ELECTRONIC SUPPLEMENTARY INFORMATION

A tetradentate metalloligand: Synthesis and coordination behaviour of a 2-pyridyl-substituted cyclobutadiene iron complex

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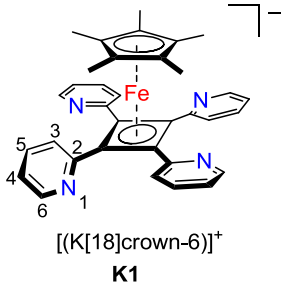
1. Full experimental details, synthesis of and spectroscopic characterisation of complexes K1 and 1–4

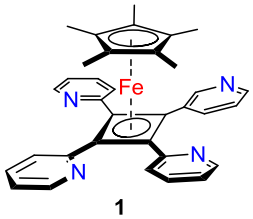
General considerations: All experiments were performed under an atmosphere of dry argon, by using standard Schlenk and glovebox techniques. Solvents were purified, dried, and degassed with an MBraun SPS800 solvent purification system. NMR spectra were recorded on Bruker Avance 300 and Avance 400 spectrometers at 300 K and internally referenced to residual solvent resonances. The assignment of the ^{1}H and ^{13}C NMR signals was confirmed by two-dimensional (COSY, HSQC, and HMBC) experiments. Melting points were measured on samples in sealed capillaries on a Stuart SMP10 melting point apparatus. UV/Vis spectra were recorded on a Varian Cary 50 spectrometer. Elemental analyses were determined by the analytical department of Regensburg University. The starting materials $FeCl_2(thf)_{1.5}$,[S1] [CuBr(tht)],[S2] [K([18]crown-6)][Cp*Fe($C_{10}H_8$)][S3] and bis(2-pyridyl)acetylene[S4] were prepared according to literature procedures. $ZnCl_2$ was purchased from ABCR and used as received.

[K([18]crown-6){Cp*Fe(C_4py_4)}] (K1): A solution of bis(2-pyridyl)acetylene (0.108 g, 0.60 mmol) in THF (10 mL) at -30 °C was added to a solution of [K([18]crown-6){Cp*Fe($C_{10}H_8$)}] (0.187 g, 0.30 mmol) in THF (20 mL) at –60 °C. The reaction mixture was stirred overnight and warmed to room temperature. A dark solid precipitated which was separated by filtration. After removal of the solvent, the crude product was extracted with diethyl ether (150 mL). Dark purple **K1** precipitated after layering this solution with *n*-hexane at room temperature. The isolated solid contains one equivalent *n*-hexane per formula unit of **K1** according to ^{1}H NMR spectroscopy and microanalysis. X-ray quality crystals of **K1** were obtained by layering a concentrated toluene solution with *n*-hexane at room temperature. Yield: 85 mg (33%); m.p.: >225 °C; UV/Vis (THF): λ_{max} (nm, (ε_{max}/L·mol^{-1}·cm^{-1})): 333 (35488), 371sh (27321), 518 (5241); ^{1}H NMR (400.13 MHz, C_6D_6): δ = 1.69 (s, 15H, CH_3), 3.03 (s, 24H, CH_2 of [18]crown-6), 6.58 (m, 4H, H_4), 7.29 (m, 4H, H_5), 8.28 (m, 4H, H_3), 8.64 (m, 4H, H_6). $^{13}C\{^{1}H\}$ NMR (400.13 MHz, C_6D_6): δ = 9.9 (s, *C*H_3), 69.8 (s, *C*H_2 of [18]crown-6), 70.3 (s, *C*$_4$py$_4$), 80.8 (s, *C*$_5$(CH$_3$)$_5$), 114.1 (s, *CH*$_{pyridine}$), 126.3 (s, *CH*$_{pyridine}$), 132.6 (s, *CH*$_{pyridine}$), 147.3 (s, *CH*$_{pyridine}$), 168.9 (s, *ipso-C*$_{pyridine}$); Elemental analysis calcd. for $C_{52}H_{69}FeKN_4O_6{\cdot}C_6H_{14}$ (Mw = 941.09 g·mol^{-1}): C 66.37, H 7.39, N 5.95, found: C 66.18, H 6.72, N 5.94.



