.87	
Temperature	100 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1 (# 2)	
Unit cell dimensions	a = 14.1069(12) Å	a = 95.150(6)°
	b = 15.1484(12) Å	b = 92.682(7)°
	c = 31.623(3) Å	g = 117.453(4)°
Volume	5942.8(9) Å ³	
Z	2	
Density (calculated)	1.684 g/cm ³	
Absorption coefficient	2.696 mm ⁻¹	
F(000)	3000	
Crystal size	0.05 x 0.13 x 0.22 mm ³	
Theta range for data collection	2.82 to 80.01°	
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 19, -40 ≤ l ≤ 40	
Reflections collected	179819	
Independent reflections	24417 [R(int) = 0.0419]	
Completeness to theta = 67.679°	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.7915	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	24417 / 0 / 1814	
Goodness-of-fit on F ²	1.072	
Final R indices [I > 2σ(I)]	R1 = 0.0338, wR2 = 0.0763	
R indices (all data)	R1 = 0.0367, wR2 = 0.0776	
Extinction coefficient	n/a	
Largest diff. peak and hole.	0.46 and -0.50 e.Å ⁻³	

Table S9. Bond lengths [\AA] and angles [$^\circ$] for **(TBA)(Ph₄As)[Fe(phen)(CN-B(C₆F₅)₃)₄].**

Fe(1)-N(1)	2.0080(14)	F(17B)-C(17B)	1.343(2)
Fe(1)-N(2)	2.0053(14)	F(18B)-C(18B)	1.344(2)
Fe(1)-C(1A)	1.8836(17)	F(19B)-C(19B)	1.350(2)
Fe(1)-C(1B)	1.9051(17)	F(3C)-C(3C)	1.350(2)
Fe(1)-C(1C)	1.8665(17)	F(4C)-C(4C)	1.344(2)
Fe(1)-C(1D)	1.9037(17)	F(5C)-C(5C)	1.344(2)
F(3A)-C(3A)	1.349(2)	F(6C)-C(6C)	1.345(2)
F(4A)-C(4A)	1.342(2)	F(7C)-C(7C)	1.359(2)
F(5A)-C(5A)	1.335(2)	F(9C)-C(9C)	1.346(2)
F(6A)-C(6A)	1.343(2)	F(10C)-C(10C)	1.346(2)
F(7A)-C(7A)	1.345(2)	F(11C)-C(11C)	1.342(2)
F(9A)-C(9A)	1.343(2)	F(12C)-C(12C)	1.348(2)
F(10A)-C(10A)	1.346(2)	F(13C)-C(13C)	1.347(2)
F(11A)-C(11A)	1.346(2)	F(15C)-C(15C)	1.355(2)
F(12A)-C(12A)	1.346(2)	F(16C)-C(16C)	1.347(2)
F(13A)-C(13A)	1.354(2)	F(17C)-C(17C)	1.345(2)
F(15A)-C(15A)	1.350(2)	F(18C)-C(18C)	1.343(2)
F(16A)-C(16A)	1.344(2)	F(19C)-C(19C)	1.353(2)
F(17A)-C(17A)	1.344(2)	F(3D)-C(3D)	1.354(2)
F(18A)-C(18A)	1.346(2)	F(4D)-C(4D)	1.347(2)
F(19A)-C(19A)	1.354(2)	F(5D)-C(5D)	1.343(2)
F(3B)-C(3B)	1.350(2)	F(6D)-C(6D)	1.343(2)
F(4B)-C(4B)	1.348(2)	F(7D)-C(7D)	1.351(2)
F(5B)-C(5B)	1.345(2)	F(9D)-C(9D)	1.349(2)
F(6B)-C(6B)	1.345(2)	F(10D)-C(10D)	1.343(2)
F(7B)-C(7B)	1.349(2)	F(11D)-C(11D)	1.343(2)
F(9B)-C(9B)	1.349(3)	F(12D)-C(12D)	1.343(2)
F(10B)-C(10B)	1.344(3)	F(13D)-C(13D)	1.352(2)
F(11B)-C(11B)	1.343(2)	F(15D)-C(15D)	1.352(2)
F(12B)-C(12B)	1.348(3)	F(16D)-C(16D)	1.342(2)
F(13B)-C(13B)	1.349(3)	F(17D)-C(17D)	1.345(2)
F(15B)-C(15B)	1.345(2)	F(18D)-C(18D)	1.341(2)
F(16B)-C(16B)	1.350(2)	F(19D)-C(19D)	1.354(2)

N(1A)-C(1A)	1.158(2)	C(3B)-C(4B)	1.381(3)
N(1A)-B(1A)	1.551(2)	C(4B)-C(5B)	1.377(3)
N(1B)-C(1B)	1.147(2)	C(5B)-C(6B)	1.375(3)
N(1B)-B(1B)	1.556(2)	C(6B)-C(7B)	1.388(3)
N(1C)-C(1C)	1.151(2)	C(8B)-C(9B)	1.391(3)
N(1C)-B(1C)	1.547(2)	C(8B)-C(13B)	1.380(3)
N(1D)-C(1D)	1.148(2)	C(8B)-B(1B)	1.639(3)
N(1D)-B(1D)	1.546(2)	C(9B)-C(10B)	1.382(3)
N(1)-C(1)	1.361(2)	C(10B)-C(11B)	1.373(4)
N(1)-C(3)	1.326(2)	C(11B)-C(12B)	1.365(4)
N(2)-C(2)	1.365(2)	C(12B)-C(13B)	1.386(3)
N(2)-C(12)	1.329(2)	C(14B)-C(15B)	1.395(2)
C(2A)-C(3A)	1.391(3)	C(14B)-C(19B)	1.386(3)
C(2A)-C(7A)	1.389(2)	C(14B)-B(1B)	1.642(3)
C(2A)-B(1A)	1.658(3)	C(15B)-C(16B)	1.376(3)
C(3A)-C(4A)	1.379(3)	C(16B)-C(17B)	1.379(3)
C(4A)-C(5A)	1.379(3)	C(17B)-C(18B)	1.374(3)
C(5A)-C(6A)	1.372(3)	C(18B)-C(19B)	1.383(3)
C(6A)-C(7A)	1.387(3)	C(2C)-C(3C)	1.389(2)
C(8A)-C(9A)	1.389(3)	C(2C)-C(7C)	1.390(2)
C(8A)-C(13A)	1.395(2)	C(2C)-B(1C)	1.641(3)
C(8A)-B(1A)	1.642(3)	C(3C)-C(4C)	1.385(3)
C(9A)-C(10A)	1.385(3)	C(4C)-C(5C)	1.383(3)
C(10A)-C(11A)	1.374(3)	C(5C)-C(6C)	1.380(3)
C(11A)-C(12A)	1.378(3)	C(6C)-C(7C)	1.374(3)
C(12A)-C(13A)	1.377(3)	C(8C)-C(9C)	1.393(3)
C(14A)-C(15A)	1.392(2)	C(8C)-C(13C)	1.387(2)
C(14A)-C(19A)	1.390(2)	C(8C)-B(1C)	1.646(2)
C(14A)-B(1A)	1.642(3)	C(9C)-C(10C)	1.381(3)
C(15A)-C(16A)	1.379(3)	C(10C)-C(11C)	1.381(3)
C(16A)-C(17A)	1.384(3)	C(11C)-C(12C)	1.371(3)
C(17A)-C(18A)	1.371(3)	C(12C)-C(13C)	1.385(3)
C(18A)-C(19A)	1.387(3)	C(14C)-C(15C)	1.390(2)
C(2B)-C(3B)	1.394(3)	C(14C)-C(19C)	1.385(2)
C(2B)-C(7B)	1.384(3)	C(14C)-B(1C)	1.649(2)
C(2B)-B(1B)	1.637(3)	C(15C)-C(16C)	1.382(2)

