Supporting Information

Synthesis of μ-Phosphido Diiron Complexes Having a P–H bond: Hydrophosphination of Phenylacetylene and Methyl Acrylate with the Cationic μ-Phosphido Diiron Complex

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Table S1. X-ray report for $[Cp_2Fe_2(CO)_2(\mu\text{-}H)(\mu\text{-}PHMes)]$ (*trans*-**1b**)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{21}H_{23}Fe_2O_2P$
Formula Weight	450.08
Crystal Color, Habit	darkviolet, platelet
Crystal Dimensions	0.20 X 0.15 X 0.10 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	4252 (5.9 - 55.0°)
Indexing Images	2 oscillations at 2.0 minutes
Camera Radius	127.40 mm
Lattice Parameters	a = 8.31944(4) Å b = 9.1436(3) Å c = 13.8510(3) Å α = 107.096(1) ° β = 95.6569(9) ° γ = 104.811(2) ° V = 956.26(4) Å^3
Space Group	P -1 (#2)
Z value	2
D_{calc}	1.563 g/cm^3
F_{000}	464.00
μ(MoKα)	16.11 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID Imaging Plate
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Temperature	-123.0 °C
Voltage, Current	50 kV, 200 mA
Collimator Size	0.3 mm
Detector Aperture	270.0 mm x 256.0 mm
Data Images	44 exposures at 3.7 minutes per degree
Oscillation Range (ϕ = 0.0°, χ = 45.0°)	ω 130.0 - 190.0° with 5.0° step
Oscillation Range (ϕ = 180.0°, χ = 45.0°)	ω 0.0 - 160.0° with 5.0° step
Camera Radius	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 9250 Unique: 4341 (R_{int} = 0.048)
Corrections	Lorentz-polarization Absorption

(trans. factors: 0.8111 - 0.9157)

C. Structure Solution and Refinement

Structure Solution (DIRDIF94 PATTY)	Patterson Methods
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\, w\, (Fo^2 - Fc^2)^2$
Least Squares Weights	$1/\sigma^2(Fo^2)$
p-factor	0.0990
Anomalous Dispersion	All non-hydrogen atoms
No. of Reflections (All, $2\sigma < 54.95°$)	4341
No. Variables	243
Reflection/Parameter Ratio	17.86
Residuals: *R*; *Rw*	0.073 ; 0.153
Residuals: *R1*	0.046
No. of Reflections to calc *R1*	3634
Goodness of Fit Indicator	1.16
Max Shift/Error in Final Cycle	0.013
Maximum peak in Final Diff. Map	0.51 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.41 $e^-/Å^3$

Table S2. Atomic coordinates and B_{iso}/B_{eq}

atom	*x*	*y*	*z*	B_{eq}
Fe1	0.07256(6)	0.37570(6)	0.31211(3)	1.25(1)
Fe2	0.27115(6)	0.19781(6)	0.34634(4)	1.29(1)
P	0.1435(1)	0.1910(1)	0.19892(6)	1.24(2)
O1	-0.2274(4)	0.1345(4)	0.3158(2)	2.80(6)
O2	0.5795(4)	0.4533(4)	0.3708(2)	2.59(6)
C1	-0.1096(5)	0.2311(5)	0.3144(3)	1.80(7)
C2	0.4548(5)	0.3523(4)	0.3592(3)	1.76(7)
C3	0.2271(4)	0.2231(4)	0.0857(2)	1.41(6)
C4	0.1211(4)	0.2530(4)	0.0119(2)	1.52(6)
C5	0.1814(5)	0.2846(5)	-0.0722(3)	1.79(7)
C6	0.3451(5)	0.2854(5)	-0.0873(3)	1.95(7)
C7	0.4440(5)	0.2472(5)	-0.0172(3)	1.97(7)
C8	0.3901(4)	0.2157(4)	0.0686(3)	1.69(7)
C9	-0.0644(5)	0.2394(5)	0.0161(3)	1.98(7)
C10	0.5080(5)	0.1673(5)	0.1338(3)	2.23(8)
C11	0.4097(6)	0.3184(6)	-0.1795(3)	2.82(9)
C12	0.1789(5)	0.6115(4)	0.4168(3)	2.02(7)
C13	0.0035(5)	0.5792(5)	0.3877(3)	2.24(8)
C14	-0.0367(5)	0.5399(5)	0.2791(3)	2.12(7)