K1

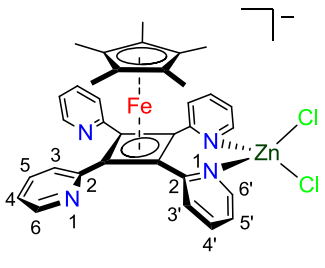
[Cp*Fe(C_4py_4)] (1): A suspension of [CuBr(tht)] (0.046 g, 0.20 mmol) in THF was added to a solution of **K1** (0.171 g, 0.20 mmol) in THF (50 mL). The color changed to brown and a black residue precipitated. The reaction mixture was stirred overnight and was filtered afterwards. The solution was removed *in vacuo*, and the crude product was extracted with benzene. Red brown crystals were isolated durig the diffusion of *n*-hexane into the benzene solution. Yield: 62 mg (56%); m.p.: >188 °C; UV/Vis (THF): λ_{max} (nm, (ε_{max}/L·mol^{-1}·cm^{-1})): 332 (36793),



1

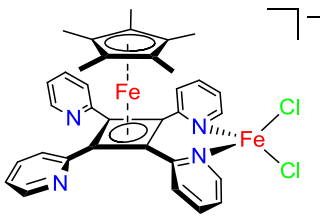
420sh (3592); Effective magnetic moment (Evans NMR Method, C_6D_6): μ_{eff} = 1.8(1) μ_B; Elemental analysis calcd. for $C_{34}H_{31}FeN_4$ (Mw = 551.49 g·mol^{-1}): C 74.05, H 5.67, N 10.16, found: C 74.24, H 5.29, N 10.30.

[K([18]crown-6){Cp*Fe(C_4py$_4$)}($ZnCl_2$)] (2): A solution of $ZnCl_2$ (0.020 g, 0.15 mmol) in THF (10 mL) was added to a solution of **K1** (0.128 g, 0.15 mmol) in THF (10 mL) at room temperature. The reaction mixture was stirred overnight and was filtered afterwards. Dark purple crystals were isolated after diffusion of diethyl ether (50 mL) into this solution. Yield: 96 mg (62%); m.p.: >260 °C; UV/Vis (THF): λ_{max} (nm, (ε_{max}/L·mol^{-1}·cm^{-1})): 327 (35658), 397sh (25066), 538 (6640); ^{1}H NMR (400.13 MHz, [D$_8$]THF): δ = 1.21 (s, 15H, C*H*$_3$), 3.55 (s, 24H, C*H*$_2$ of [18]crown-6), 6.53 (m, 2H, *H*$_5$), 6.83 (m, 2H, *H*$_{5'}$), 7.07 (m, 2H, *H*$_4$), 7.23 (m, 2H, *H*$_{4'}$), 7.51 (br d, *J* = 8.0 Hz, 2H, *H*$_3$), 7.74 (br d, *J* = 8.0 Hz, 2H, *H*$_{3'}$), 8.30-8.33 (overlapping m, 4H, *H*$_6$ and *H*$_{6'}$). ^{13}C{^{1}H} NMR (400.13 MHz, C_6D_6): δ = 8.9 (s, *C*H$_3$), 71.1 (s, *C*H$_2$ of [18]crown-6), 83.1 (s, *C*$_5$(CH$_3$)$_5$), 112.4 (s, *CH*$_{pyridine}$), 117.2 (s, *CH*$_{pyridine}$), 125.4 (br s, *CH*$_{pyridine}$), 134.2 (s, *CH*$_{pyridine}$), 148.0 (s, *CH*$_{pyridine}$), 148.8 (s, *CH*$_{pyridine}$), 166.6 (s, *CH*$_{pyridine}$), 169.0 (s, *CH*$_{pyridine}$), the signal for the carbons of the C_4py_4 moiety were not detected due to overlap with solvent; Elemental analysis calcd. for $C_{48}H_{61}Cl_2FeKN_4O_6Zn$ (Mw = 1021.26 g·mol^{-1}): C 55.74, H 5.59, N 5.65, found: C 56.02, H 5.59, N 5.73.