C(16C)-C(17C)	1.376(3)	C(8)-H(8)	0.9500
C(17C)-C(18C)	1.379(3)	C(8)-C(9)	1.435(3)
C(18C)-C(19C)	1.383(2)	C(9)-C(10)	1.406(3)
C(2D)-C(3D)	1.388(3)	C(10)-H(10)	0.9500
C(2D)-C(7D)	1.386(3)	C(10)-C(11)	1.368(3)
C(2D)-B(1D)	1.650(3)	C(11)-H(11)	0.9500
C(3D)-C(4D)	1.382(3)	C(11)-C(12)	1.402(3)
C(4D)-C(5D)	1.374(3)	C(12)-H(12)	0.9500
C(5D)-C(6D)	1.374(3)	As(1)-C(13)	1.9113(18)
C(6D)-C(7D)	1.388(2)	As(1)-C(19)	1.9210(19)
C(8D)-C(9D)	1.390(3)	As(1)-C(25)	1.9182(19)
C(8D)-C(13D)	1.390(2)	As(1)-C(31)	1.9123(19)
C(8D)-B(1D)	1.648(3)	C(13)-C(14)	1.389(3)
C(9D)-C(10D)	1.387(3)	C(13)-C(18)	1.388(3)
C(10D)-C(11D)	1.370(3)	C(14)-H(14)	0.9500
C(11D)-C(12D)	1.379(3)	C(14)-C(15)	1.388(3)
C(12D)-C(13D)	1.377(3)	C(15)-H(15)	0.9500
C(14D)-C(15D)	1.385(3)	C(15)-C(16)	1.379(3)
C(14D)-C(19D)	1.391(3)	C(16)-H(16)	0.9500
C(14D)-B(1D)	1.642(3)	C(16)-C(17)	1.380(4)
C(15D)-C(16D)	1.390(3)	C(17)-H(17)	0.9500
C(16D)-C(17D)	1.373(3)	C(17)-C(18)	1.388(3)
C(17D)-C(18D)	1.378(3)	C(18)-H(18)	0.9500
C(18D)-C(19D)	1.383(3)	C(19)-C(20)	1.391(3)
C(1)-C(2)	1.421(2)	C(19)-C(24)	1.388(3)
C(1)-C(6)	1.406(2)	C(20)-H(20)	0.9500
C(2)-C(9)	1.404(2)	C(20)-C(21)	1.390(3)
C(3)-H(3)	0.9500	C(21)-H(21)	0.9500
C(3)-C(4)	1.403(3)	C(21)-C(22)	1.385(3)
C(4)-H(4)	0.9500	C(22)-H(22)	0.9500
C(4)-C(5)	1.372(3)	C(22)-C(23)	1.380(3)
C(5)-H(5)	0.9500	C(23)-H(23)	0.9500
C(5)-C(6)	1.408(3)	C(23)-C(24)	1.390(3)
C(6)-C(7)	1.434(3)	C(24)-H(24)	0.9500
C(7)-H(7)	0.9500	C(25)-C(26)	1.394(3)
C(7)-C(8)	1.350(3)	C(25)-C(30)	1.388(3)

C(26)-H(26)	0.9500	C(41)-H(41A)	0.9900
C(26)-C(27)	1.388(3)	C(41)-H(41B)	0.9900
C(27)-H(27)	0.9500	C(41)-C(42)	1.521(2)
C(27)-C(28)	1.385(3)	C(42)-H(42A)	0.9900
C(28)-H(28)	0.9500	C(42)-H(42B)	0.9900
C(28)-C(29)	1.383(3)	C(42)-C(43)	1.526(3)
C(29)-H(29)	0.9500	C(43)-H(43A)	0.9900
C(29)-C(30)	1.395(3)	C(43)-H(43B)	0.9900
C(30)-H(30)	0.9500	C(43)-C(44)	1.521(3)
C(31)-C(32)	1.395(3)	C(44)-H(44A)	0.9800
C(31)-C(36)	1.389(3)	C(44)-H(44B)	0.9800
C(32)-H(32)	0.9500	C(44)-H(44C)	0.9800
C(32)-C(33)	1.385(3)	C(45)-H(45A)	0.9900
C(33)-H(33)	0.9500	C(45)-H(45B)	0.9900
C(33)-C(34)	1.382(3)	C(45)-C(46)	1.522(2)
C(34)-H(34)	0.9500	C(46)-H(46A)	0.9900
C(34)-C(35)	1.388(3)	C(46)-H(46B)	0.9900
C(35)-H(35)	0.9500	C(46)-C(47)	1.529(3)
C(35)-C(36)	1.387(3)	C(47)-H(47A)	0.9900
C(36)-H(36)	0.9500	C(47)-H(47B)	0.9900
N(3)-C(37)	1.518(2)	C(47)-C(48)	1.519(3)
N(3)-C(41)	1.525(2)	C(48)-H(48A)	0.9800
N(3)-C(45)	1.521(2)	C(48)-H(48B)	0.9800
N(3)-C(49)	1.520(2)	C(48)-H(48C)	0.9800
C(37)-H(37A)	0.9900	C(49)-H(49A)	0.9900
C(37)-H(37B)	0.9900	C(49)-H(49B)	0.9900
C(37)-C(38)	1.516(3)	C(49)-C(50)	1.522(3)
C(38)-H(38A)	0.9900	C(50)-H(50A)	0.9900
C(38)-H(38B)	0.9900	C(50)-H(50B)	0.9900
C(38)-C(39)	1.528(3)	C(50)-C(51)	1.524(3)
C(39)-H(39A)	0.9900	C(51)-H(51A)	0.9900
C(39)-H(39B)	0.9900	C(51)-H(51B)	0.9900
C(39)-C(40)	1.518(3)	C(51)-C(52)	1.526(3)
C(40)-H(40A)	0.9800	C(52)-H(52A)	0.9800
C(40)-H(40B)	0.9800	C(52)-H(52B)	0.9800
C(40)-H(40C)	0.9800	C(52)-H(52C)	0.9800