Table S2. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	*x*	*y*	*z*	B_{eq}
C15	0.1182(5)	0.5512(4)	0.2410(3)	1.85(7)
C16	0.2513(5)	0.5951(4)	0.3265(3)	1.78(7)
C17	0.2472(6)	-0.0451(5)	0.3081(3)	2.57(9)
C18	0.1057(5)	-0.0148(5)	0.3487(3)	2.23(8)
C19	0.1618(6)	0.0908(5)	0.4504(3)	2.61(9)
C20	0.3391(6)	0.1280(6)	0.4723(3)	3.04(9)
C21	0.3924(5)	0.0437(6)	0.3839(4)	3.1(1)
H1	0.171(6)	0.330(6)	0.396(4)	3.4(8)
H2	0.020(6)	0.045(6)	0.157(3)	3.0(8)
H3	0.1088	0.3045	-0.1214	2.2
H4	0.5549	0.2430	-0.0282	2.3
H5	-0.0854	0.3368	0.0152	2.4
H6	-0.1342	0.1537	-0.0424	2.4
H7	-0.0909	0.2193	0.0768	2.4
H8	0.4599	0.1499	0.1902	2.7
H9	0.5274	0.0716	0.0937	2.7
H10	0.6137	0.2502	0.1591	2.7
H11	0.4355	0.2276	-0.2205	3.4
H12	0.3271	0.3432	-0.2186	3.4
H13	0.5107	0.4081	-0.1563	3.4
H14	0.2392	0.6392	0.4852	2.4
H15	-0.0769	0.5828	0.4333	2.6
H16	-0.1463	0.5124	0.2385	2.5
H17	0.1296	0.5321	0.1707	2.2
H18	0.3684	0.6108	0.3238	2.2
H19	0.2452	-0.1136	0.2402	3.0
H20	-0.0101	-0.0605	0.3132	2.7
H21	0.0919	0.1302	0.4954	3.1
H22	0.4125	0.1984	0.5359	3.7
H23	0.5061	0.0480	0.3780	3.7

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S3. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.0173(3)	0.0151(3)	0.0171(3)	0.0056(2)	0.0062(2)	0.0064(2)
Fe2	0.0171(3)	0.0161(3)	0.0177(3)	0.0047(2)	0.0044(2)	0.0079(2)
P	0.0163(4)	0.0150(4)	0.0157(4)	0.0040(3)	0.0044(3)	0.0049(3)
O1	0.025(1)	0.035(2)	0.050(2)	0.006(1)	0.013(1)	0.019(1)
O2	0.025(1)	0.028(2)	0.040(2)	0.000(1)	0.001(1)	0.013(1)
C1	0.021(2)	0.024(2)	0.026(2)	0.010(1)	0.009(1)	0.009(1)
C2	0.022(2)	0.023(2)	0.024(2)	0.007(1)	0.004(1)	0.010(1)
C3	0.019(2)	0.016(2)	0.018(2)	0.004(1)	0.006(1)	0.005(1)
C4	0.021(2)	0.019(2)	0.016(2)	0.004(1)	0.004(1)	0.005(1)
C5	0.025(2)	0.026(2)	0.020(2)	0.009(1)	0.006(1)	0.010(1)
C6	0.028(2)	0.025(2)	0.025(2)	0.008(2)	0.013(1)	0.012(1)
C7	0.020(2)	0.030(2)	0.024(2)	0.008(2)	0.009(1)	0.005(1)
C8	0.019(2)	0.020(2)	0.024(2)	0.005(1)	0.008(1)	0.005(1)
C9	0.021(2)	0.035(2)	0.020(2)	0.009(2)	0.002(1)	0.008(1)
C10	0.025(2)	0.038(2)	0.029(2)	0.017(2)	0.008(2)	0.015(2)
C11	0.040(2)	0.042(2)	0.037(2)	0.017(2)	0.023(2)	0.022(2)
C12	0.039(2)	0.016(2)	0.021(2)	0.007(2)	0.006(2)	0.007(1)
C13	0.036(2)	0.018(2)	0.038(2)	0.014(2)	0.019(2)	0.011(2)
C14	0.026(2)	0.020(2)	0.037(2)	0.009(1)	0.001(2)	0.012(2)
C15	0.034(2)	0.017(2)	0.025(2)	0.009(1)	0.009(1)	0.012(1)
C16	0.027(2)	0.014(2)	0.027(2)	0.004(1)	0.007(1)	0.008(1)
C17	0.053(3)	0.019(2)	0.035(2)	0.016(2)	0.018(2)	0.015(2)
C18	0.023(2)	0.021(2)	0.041(2)	-0.001(1)	0.001(2)	0.017(2)
C19	0.047(2)	0.029(2)	0.035(2)	0.015(2)	0.025(2)	0.020(2)
C20	0.049(3)	0.036(2)	0.029(2)	0.001(2)	-0.008(2)	0.025(2)
C21	0.029(2)	0.038(2)	0.071(3)	0.016(2)	0.016(2)	0.042(2)