N(2)-Fe(1)-N(1)	81.30(6)	F(5A)-C(5A)-C(4A)	120.01(19)
C(1A)-Fe(1)-N(1)	93.19(6)	F(5A)-C(5A)-C(6A)	120.60(18)
C(1A)-Fe(1)-N(2)	174.34(7)	C(6A)-C(5A)-C(4A)	119.39(18)
C(1A)-Fe(1)-C(1B)	91.32(7)	F(6A)-C(6A)-C(5A)	119.44(18)
C(1A)-Fe(1)-C(1D)	92.72(7)	F(6A)-C(6A)-C(7A)	120.49(18)
C(1B)-Fe(1)-N(1)	89.43(6)	C(5A)-C(6A)-C(7A)	120.07(17)
C(1B)-Fe(1)-N(2)	87.38(6)	F(7A)-C(7A)-C(2A)	120.86(17)
C(1C)-Fe(1)-N(1)	175.12(6)	F(7A)-C(7A)-C(6A)	116.07(16)
C(1C)-Fe(1)-N(2)	94.11(6)	C(6A)-C(7A)-C(2A)	123.06(18)
C(1C)-Fe(1)-C(1A)	91.37(7)	C(9A)-C(8A)-C(13A)	113.96(16)
C(1C)-Fe(1)-C(1B)	88.73(7)	C(9A)-C(8A)-B(1A)	127.24(15)
C(1C)-Fe(1)-C(1D)	90.75(7)	C(13A)-C(8A)-B(1A)	118.38(15)
C(1D)-Fe(1)-N(1)	90.77(6)	F(9A)-C(9A)-C(8A)	120.98(16)
C(1D)-Fe(1)-N(2)	88.63(6)	F(9A)-C(9A)-C(10A)	115.97(16)
C(1D)-Fe(1)-C(1B)	175.93(7)	C(10A)-C(9A)-C(8A)	123.03(17)
C(1A)-N(1A)-B(1A)	167.33(16)	F(10A)-C(10A)-C(9A)	120.62(17)
C(1B)-N(1B)-B(1B)	172.33(17)	F(10A)-C(10A)-C(11A)	119.02(17)
C(1C)-N(1C)-B(1C)	166.58(16)	C(11A)-C(10A)-C(9A)	120.36(17)
C(1D)-N(1D)-B(1D)	176.13(17)	F(11A)-C(11A)-C(10A)	120.38(17)
C(1)-N(1)-Fe(1)	113.15(11)	F(11A)-C(11A)-C(12A)	120.58(17)
C(3)-N(1)-Fe(1)	129.23(12)	C(10A)-C(11A)-C(12A)	119.04(17)
C(3)-N(1)-C(1)	117.60(15)	F(12A)-C(12A)-C(11A)	120.02(17)
C(2)-N(2)-Fe(1)	113.02(11)	F(12A)-C(12A)-C(13A)	120.93(17)
C(12)-N(2)-Fe(1)	129.48(12)	C(13A)-C(12A)-C(11A)	119.03(17)
C(12)-N(2)-C(2)	117.49(15)	F(13A)-C(13A)-C(8A)	119.10(16)
N(1A)-C(1A)-Fe(1)	176.39(15)	F(13A)-C(13A)-C(12A)	116.37(15)
C(3A)-C(2A)-B(1A)	117.42(15)	C(12A)-C(13A)-C(8A)	124.52(17)
C(7A)-C(2A)-C(3A)	114.13(16)	C(15A)-C(14A)-B(1A)	119.79(15)
C(7A)-C(2A)-B(1A)	128.23(16)	C(19A)-C(14A)-C(15A)	113.43(16)
F(3A)-C(3A)-C(2A)	119.80(15)	C(19A)-C(14A)-B(1A)	126.78(16)
F(3A)-C(3A)-C(4A)	115.62(16)	F(15A)-C(15A)-C(14A)	119.33(16)
C(4A)-C(3A)-C(2A)	124.59(16)	F(15A)-C(15A)-C(16A)	116.35(16)
F(4A)-C(4A)-C(3A)	121.26(16)	C(16A)-C(15A)-C(14A)	124.28(17)
F(4A)-C(4A)-C(5A)	119.96(17)	F(16A)-C(16A)-C(15A)	121.17(17)
C(3A)-C(4A)-C(5A)	118.77(18)	F(16A)-C(16A)-C(17A)	119.30(17)
		C(15A)-C(16A)-C(17A)	119.51(17)

F(17A)-C(17A)-C(16A)	120.38(17)	C(11B)-C(10B)-C(9B)	119.2(2)
F(17A)-C(17A)-C(18A)	120.69(17)	F(11B)-C(11B)-C(10B)	119.6(3)
C(18A)-C(17A)-C(16A)	118.94(17)	F(11B)-C(11B)-C(12B)	120.9(3)
F(18A)-C(18A)-C(17A)	119.92(17)	C(12B)-C(11B)-C(10B)	119.5(2)
F(18A)-C(18A)-C(19A)	120.48(16)	F(12B)-C(12B)-C(11B)	119.8(2)
C(17A)-C(18A)-C(19A)	119.60(17)	F(12B)-C(12B)-C(13B)	120.4(3)
F(19A)-C(19A)-C(14A)	120.94(16)	C(11B)-C(12B)-C(13B)	119.8(2)
F(19A)-C(19A)-C(18A)	114.88(15)	F(13B)-C(13B)-C(8B)	120.86(18)
C(18A)-C(19A)-C(14A)	124.18(17)	F(13B)-C(13B)-C(12B)	115.8(2)
N(1B)-C(1B)-Fe(1)	174.15(15)	C(8B)-C(13B)-C(12B)	123.3(2)
C(3B)-C(2B)-B(1B)	118.53(16)	C(15B)-C(14B)-B(1B)	119.48(16)
C(7B)-C(2B)-C(3B)	114.41(16)	C(19B)-C(14B)-C(15B)	113.90(17)
C(7B)-C(2B)-B(1B)	127.06(16)	C(19B)-C(14B)-B(1B)	126.13(16)
F(3B)-C(3B)-C(2B)	119.67(16)	F(15B)-C(15B)-C(14B)	119.40(16)
F(3B)-C(3B)-C(4B)	116.29(17)	F(15B)-C(15B)-C(16B)	116.84(17)
C(4B)-C(3B)-C(2B)	124.01(18)	C(16B)-C(15B)-C(14B)	123.76(18)
F(4B)-C(4B)-C(3B)	120.87(18)	F(16B)-C(16B)-C(15B)	120.59(19)
F(4B)-C(4B)-C(5B)	120.00(17)	F(16B)-C(16B)-C(17B)	119.72(18)
C(5B)-C(4B)-C(3B)	119.13(18)	C(15B)-C(16B)-C(17B)	119.69(19)
F(5B)-C(5B)-C(4B)	120.10(19)	F(17B)-C(17B)-C(16B)	120.1(2)
F(5B)-C(5B)-C(6B)	120.54(18)	F(17B)-C(17B)-C(18B)	120.9(2)
C(6B)-C(5B)-C(4B)	119.36(17)	C(18B)-C(17B)-C(16B)	119.04(18)
F(6B)-C(6B)-C(5B)	119.64(17)	F(18B)-C(18B)-C(17B)	119.88(19)
F(6B)-C(6B)-C(7B)	120.50(18)	F(18B)-C(18B)-C(19B)	120.66(19)
C(5B)-C(6B)-C(7B)	119.86(18)	C(17B)-C(18B)-C(19B)	119.47(19)
F(7B)-C(7B)-C(2B)	120.77(16)	F(19B)-C(19B)-C(14B)	120.70(16)
F(7B)-C(7B)-C(6B)	115.99(16)	F(19B)-C(19B)-C(18B)	115.25(17)
C(2B)-C(7B)-C(6B)	123.23(18)	C(18B)-C(19B)-C(14B)	124.04(18)
C(9B)-C(8B)-B(1B)	121.51(16)	N(1C)-C(1C)-Fe(1)	177.80(15)
C(13B)-C(8B)-C(9B)	114.43(18)	C(3C)-C(2C)-C(7C)	114.08(16)
C(13B)-C(8B)-B(1B)	124.05(17)	C(3C)-C(2C)-B(1C)	127.16(15)
F(9B)-C(9B)-C(8B)	120.13(17)	C(7C)-C(2C)-B(1C)	118.63(15)
F(9B)-C(9B)-C(10B)	116.2(2)	F(3C)-C(3C)-C(2C)	121.20(15)
C(10B)-C(9B)-C(8B)	123.6(2)	F(3C)-C(3C)-C(4C)	115.45(15)
F(10B)-C(10B)-C(9B)	120.7(3)	C(4C)-C(3C)-C(2C)	123.34(16)
F(10B)-C(10B)-C(11B)	120.1(2)	F(4C)-C(4C)-C(3C)	120.92(16)

F(4C)-C(4C)-C(5C)	119.32(16)	F(16C)-C(16C)-C(17C)	119.62(16)
C(5C)-C(4C)-C(3C)	119.76(16)	C(17C)-C(16C)-C(15C)	119.34(16)
F(5C)-C(5C)-C(4C)	120.55(16)	F(17C)-C(17C)-C(16C)	120.26(16)
F(5C)-C(5C)-C(6C)	120.28(16)	F(17C)-C(17C)-C(18C)	120.50(17)
C(6C)-C(5C)-C(4C)	119.16(16)	C(16C)-C(17C)-C(18C)	119.18(16)
F(6C)-C(6C)-C(5C)	119.61(16)	F(18C)-C(18C)-C(17C)	120.12(16)
F(6C)-C(6C)-C(7C)	121.45(16)	F(18C)-C(18C)-C(19C)	120.42(16)
C(7C)-C(6C)-C(5C)	118.94(16)	C(17C)-C(18C)-C(19C)	119.43(16)
F(7C)-C(7C)-C(2C)	118.81(15)	F(19C)-C(19C)-C(14C)	120.71(15)
F(7C)-C(7C)-C(6C)	116.48(15)	F(19C)-C(19C)-C(18C)	115.29(15)
C(6C)-C(7C)-C(2C)	124.71(16)	C(18C)-C(19C)-C(14C)	123.98(16)
C(9C)-C(8C)-B(1C)	119.61(15)	N(1D)-C(1D)-Fe(1)	174.21(15)
C(13C)-C(8C)-C(9C)	114.09(16)	C(3D)-C(2D)-B(1D)	119.98(16)
C(13C)-C(8C)-B(1C)	125.65(16)	C(7D)-C(2D)-C(3D)	114.16(16)
F(9C)-C(9C)-C(8C)	119.61(15)	C(7D)-C(2D)-B(1D)	125.79(16)
F(9C)-C(9C)-C(10C)	116.32(16)	F(3D)-C(3D)-C(2D)	120.03(16)
C(10C)-C(9C)-C(8C)	124.07(17)	F(3D)-C(3D)-C(4D)	116.12(17)
F(10C)-C(10C)-C(9C)	121.18(17)	C(4D)-C(3D)-C(2D)	123.85(18)
F(10C)-C(10C)-C(11C)	119.65(16)	F(4D)-C(4D)-C(3D)	120.50(18)
C(9C)-C(10C)-C(11C)	119.16(18)	F(4D)-C(4D)-C(5D)	119.96(17)
F(11C)-C(11C)-C(10C)	120.88(18)	C(5D)-C(4D)-C(3D)	119.53(18)
F(11C)-C(11C)-C(12C)	119.84(17)	F(5D)-C(5D)-C(4D)	119.90(18)
C(12C)-C(11C)-C(10C)	119.28(17)	F(5D)-C(5D)-C(6D)	120.81(18)
F(12C)-C(12C)-C(11C)	119.56(17)	C(6D)-C(5D)-C(4D)	119.30(17)
F(12C)-C(12C)-C(13C)	120.62(18)	F(6D)-C(6D)-C(5D)	120.19(16)
C(11C)-C(12C)-C(13C)	119.82(17)	F(6D)-C(6D)-C(7D)	120.38(18)
F(13C)-C(13C)-C(8C)	121.31(16)	C(5D)-C(6D)-C(7D)	119.41(17)
F(13C)-C(13C)-C(12C)	115.14(16)	F(7D)-C(7D)-C(2D)	120.70(16)
C(12C)-C(13C)-C(8C)	123.55(17)	F(7D)-C(7D)-C(6D)	115.57(16)
C(15C)-C(14C)-B(1C)	119.01(15)	C(2D)-C(7D)-C(6D)	123.73(18)
C(19C)-C(14C)-C(15C)	114.00(15)	C(9D)-C(8D)-C(13D)	113.37(17)
C(19C)-C(14C)-B(1C)	126.84(15)	C(9D)-C(8D)-B(1D)	126.80(16)
F(15C)-C(15C)-C(14C)	119.92(15)	C(13D)-C(8D)-B(1D)	119.43(16)
F(15C)-C(15C)-C(16C)	115.99(15)	F(9D)-C(9D)-C(8D)	121.10(17)
C(16C)-C(15C)-C(14C)	124.05(16)	F(9D)-C(9D)-C(10D)	114.94(17)
F(16C)-C(16C)-C(15C)	121.02(17)	C(10D)-C(9D)-C(8D)	123.95(18)