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S4. Bond Lengths (Å)

atom	atom	distance		atom	atom	distance
FE1	FE2	2.6968(6)		FE1	P	2.1897(9)
FE1	C1	1.748(4)		FE1	C12	2.113(4)
FE1	C13	2.100(4)		FE1	C14	2.076(4)
FE1	C15	2.094(3)		FE1	C16	2.112(4)
FE2	P	2.1827(9)		FE2	O2	2.907(3)
FE2	C1	3.258(3)		FE2	C2	1.748(4)
FE2	C17	2.077(4)		FE2	C18	2.087(4)
FE2	C19	2.120(4)		FE2	C20	2.102(4)
FE2	C21	2.080(4)		P	C3	1.847(3)
O1	C1	1.146(5)		O2	C2	1.160(5)
C3	C4	1.417(5)	C3	C8	1.414(4)	
C4	C5	1.390(4)		C4	C9	1.525(5)
C5	C6	1.396(5)		C6	C7	1.389(5)
C6	C11	1.514(5)		C7	C8	1.392(5)
C8	C10	1.502(5)		C12	C13	1.405(6)
C12	C14	2.296(5)		C12	C15	2.306(5)
C12	C16	1.427(5)		C13	C14	1.422(6)
C14	C15	1.432(5)		C15	C1	1.423(5)
C17	C18	1.409(6)		C17	C21	1.403(7)
C18	C19	1.406(6)		C19	C20	1.406(6)
C20	C21	1.421(7)				
FE1	H1	1.58(5)		FE2	H1	1.66(5)
P	H2	1.38(5)		C5	H3	0.95
C7	H4	0.96		C9	H5	0.95
C9	H6	0.95		C9	H7	0.95
C10	H8	0.95		C10	H9	0.95
C10	H10	0.96		C11	H11	0.95
C11	H12	0.95		C11	H13	0.96
C12	H14	0.96		C13	H15	0.96
C14	H16	0.95		C15	H17	0.96
C16	H18	0.95		C17	H19	0.96
C18	H20	0.96		C19	H21	0.95
C20	H22	0.96		C21	H23	0.95

Table S5. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
FE2	FE1	P	51.80(3)	FE2	FE1	O1	91.31(6)
FE2	FE1	C12	108.3(1)	FE2	FE1	C13	141.1(1)
FE2	FE1	C14	168.4(1)	FE2	FE1	C15	128.6(1)
FE2	FE1	C16	102.46(10)	P	FE1	C1	89.9(1)
P	FE1	C12	140.5(1)	P	FE1	C13	164.2(1)
P	FE1	C14	125.3(1)	P	FE1	C15	98.20(10)
P	FE1	C16	105.58(10)	C1	FE1	C12	127.6(2)
C1	FE1	C13	97.6(2)	C1	FE1	C14	99.6(2)
C1	FE1	C15	133.6(2)	C1	FE1	C16	163.4(1)
C12	FE1	C13	38.9(2)	C12	FE1	C14	66.5(2)
C12	FE1	C15	66.5(1)	C12	FE1	C16	39.5(1)
C13	FE1	C14	39.8(2)	C13	FE1	C15	66.6(1)
C13	FE1	C16	66.0(1)	C14	FE1	C15	40.2(1)
C14	FE1	C16	66.7(1)	C15	FE1	C16	39.5(1)
FE1	FE2	P	52.04(2)	FE1	FE2	C2	91.7(1)
FE1	FE2	C17	136.1(1)	FE1	FE2	C18	105.4(1)
FE1	FE2	C19	104.6(1)	FE1	FE2	C20	133.7(1)
FE1	FE2	C21	170.5(1)	P	FE2	C2	97.4(1)
P	FE2	C17	97.8(1)	P	FE2	C18	96.0(1)
P	FE2	C19	127.1(1)	P	FE2	C20	161.2(1)
P	FE2	C21	131.2(2)	C2	FE2	C17	126.8(2)
C2	FE2	C18	162.5(2)	C2	FE2	C19	133.5(2)
C2	FE2	C20	100.1(2)	C2	FE2	C21	96.5(2)
C17	FE2	C18	39.6(2)	C17	FE2	C19	66.0(2)
C17	FE2	C20	66.0(2)	C17	FE2	C21	39.4(2)
C18	FE2	C19	39.0(2)	C18	FE2	C20	65.5(2)
C18	FE2	C21	66.2(2)	C19	FE2	C20	38.9(2)
C19	FE2	C21	66.1(2)	C20	FE2	C21	39.7(2)
FE1	P	FE2	76.16(3)	FE1	P	C3	122.7(1)
FE2	P	C3	131.3(1)	FE1	C1	O1	178.9(3)
FE2	C2	O2	177.3(3)	P	C3	C4	118.2(2)
P	C3	C8	122.9(3)	C4	C3	C8	118.8(3)
C3	C4	C5	120.1(3)	C3	C4	C5	122.3(3)
C5	C4	C9	117.4(3)	C4	C5	C6	121.5(3)
C5	C6	C7	117.6(3)	C5	C6	C11	121.3(3)
C7	C6	C11	121.0(3)	C6	C7	C8	123.1(3)
C3	C8	C7	118.7(3)	C3	C8	C10	124.6(3)
C7	C8	C10	116.7(3)	FE1	C12	C13	70.0(2)
FE1	C12	C16	70.2(2)	C13	C12	C16	108.1(3)
FE1	C13	C12	71.1(2)	FE1	C13	C14	69.2(2)
C12	C13	C14	108.6(3)	FE1	C14	C13	71.0(2)
FE1	C14	C15	70.6(2)	C13	C14	C15	107.6(3)
FE1	C15	C14	69.3(2)	FE1	C15	C16	70.9(2)
C14	C15	C16	107.6(3)	FE1	C16	C12	70.3(2)
FE1	C16	C15	69.6(2)	C12	C16	C15	108.0(3)
FE2	C17	C18	70.6(2)	FE2	C17	C21	70.4(2)
C18	C17	C21	108.1(4)	FE2	C18	C17	69.8(2)
FE2	C18	C19	71.8(2)	C17	C18	C19	108.6(4)
FE2	C19	C18	69.2(2)	FE2	C19	C20	69.8(2)
C18	C19	C20	107.5(3)	FE2	C20	C19	71.2(2)

Table S5. Bond Angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
FE2	C20	C21	69.3(2)	C19	C20	C21	108.3(4)
FE2	C21	C17	70.1(2)	FE2	C21	C20	71.0(2)
C17	C21	C20	107.5(4)				
FE2	FE1	H1	34(1)	P	FE1	H1	86(1)
C1	FE1	H1	87(1)	C12	FE1	H1	83(1)
C13	FE1	H1	107(1)	C14	FE1	H1	147(1)
C15	FE1	H1	137(1)	C16	FE1	H1	98(1)
FE1	FE2	H1	32(1)	P	FE2	H1	84(1)
C2	FE2	H1	91(1)	C17	FE2	H1	140(1)
C18	FE2	H1	101(1)	C19	FE2	H1	81(1)
C20	FE2	H1	101(1)	C21	FE2	H1	141(1)
FE1	P	H2	115(1)	FE2	P	H2	107(1)
C3	P	H2	102(1)	C4	C5	H3	119.3
C6	C5	H3	119.2	C6	C7	H4	118.5
C8	H7	H4	118.4	C4	C9	H5	109.6
C4	C9	H6	109.4	C4	C9	H7	110.1
H5	C9	H6	108.9	H5	C9	H7	109.5
H6	C9	H7	109.4	C8	C10	H8	109.8
C8	C10	H9	109.7	C8	C10	H10	109.7
H8	C10	H9	109.5	H8	C10	H10	109.1
H9	C10	H10	108.9	C6	C11	H11	109.7
C6	C11	H12	109.9	C6	C11	H13	109.2
H11	C11	H12	110.1	H11	C11	H13	108.9
H12	C11	H13	108.9	FE1	C12	H14	125.3
C13	C12	H14	126.0	C16	C12	H14	125.9
FE1	C13	H15	125.6	C12	C13	H15	126.0
C14	C13	H15	125.4	FE1	C14	H16	124.5
C13	C14	H16	126.8	C15	C14	H16	125.6
FE1	C15	H17	125.0	C14	C15	H17	126.0
C16	C15	H17	126.4	FE1	C16	H18	125.7
C12	C16	H18	126.0	C15	C16	H18	126.0
FE2	C17	H19	124.2	C18	C17	H19	126.1
C21	C17	H19	125.8	FE2	C18	H20	125.1
C17	C18	H20	125.7	C19	C18	H20	125.7
FE2	C19	H21	125.8	C18	C19	H21	125.8
C20	C19	H21	126.8	FE2	C20	H22	125.0
C19	C20	H22	126.3	C21	C20	H22	125.4
FE2	C21	H23	124.1	C17	C21	H23	126.9
C20	C21	H23	125.6				