F(10D)-C(10D)-C(9D)	120.29(19)	N(1B)-B(1B)-C(2B)	104.93(13)
F(10D)-C(10D)-C(11D)	120.03(18)	N(1B)-B(1B)-C(8B)	107.56(14)
C(11D)-C(10D)-C(9D)	119.68(19)	N(1B)-B(1B)-C(14B)	103.79(13)
F(11D)-C(11D)-C(10D)	120.6(2)	C(2B)-B(1B)-C(8B)	110.47(14)
F(11D)-C(11D)-C(12D)	120.39(19)	C(2B)-B(1B)-C(14B)	116.48(14)
C(10D)-C(11D)-C(12D)	119.00(18)	C(8B)-B(1B)-C(14B)	112.70(14)
F(12D)-C(12D)-C(11D)	119.79(18)	N(1C)-B(1C)-C(2C)	112.22(14)
F(12D)-C(12D)-C(13D)	120.77(19)	N(1C)-B(1C)-C(8C)	102.31(13)
C(13D)-C(12D)-C(11D)	119.43(18)	N(1C)-B(1C)-C(14C)	106.79(14)
F(13D)-C(13D)-C(8D)	119.17(16)	C(2C)-B(1C)-C(8C)	114.46(14)
F(13D)-C(13D)-C(12D)	116.39(17)	C(2C)-B(1C)-C(14C)	105.06(13)
C(12D)-C(13D)-C(8D)	124.44(18)	C(8C)-B(1C)-C(14C)	115.93(14)
C(15D)-C(14D)-C(19D)	113.87(16)	N(1D)-B(1D)-C(2D)	106.91(14)
C(15D)-C(14D)-B(1D)	127.47(16)	N(1D)-B(1D)-C(8D)	109.67(14)
C(19D)-C(14D)-B(1D)	118.48(16)	N(1D)-B(1D)-C(14D)	103.96(14)
F(15D)-C(15D)-C(14D)	120.57(17)	C(8D)-B(1D)-C(2D)	105.82(14)
F(15D)-C(15D)-C(16D)	115.72(16)	C(14D)-B(1D)-C(2D)	114.04(14)
C(14D)-C(15D)-C(16D)	123.71(17)	C(14D)-B(1D)-C(8D)	116.11(15)
F(16D)-C(16D)-C(15D)	121.03(18)	N(1)-C(1)-C(2)	115.86(15)
F(16D)-C(16D)-C(17D)	119.32(17)	N(1)-C(1)-C(6)	123.69(16)
C(17D)-C(16D)-C(15D)	119.63(17)	C(6)-C(1)-C(2)	120.42(16)
F(17D)-C(17D)-C(16D)	120.64(18)	N(2)-C(2)-C(1)	116.07(15)
F(17D)-C(17D)-C(18D)	120.01(18)	N(2)-C(2)-C(9)	123.94(16)
C(16D)-C(17D)-C(18D)	119.35(17)	C(9)-C(2)-C(1)	119.93(16)
F(18D)-C(18D)-C(17D)	119.92(17)	N(1)-C(3)-H(3)	118.7
F(18D)-C(18D)-C(19D)	121.04(17)	N(1)-C(3)-C(4)	122.55(17)
C(17D)-C(18D)-C(19D)	119.03(17)	C(4)-C(3)-H(3)	118.7
F(19D)-C(19D)-C(14D)	119.80(16)	C(3)-C(4)-H(4)	119.9
F(19D)-C(19D)-C(18D)	115.79(16)	C(5)-C(4)-C(3)	120.12(17)
C(18D)-C(19D)-C(14D)	124.41(17)	C(5)-C(4)-H(4)	119.9
N(1A)-B(1A)-C(2A)	105.79(14)	C(4)-C(5)-H(5)	120.6
N(1A)-B(1A)-C(8A)	113.37(14)	C(4)-C(5)-C(6)	118.87(17)
N(1A)-B(1A)-C(14A)	105.73(14)	C(6)-C(5)-H(5)	120.6
C(8A)-B(1A)-C(2A)	102.77(14)	C(1)-C(6)-C(5)	117.13(16)
C(8A)-B(1A)-C(14A)	114.31(14)	C(1)-C(6)-C(7)	118.66(17)
C(14A)-B(1A)-C(2A)	114.78(14)	C(5)-C(6)-C(7)	124.18(17)

C(6)-C(7)-H(7)	119.6	C(16)-C(17)-H(17)	119.7
C(8)-C(7)-C(6)	120.83(18)	C(16)-C(17)-C(18)	120.6(2)
C(8)-C(7)-H(7)	119.6	C(18)-C(17)-H(17)	119.7
C(7)-C(8)-H(8)	119.3	C(13)-C(18)-C(17)	118.6(2)
C(7)-C(8)-C(9)	121.42(17)	C(13)-C(18)-H(18)	120.7
C(9)-C(8)-H(8)	119.3	C(17)-C(18)-H(18)	120.7
C(2)-C(9)-C(8)	118.67(17)	C(20)-C(19)-As(1)	120.72(15)
C(2)-C(9)-C(10)	116.78(17)	C(24)-C(19)-As(1)	118.30(14)
C(10)-C(9)-C(8)	124.54(17)	C(24)-C(19)-C(20)	120.98(18)
C(9)-C(10)-H(10)	120.4	C(19)-C(20)-H(20)	120.6
C(11)-C(10)-C(9)	119.19(17)	C(21)-C(20)-C(19)	118.8(2)
C(11)-C(10)-H(10)	120.4	C(21)-C(20)-H(20)	120.6
C(10)-C(11)-H(11)	119.8	C(20)-C(21)-H(21)	119.7
C(10)-C(11)-C(12)	120.32(17)	C(22)-C(21)-C(20)	120.6(2)
C(12)-C(11)-H(11)	119.8	C(22)-C(21)-H(21)	119.7
N(2)-C(12)-C(11)	122.25(17)	C(21)-C(22)-H(22)	120.0
N(2)-C(12)-H(12)	118.9	C(23)-C(22)-C(21)	120.05(19)
C(11)-C(12)-H(12)	118.9	C(23)-C(22)-H(22)	120.0
C(13)-As(1)-C(19)	109.23(8)	C(22)-C(23)-H(23)	119.9
C(13)-As(1)-C(25)	111.09(8)	C(22)-C(23)-C(24)	120.2(2)
C(13)-As(1)-C(31)	106.23(8)	C(24)-C(23)-H(23)	119.9
C(25)-As(1)-C(19)	109.43(8)	C(19)-C(24)-C(23)	119.35(19)
C(31)-As(1)-C(19)	112.26(8)	C(19)-C(24)-H(24)	120.3
C(31)-As(1)-C(25)	108.59(8)	C(23)-C(24)-H(24)	120.3
C(14)-C(13)-As(1)	119.43(14)	C(26)-C(25)-As(1)	119.36(14)
C(18)-C(13)-As(1)	118.69(15)	C(30)-C(25)-As(1)	119.71(15)
C(18)-C(13)-C(14)	121.32(18)	C(30)-C(25)-C(26)	120.94(18)
C(13)-C(14)-H(14)	120.5	C(25)-C(26)-H(26)	120.4
C(15)-C(14)-C(13)	118.95(19)	C(27)-C(26)-C(25)	119.27(19)
C(15)-C(14)-H(14)	120.5	C(27)-C(26)-H(26)	120.4
C(14)-C(15)-H(15)	119.9	C(26)-C(27)-H(27)	119.9
C(16)-C(15)-C(14)	120.3(2)	C(28)-C(27)-C(26)	120.1(2)
C(16)-C(15)-H(15)	119.9	C(28)-C(27)-H(27)	119.9
C(15)-C(16)-H(16)	119.9	C(27)-C(28)-H(28)	119.8
C(15)-C(16)-C(17)	120.3(2)	C(29)-C(28)-C(27)	120.4(2)
C(17)-C(16)-H(16)	119.9	C(29)-C(28)-H(28)	119.8