Table S6. Crystal data of $[Cp_2Fe_2(CO)_2(\mu\text{-}CO)(\mu\text{-}(E)\text{-}PPhCH{=}CHPh)]OTf$ (**3a**)

formula	$C_{28}H_{22}F_3Fe_2O_6PS$
fw	686.19
cryst system	monoclinic
space group	$P2_1/n$
syst absence	$h\,0\,l : h + l = 2n + 1$
	$0\,k\,0 : k = 2n + 1$
	$h\,0\,0 : h = 2n + 1$
	$0\,0\,l : l = 2n + 1$
	a = 15.255(2) Å
	b = 13.4334(11) Å
	c = 14.402(2) Å
	β = 106.99(2) °
	V = 2822.8(6) Å^3
Z value	4
$d$calcd / gcm^{-1}	1.615
μ(Mo Kα) / cm^{-1}	21.9
cryst size / mm	0.45 x 0.30 x 0.10
radiation	Mo Ka (λ = 0.71073)
monochromator	graphite
temp / °C	20
reflcn measd	h, k, l
2θ range / deg	3 - 55
scan mode	2θ - ω
ω - scan width / deg	1.2 + 0.35 tanθ
bkgd(count time) / s	4.0
ω - scan rate / deg min^{-1}	4.0
Index ranges	$-19 \le h \le 18$, $0 \le k \le 17$, $0 \le l \le 17$
Reflections collected	6519
Independent reflections	6427 [R(int) = 0.5490]
Refinement method	Full-matrix least-squares on $F2$
Data / restraints / parameters	6426 / 0 / 458
Goodness-of-fit on F^2	1.042
Final R indices [$I > 2\sigma(I)$]	$R1$[a] = 0.0545, $\omega R2$[b] = 0.1168
R indices (all data)	$R1$[a] = 0.1276, $\omega R2$[b] = 0.1484
Largest diff. peak and hole	0.571 and -0.448 e^{-3}

[a] $R1 = \Sigma||Fo| - |Fc|| / \Sigma|Fo|$.
[b] $\omega R2 = [\Sigma[\omega(Fo^2 - Fc^2)^2] / \Sigma[\omega(Fo^2)^2]]^{0.5}$,
calc $\omega = 1/[\sigma^2 (Fo^2)+(0.0628P)^2+0.4253P]$ where $P = (Fo^2+2Fc^2)/3$.

Table S7. Atomic coordinates and U_{eq}

atom	*x*	*y*	*z*	*U(eq)*
Fe1	0.1424(1)	0.1080(1)	0.3723(1)	0.037(1)
Fe2	0.0202(1)	-0.0128(1)	0.2635(1)	0.041(1)
P	0.0335(1)	0.1468(1)	0.2399(1)	0.037(1)
O1	0.1193(3)	-0.0849(3)	0.4556(3)	0.068(1)
O2	0.0486(3)	0.1897(3)	0.5040(3)	0.071(1)
O3	-0.1292(3)	0.0140(3)	0.3477(3)	0.072(1)
C1	0.1023(3)	-0.0248(4)	0.3954(4)	0.047(1)
C2	0.0818(3)	0.1562(4)	0.4497(4)	0.046(1)
C3	-0.0703(4)	0.0061(4)	0.3151(4)	0.050(1)
C4	-0.0605(3)	0.2270(4)	0.2432(3)	0.043(1)
C5	-0.0439(4)	0.3165(4)	0.2941(4)	0.056(1)
C6	-0.1153(7)	0.3749(7)	0.2989(6)	0.084(3)
C7	-0.2046(7)	0.3472(8)	0.2518(7)	0.101(3)
C8	-0.2218(5)	0.2598(9)	0.2004(7)	0.092(3)
C9	-0.1499(4)	0.1995(6)	0.1949(5)	0.063(2)
C10	0.0684(3)	0.1894(4)	0.1385(3)	0.041(1)
C11	0.0359(3)	0.2690(4)	0.0848(3)	0.042(1)
C12	0.0687(3)	0.3113(3)	0.0077(3)	0.039(1)
C13	0.1521(4)	0.2844(4)	-0.0061(4)	0.045(1)
C14	0.1805(4)	0.3268(4)	-0.0791(4)	0.053(1)
C15	0.1267(5)	0.3958(4)	-0.1419(4)	0.061(2)
C16	0.0454(5)	0.4226(5)	-0.1292(4)	0.066(2)
C17	0.0158(4)	0.3817(4)	-0.0549(4)	0.054(1)
C18	0.2713(3)	0.1045(5)	0.4758(5)	0.058(2)
C19	0.2512(4)	0.2019(5)	0.4381(4)	0.056(1)
C20	0.2410(4)	0.1986(5)	0.3389(5)	0.057(2)
C21	0.2535(4)	0.1013(5)	0.3134(5)	0.062(2)
C22	0.2729(4)	0.0431(5)	0. 3986(5)	0.058(2)
C23	-0.0655(5)	-0.1044(6)	0.1588(5)	0.076(2)
C24	-0.0088(6)	-0.1621(5)	0.2285(5)	0.073(2)
C25	0.0820(6)	-0.1447(6)	0.2328(6)	0.079(2)
C26	0.0769(7)	-0.0690(6)	0.1592(7)	0.086(3)
C27	-0.0145(6)	-0.0492(6)	0.1150(5)	0.077(2)
S	0.2978(1)	-0.0074(1)	0.0615(1)	0.068(1)
F1	0.3850(5)	0.1394(5)	0.1556(4)	0.171(3)
F2	0.3612(3)	0.1557(4)	0.0079(4)	0.122(2)
F3	0.4618(3)	0.0588(5)	0.0835(6)	0.190(3)
O4	0.2175(3)	0.0441(4)	0.0593(4)	0.099(2)
O5	0.3299(4)	-0.0664(4)	0.1495(5)	0.127(2)
O6	0.3001(6)	-0.0522(6)	-0.0232(6)	0.197(4)
C28	0.3820(5)	0.0898(6)	0.0767(6)	0.081(2)