C(28)-C(29)-H(29)	119.9	C(37)-C(38)-H(38A)	110.0
C(28)-C(29)-C(30)	120.18(19)	C(37)-C(38)-H(38B)	110.0
C(30)-C(29)-H(29)	119.9	C(37)-C(38)-C(39)	108.51(15)
C(25)-C(30)-C(29)	119.06(19)	H(38A)-C(38)-H(38B)	108.4
C(25)-C(30)-H(30)	120.5	C(39)-C(38)-H(38A)	110.0
C(29)-C(30)-H(30)	120.5	C(39)-C(38)-H(38B)	110.0
C(32)-C(31)-As(1)	120.60(14)	C(38)-C(39)-H(39A)	109.1
C(36)-C(31)-As(1)	118.64(14)	C(38)-C(39)-H(39B)	109.1
C(36)-C(31)-C(32)	120.74(18)	H(39A)-C(39)-H(39B)	107.9
C(31)-C(32)-H(32)	120.5	C(40)-C(39)-C(38)	112.33(17)
C(33)-C(32)-C(31)	118.95(18)	C(40)-C(39)-H(39A)	109.1
C(33)-C(32)-H(32)	120.5	C(40)-C(39)-H(39B)	109.1
C(32)-C(33)-H(33)	119.7	C(39)-C(40)-H(40A)	109.5
C(34)-C(33)-C(32)	120.62(18)	C(39)-C(40)-H(40B)	109.5
C(34)-C(33)-H(33)	119.7	C(39)-C(40)-H(40C)	109.5
C(33)-C(34)-H(34)	119.9	H(40A)-C(40)-H(40B)	109.5
C(33)-C(34)-C(35)	120.20(19)	H(40A)-C(40)-H(40C)	109.5
C(35)-C(34)-H(34)	119.9	H(40B)-C(40)-H(40C)	109.5
C(34)-C(35)-H(35)	120.0	N(3)-C(41)-H(41A)	108.5
C(36)-C(35)-C(34)	119.97(19)	N(3)-C(41)-H(41B)	108.5
C(36)-C(35)-H(35)	120.0	H(41A)-C(41)-H(41B)	107.5
C(31)-C(36)-H(36)	120.2	C(42)-C(41)-N(3)	114.99(15)
C(35)-C(36)-C(31)	119.51(18)	C(42)-C(41)-H(41A)	108.5
C(35)-C(36)-H(36)	120.2	C(42)-C(41)-H(41B)	108.5
C(37)-N(3)-C(41)	110.36(13)	C(41)-C(42)-H(42A)	109.5
C(37)-N(3)-C(45)	106.76(13)	C(41)-C(42)-H(42B)	109.5
C(37)-N(3)-C(49)	110.61(13)	C(41)-C(42)-C(43)	110.81(15)
C(45)-N(3)-C(41)	110.58(13)	H(42A)-C(42)-H(42B)	108.1
C(49)-N(3)-C(41)	107.70(13)	C(43)-C(42)-H(42A)	109.5
C(49)-N(3)-C(45)	110.86(14)	C(43)-C(42)-H(42B)	109.5
N(3)-C(37)-H(37A)	108.1	C(42)-C(43)-H(43A)	109.4
N(3)-C(37)-H(37B)	108.1	C(42)-C(43)-H(43B)	109.4
H(37A)-C(37)-H(37B)	107.3	H(43A)-C(43)-H(43B)	108.0
C(38)-C(37)-N(3)	116.78(15)	C(44)-C(43)-C(42)	111.26(17)
C(38)-C(37)-H(37A)	108.1	C(44)-C(43)-H(43A)	109.4
C(38)-C(37)-H(37B)	108.1	C(44)-C(43)-H(43B)	109.4

C(43)-C(44)-H(44A)	109.5	H(48A)-C(48)-H(48B)	109.5
C(43)-C(44)-H(44B)	109.5	H(48A)-C(48)-H(48C)	109.5
C(43)-C(44)-H(44C)	109.5	H(48B)-C(48)-H(48C)	109.5
H(44A)-C(44)-H(44B)	109.5	N(3)-C(49)-H(49A)	108.6
H(44A)-C(44)-H(44C)	109.5	N(3)-C(49)-H(49B)	108.6
H(44B)-C(44)-H(44C)	109.5	N(3)-C(49)-C(50)	114.60(15)
N(3)-C(45)-H(45A)	108.5	H(49A)-C(49)-H(49B)	107.6
N(3)-C(45)-H(45B)	108.5	C(50)-C(49)-H(49A)	108.6
N(3)-C(45)-C(46)	115.22(15)	C(50)-C(49)-H(49B)	108.6
H(45A)-C(45)-H(45B)	107.5	C(49)-C(50)-H(50A)	109.7
C(46)-C(45)-H(45A)	108.5	C(49)-C(50)-H(50B)	109.7
C(46)-C(45)-H(45B)	108.5	C(49)-C(50)-C(51)	109.86(16)
C(45)-C(46)-H(46A)	109.5	H(50A)-C(50)-H(50B)	108.2
C(45)-C(46)-H(46B)	109.5	C(51)-C(50)-H(50A)	109.7
C(45)-C(46)-C(47)	110.67(16)	C(51)-C(50)-H(50B)	109.7
H(46A)-C(46)-H(46B)	108.1	C(50)-C(51)-H(51A)	109.2
C(47)-C(46)-H(46A)	109.5	C(50)-C(51)-H(51B)	109.2
C(47)-C(46)-H(46B)	109.5	C(50)-C(51)-C(52)	111.93(16)
C(46)-C(47)-H(47A)	108.8	H(51A)-C(51)-H(51B)	107.9
C(46)-C(47)-H(47B)	108.8	C(52)-C(51)-H(51A)	109.2
H(47A)-C(47)-H(47B)	107.7	C(52)-C(51)-H(51B)	109.2
C(48)-C(47)-C(46)	113.69(17)	C(51)-C(52)-H(52A)	109.5
C(48)-C(47)-H(47A)	108.8	C(51)-C(52)-H(52B)	109.5
C(48)-C(47)-H(47B)	108.8	C(51)-C(52)-H(52C)	109.5
C(47)-C(48)-H(48A)	109.5	H(52A)-C(52)-H(52B)	109.5
C(47)-C(48)-H(48B)	109.5	H(52A)-C(52)-H(52C)	109.5
C(47)-C(48)-H(48C)	109.5	H(52B)-C(52)-H(52C)	109.5

S.6. Theoretical Calculations

Below are sample input files for structural optimizations and CASSCF-NEVPT2 calculations.

Figures S65-S67 depict the active space orbitals for CASSCF-NEVPT2 calculations.