Table S8. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.034(1)	0.036(1)	0.038(1)	0.003(1)	0.006(1)	-0.004(1)
Fe2	0.048(1)	0.037(1)	0.037(1)	-0.002(1)	0.011(1)	-0.009(1)
P	0.037(1)	0.038(1)	0.035(1)	0.003(1)	0.009(1)	-0.002(1)
O1	0.076(3)	0.056(2)	0.060(2)	0.027(2)	0.001(2)	-0.012(2)
O2	0.075(3)	0.087(3)	0.059(2)	-0.011(2)	0.032(2)	-0.003(2)
O3	0.060(2)	0.093(3)	0.073(3)	-0.009(2)	0.034(2)	-0.020(2)
C1	0.047(3)	0.044(3)	0.049(3)	0.005(2)	0.011(2)	-0.009(2)
C2	0.045(3)	0.046(3)	0.042(3)	0.002(2)	0.003(2)	-0.010(2)
C3	0.049(3)	0.054(3)	0.045(3)	-0.003(2)	0.010(2)	-0.017(3)
C4	0.031(2)	0.061(3)	0.036(2)	0.015(2)	0.009(2)	0.006(2)
C5	0.063(4)	0.050(3)	0.058(3)	0.009(3)	0.019(3)	0.012(3)
C6	0.111(7)	0.075(5)	0.082(5)	0.024(4)	0.050(5)	0.047(5)
C7	0.094(7)	0.122(8)	0.106(7)	0.065(6)	0.061(6)	0.071(6)
C8	0.044(4)	0.142(9)	0.087(5)	0.052(6)	0.016(4)	0.016(5)
C9	0.040(3)	0.087(5)	0.056(4)	0.022(4)	0.004(3)	0.007(3)
C10	0.041(3)	0.044(3)	0.040(3)	0.008(2)	0.013(2)	0.003(2)
C11	0.043(3)	0.046(3)	0.039(3)	0.003(2)	0.013(2)	0.003(2)
C12	0.044(3)	0.037(3)	0.035(2)	0.003(2)	0.008(2)	-0.006(2)
C13	0.053(3)	0.037(3)	0.043(3)	-0.002(2)	0.013(2)	-0.005(2)
C14	0.064(4)	0.048(3)	0.050(3)	-0.006(3)	0.022(3)	-0.011(3)
C15	0.090(5)	0.053(3)	0.042(3)	-0.001(3)	0.024(3)	-0.022(3)
C16	0.087(5)	0.055(4)	0.048(3)	0.020(3)	0.007(3)	-0.003(3)
C17	0.055(3)	0.051(3)	0.053(3)	0.012(3)	0.010(3)	0.005(3)
C18	0.038(3)	0.072(4)	0.057(4)	0.012(3)	0.002(2)	-0.005(3)
C19	0.039(3)	0.054(3)	0.065(4)	-0.004(3)	0.002(3)	-0.011(2)
C20	0.041(3)	0.049(4)	0.076(4)	0.016(3)	0.010(3)	-0.013(3)
C21	0.038(3)	0.090(5)	0.062(4)	-0.009(4)	0.023(3)	-0.015(3)
C22	0.036(3)	0.050(4)	0.080(4)	0.007(3)	0.006(3)	0.003(2)
C22	0.036(3)	0.050(4)	0.080(4)	0.007(3)	0.006(3)	0.003(2)
C23	0.079(5)	0.074(5)	0.067(4)	-0.029(4)	0.006(4)	-0.020(4)
C24	0.102(6)	0.046(4)	0.076(5)	-0.020(3)	0.034(4)	-0.026(4)
C25	0.088(6)	0.053(4)	0.091(6)	-0.027(4)	0.018(5)	0.010(4)
C26	0.117(7)	0.066(5)	0.108(6)	-0.047(5)	0.086(6)	-0.048(5)
C27	0.111(6)	0.074(5)	0.049(4)	-0.017(3)	0.026(4)	-0.015(4)
S	0.060(1)	0.055(1)	0.091(1)	-0.015(1)	0.024(1)	-0.002(1)
F1	0.247(7)	0.159(5)	0.104(4)	-0.050(4)	0.046(4)	-0.122(5)
F2	0.136(4)	0.124(4)	0.113(4)	0.045(3)	0.047(3)	-0.013(3)
F3	0.057(3)	0.154(5)	0.356(10)	0.042(6)	0.055(4)	-0.006(3)
O4	0.063(3)	0.104(4)	0.138(5)	0.039(3)	0.043(3)	0.020(3)
O5	0.107(4)	0.083(4)	0.179(6)	0.057(4)	0.020(4)	0.007(3)
O6	0.215(8)	0.215(8)	0.212(8)	-0.160(7)	0.143(7)	-0.118(7)
C28	0.081(5)	0.081(5)	0.079(5)	-0.002(4)	0.017(4)	-0.013(4)