Structural Optimization for Ru-bpy-BH₃

```
! PBE0 def2-TZVP Opt TightSCF LargePrint printbasis
!Grid4 FinalGrid6
!PCM(Acetonitrile)
```

```
%basis
NewGTO Ru "def2-QZVPP" end
end
```

```
%pal
  nprocs 16
end
```

```
%scf
maxiter 2000
end
```

```
%maxcore 12000
```

```
* xyzfile -2 1 Ru_bpy_XRay.xyz
```

CASSCF-NEVPT2 Calculation for Ru-bpy-BH₃

```
! RI DKH DKH-def2-tzvp SARC/J RIJK AutoAux CONV NEVPT2 CPCM(Acetonitrile)  
MOREAD LargePrint
```

```
! NoFrozenCore
```

```
%basis
```

```
NewGTO Ru "old-DKH-TZVP" end
```

```
end
```

```
%moinp "Ru_bpy_BH3_CASSCF5_12.gbwn"
```

```
%rel method DKH picturechange 2 end
```

```
%casscf
```

```
trafostep ri
```

```
nel 12
```

```
norb 13
```

```
MaxIter 200
```

```
Mult 5,3,1
```

```
NRroots 1,9,10 end
```

```
%pal
```

```
nprocs 6
```

```
end
```

```
%scf
```

```
%maxcore 31000
```

```
* xyzfile -2 1 Ru_bpy_BH3_Aligned.xyz
```

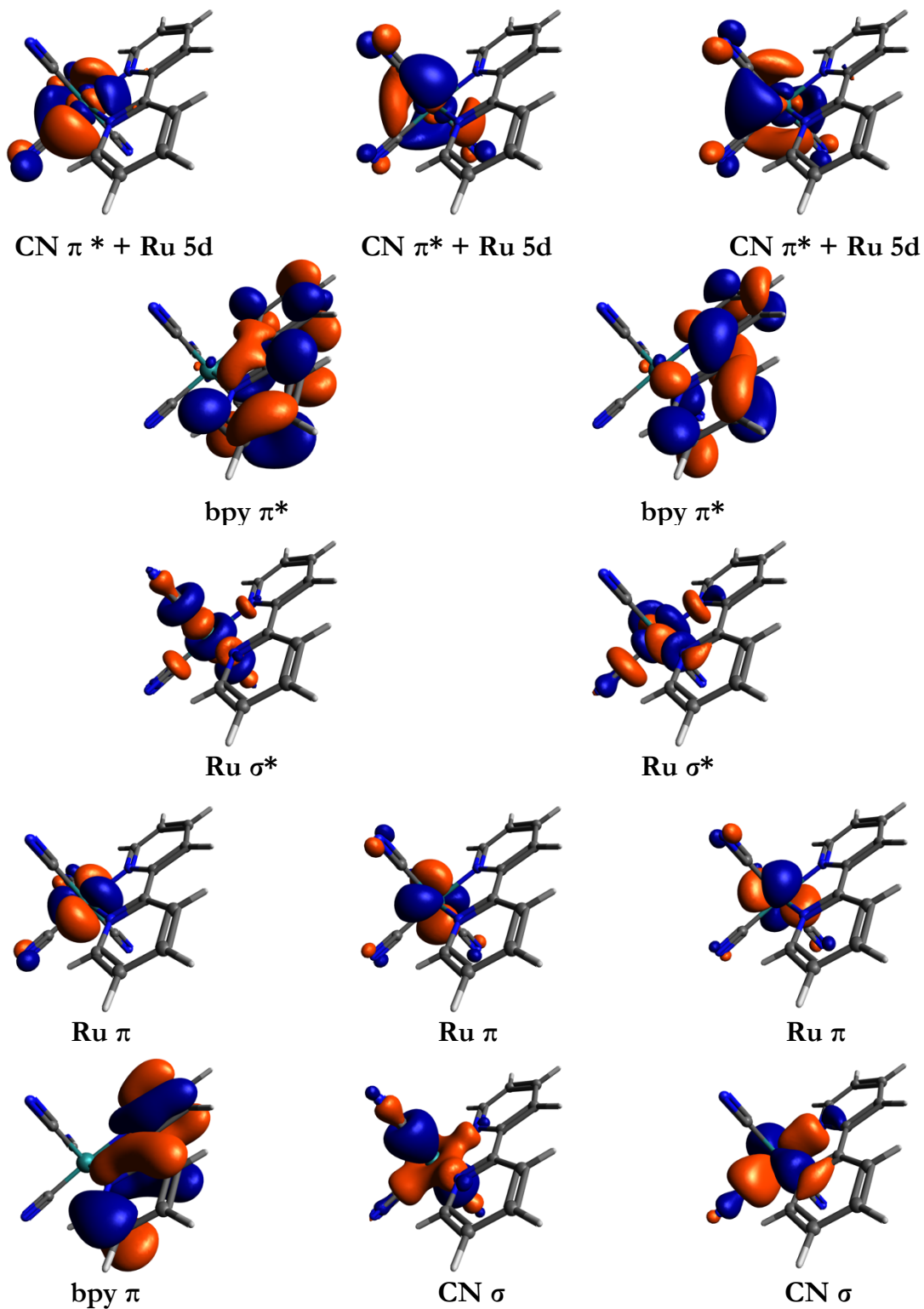



Figure S71. Active space molecular orbitals for the state-averaged CAS(12,13) of $[\text{Ru}(\text{bpy})(\text{CN})_4]^{2-}$. Isosurface values set to 0.04

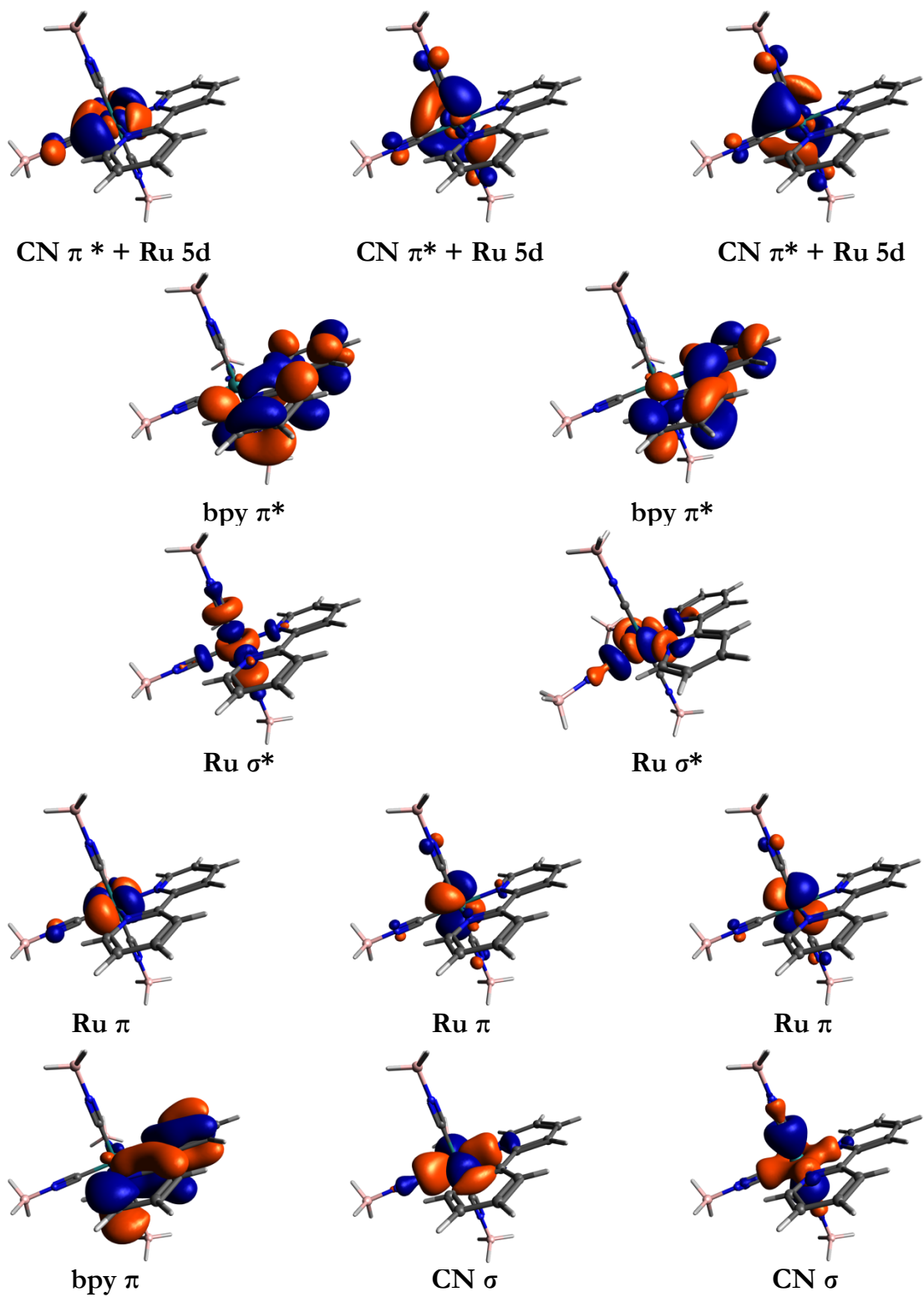


Figure S72. Active space molecular orbitals for the state-averaged CAS(12,13) of $[\text{Ru}(\text{bpy})(\text{CN-BH}_3)_4]^{2-}$. Isosurface values set to 0.04.

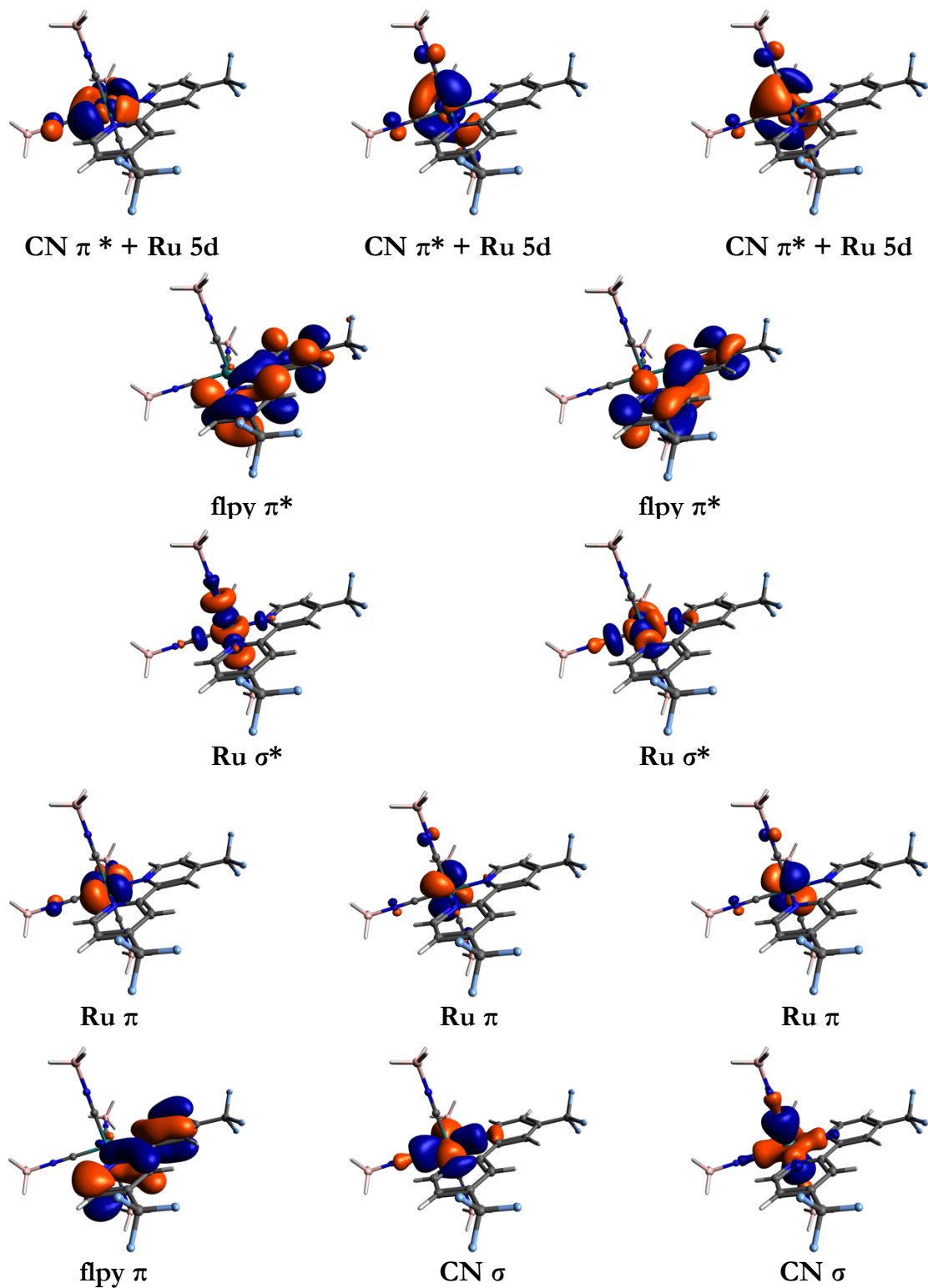


Figure S73. Active space molecular orbitals for the state-averaged CAS(12,13) of $[\text{Ru}(\text{flpy})(\text{CN-BH}_3)_4]^{2-}$. Isosurface values set to 0.04.

S.7. References

1. Kjær, K. S.; Kunnus, K.; Harlang, T. C. B.; Van Driel, T. B.; Ledbetter, K.; Hartsock, R. W.; Reinhard, M. E.; Koroidov, S.; Li, L.; Laursen, M. G.; Biasin, E.; Hansen, F. B.; Vester, P.; Christensen, M.; Haldrup, K.; Nielsen, M. M.; Chabera, P.; Liu, Y.; Tatsuno, H.; Timm, C.; Uhlig, J.; Sundstöm, V.; Németh, Z.; Szemes, D. S.; Bajnóczi, É.; Vankó, G.; Alonso-Mori, R.; Glowina, J. M.; Nelson, S.; Sikorski, M.; Sokaras, D.; Lemke, H. T.; Canton, S. E.; Wärnmark, K.; Persson, P.; Cordones, A. A.; Gaffney, K. J. Solvent Control of Charge Transfer Excited State Relaxation Pathways in $[\text{Fe}(2,2'\text{-Bipyridine})(\text{CN})_4]^{2-}$. *Phys. Chem. Chem. Phys.* **2018**, *20* (6), 4238–4249. <https://doi.org/10.1039/C7CP07838B>.