Table S9. Bond Lengths (Å)

atom	atom	distance	atom	atom	distance
FE1	C2	1.767(6)	FE1	C1	1.946(5)
FE1	C19	2.081(5)	FE1	C18	2.094(5)
FE1	C20	2.098(5)	FE1	C22	2.105(5)
FE1	C21	2.108(6)	FE1	P	2.1947(14)
FE1	FE2	2.6175(10)	FE2	C3	1.767(6)
FE2	C1	1.953(5)	FE2	C26	2.082(7)
FE2	C24	2.084(6)	FE2	C23	2.085(6)
FE2	C27	2.105(6)	FE2	C25	2.113(7)
FE2	P	2.1891(14)	P	C10	1.788(5)
P	C4	1.805(5)	O1	C1	1.157(6)
O2	C2	1.140(6)	O3	C3	1.135(6)
C4	C9	1.387(7)	C4	C5	1.392(8)
C5	C6	1.361(9)	C6	C7	1.383(13)
C7	C8	1.372(13)	C8	C9	1.383(11)
C10	C11	1.328(7)	C11	C12	1.459(6)
C12	C17	1.391(7)	C12	C13	1.391(7)
C13	C14	1.373(7)	C14	C15	1.385(8)
C15	C16	1.354(9)	C16	C17	1.390(8)
C18	C22	1.391(9)	C18	C19	1.415(8)
C19	C20	1.392(8)	C20	C21	1.386(9)
C21	C22	1.411(9)	C23	C27	1.356(10)
C23	C24	1.361(10)	C24	C25	1.388(11)
C25	C26	1.455(12)	C26	C27	1.380(12)
S	O6	1.370(6)	S	O4	1.399(5)
S	O5	1.454(6)	S	C28	1.800(7)
F1	C28	1.306(8)	F2	C28	1.298(8)
F3	C28	1.263(8)			

Table S10. Bond Angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C2	FE1	C1	88.9(2)	C2	FE1	C19	89.1(2)
C1	FE1	C19	136.6(2)	C2	FE1	C18	96.6(2)
C1	FE1	C18	97.8(2)	C19	FE1	C18	39.6(2)
C2	FE1	C20	118.3(2)	C1	FE1	C20	148.6(2)
C19	FE1	C20	38.9(2)	C18	FE1	C20	65.7(2)
C2	FE1	C22	132.9(2)	C1	FE1	C22	85.3(2)
C19	FE1	C22	65.3(2)	C18	FE1	C22	38.7(2)
C20	FE1	C22	65.0(2)	C2	FE1	C21	154.2(2)
C1	FE1	C21	111.1(3)	C19	FE1	C21	65.2(3)
C18	FE1	C21	65.6(3)	C20	FE1	C21	38.5(2)
C22	FE1	C21	39.2(2)	C2	FE1	P	93.4(2)
C1	FE1	P	99.8(2)	C19	FE1	P	123.5(2)
C18	FE1	P	159.9(2)	C20	FE1	P	94.3(2)
C22	FE1	P	133.7(2)	C21	FE1	P	98.8(2)
C2	FE1	FE2	101.2(2)	C1	FE1	FE2	47.9(2)
C19	FE1	FE2	169.2(2)	C18	FE1	FE2	140.3(2)
C20	FE1	FE2	130.9(2)	C22	FE1	FE2	108.8(2)
C21	FE1	FE2	104.3(2)	P	FE1	FE2	53.24(4)
C3	FE2	C1	87.7(2)	C3	FE2	C26	153.6(3)
C1	FE2	C26	112.9(4)	C3	FE2	C24	95.9(3)
C1	FE2	C24	100.7(3)	C26	FE2	C24	65.2(3)
C3	FE2	C23	89.2(3)	C1	FE2	C23	138.0(3)
C26	FE2	C23	64.5(3)	C24	FE2	C23	38.1(3)
C3	FE2	C27	117.7(3)	C1	FE2	C27	150.3(3)
C26	FE2	C27	38.5(3)	C24	FE2	C27	63.8(3)
C23	FE2	C27	37.8(3)	C3	FE2	C25	131.2(3)
C1	FE2	C25	86.3(3)	C26	FE2	C25	40.6(3)
C24	FE2	C25	38.6(3)	C23	FE2	C25	65.0(3)
C27	FE2	C25	65.7(3)	C3	FE2	P	92.5(2)
C1	FE2	P	99.8(2)	C26	FE2	P	99.6(2)
C24	FE2	P	158.1(2)	C23	FE2	P	122.2(2)
C27	FE2	P	94.4(2)	C25	FE2	P	136.2(3)
C3	FE2	FE1	99.6(2)	C1	FE2	FE1	47.7(2)
C26	FE2	FE1	106.5(2)	C24	FE2	FE1	143.6(2)
C23	FE2	FE1	170.1(2)	C27	FE2	FE1	132.6(2)
C25	FE2	FE1	111.2(2)	P	FE2	FE1	53.44(4)
C10	P	C4	105.0(2)	C10	P	FE2	120.2(2)
C4	P	FE2	118.0(2)	C10	P	FE1	117.1(2)
C4	P	FE1	121.6(2)	FE2	P	FE1	73.32(5)
O1	C1	FE1	139.0(4)	O1	C1	FE2	136.6(4)
FE1	C1	FE2	84.4(2)	O2	C2	FE1	175.1(4)
O3	C3	FE2	177.1(5)	C9	C4	C5	119.6(5)

Table S10. Bond Angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C9	C4	P	120.1(5)	C5	C4	P	120.3(4)
C6	C5	C4	119.9(7)	C5	C6	C7	120.5(9)
C8	C7	C6	120.0(7)	C7	C8	C9	120.1(8)
C8	C9	C4	119.7(8)	C11	C10	P	125.8(4)
C10	C11	C12	127.2(5)	C17	C12	C13	117.7(5)
C17	C12	C11	119.7(5)	C13	C12	C11	122.6(4)
C14	C13	C12	120.6(5)	C13	C14	C15	121.2(6)
C16	C15	C14	118.8(5)	C15	C16	C17	121.0(6)
C12	C17	C16	120.7(6)	C22	C18	C19	107.1(6)
C22	C18	FE1	71.1(3)	C19	C18	FE1	69.7(3)
C20	C19	C18	108.1(6)	C20	C19	FE1	71.2(3)
C18	C19	FE1	70.7(3)	C21	C20	C19	108.6(6)
C21	C20	FE1	71.1(3)	C19	C20	FE1	69.9(3)
C20	C21	C22	107.6(6)	C20	C21	FE1	70.4(3)
C22	C21	FE1	70.3(3)	C18	C22	C21	108.6(6)
C18	C22	FE1	70.2(3)	C21	C22	FE1	70.5(3)
C27	C23	C24	109.1(7)	C27	C23	FE2	71.9(4)
C24	C23	FE2	70.9(4)	C23	C24	C25	110.3(7)
C23	C24	FE2	71.0(4)	C25	C24	FE2	71.8(4)
C24	C25	C26	104.3(8)	C24	C25	FE2	69.6(4)
C26	C25	FE2	68.6(4)	C27	C26	C25	107.6(7)
C27	C26	FE2	71.7(4)	C25	C26	FE2	70.9(4)
C23	C27	C26	108.7(7)	C23	C27	FE2	70.3(4)
C26	C27	FE2	69.8(4)	O6	S	O4	116.6(5)
O6	S	O5	116.6(5)	O4	S	O5	111.1(4)
O6	S	C28	102.9(4)	O4	S	C28	103.5(4)
O5	S	C28	104.0(4)	F3	C28	F2	107.4(7)
F3	C28	F1	108.3(8)	F2	C28	F1	104.8(7)
F3	C28	S	114.0(6)	F2	C28	S	113.3(5)
F1	C28	S	108.6(5)				