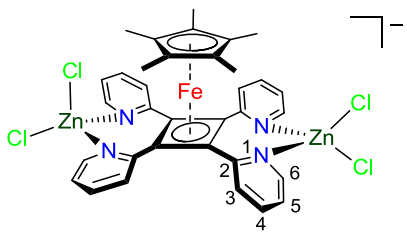
[(K[18]crown-6)]$^+$
2

[K([18]crown-6){Cp*Fe(C_4py$_4$)}($FeCl_2$)] (3): A suspension of $FeCl_2(thf)_{1.5}$ (0.030 g, 0.13 mmol) in THF (10 mL) was added to a solution of **K1** (0.111 g, 0.13 mmol) in THF (10 mL) at room temperature. The reaction mixture was stirred overnight and was filtered afterwards. Dark purple crystals were isolated by diffusion of *n*-hexane (50 mL) into this solution. Yield: 67 mg (52%); m.p.: >165 °C; UV/Vis (THF): λ_{max} (nm, (ε_{max}/L·mol^{-1}·cm^{-1})): 320 (32821), 402sh (16125), 532 (4593); Effective magnetic moment (Evans NMR Method, [D$_8$]THF): μ_{eff} = 4.1(1) μ_B; Elemental analysis calcd. for $C_{48}H_{61}Cl_2Fe_2KN_4O_6$ (Mw = 981.64 g·mol^{-1}): C 56.28, H 5.65, N 5.71, found: C 56.26, H 5.66, N 5.81.



[K[18]crown-6]$^+$
3

[K([18]crown-6)(thf)][Cp*Fe(C_4py$_4$)($ZnCl_2$)$_2$] (4): A solution of $ZnCl_2$ (0.031 g, 0.23 mmol) in THF (10 mL) was added to a solution of **K1** (0.094 g, 0.11 mmol) in THF (10 mL) at room temperature. The reaction mixture was stirred overnight. A purple microcrystalline solid precipitated after 15 min. Solid residue was isolated by filtration and dissolved in 20 mL THF/acetonitrile (10:1). Dark purple crystals of **4**·THF formed during the diffusion of diethyl ether (70 mL) into this solution. ^{1}H NMR spectroscopy and elemental analysis confirmed the presence of one THF solvate molecule per formula unit. Yield: 38 mg (28%); m.p.: >290 °C, decomposition to a black solid; UV/Vis (1,2-DFB): λ_{max} (nm, (ε_{max} /L·mol^{-1}·cm^{-1})): 391 (23006), 405sh (12644), 527



[K([18]crown-6)(thf)]$^+$
4

(3802); ^{1}H NMR (400.13 MHz, CD_3CN): δ = 1.22 (s, 15H, CH_3), 1.29 (m, 8H, THF), 3.57 (s, 24H, CH_2 of [18]crown-6), 3.62 (m, 8H, THF), 7.11 (t, *J* = 6.3 Hz, 4H, H_5), 7.20 (d, *J* = 8.3 Hz, 4H, H_3), 7.58 (t, *J* = 8.0 Hz, 4H, H_4), 8.53 (d, *J* = 4.9 Hz, 4H, H_6). $^{13}C\{^{1}H\}$ NMR (400.13 MHz, CD_3CN): δ = 10.3 (s, *C*H_3), 26.2 (s, THF), 62.2 (s, THF), 70.0 (s, *C*$_4$py$_4$), 70.9 (s, *C*H_2 of [18]crown-6), 84.0 (s, *C*$_5$(CH$_3$)$_5$), 118.5 (s, *CH*$_{pyridine}$), 127.1 (s, *CH*$_{pyridine}$), 138.4 (s, *CH*$_{pyridine}$), 149.2 (s, *CH*$_{pyridine}$), 165.9 (s, *ipso-C*$_{pyridine}$); Elemental analysis calcd. for $C_{48}H_{61}Cl_4FeKN_4O_6Zn_2 \cdot OC_4H_8$ (Mw = 1229.65): C 50.79, H 5.66, N 4.56, found: C 50.36, H 5.40, N 4.56.

Cyclic voltammetry:

Cyclic Voltammetry experiments were performed in an airtight single-compartment cell connected to a Metrohm Autolab PGSTAT101 potentiostat. The cell was equipped with a Pt disk working electrode that was polished with 0.25 µm diamond paste, a Pt coil counter eletrode and an Ag wire pseudoreference electrode. The solutions of the studied complexes were prepared under an argon atmosphere in dry acetonitrile. The supporting electrolyte, tetrabutylammonium hexafluorophosphate, was predried in vacuo at 110 °C. All redox potentials are reported versus the ferrocene / ferrocenium (Fc/Fc^+) couple used as an internal standard.

X-ray crystallography:

Crystals were mounted in paratone oil and transferred to the cold N_2 gas stream of an Agilent Technologies SuperNova diffractometer with Cu/Ka radiation (λ = 1.54178 Å). Semi-empirical multi-scan absorption corrections were applied to the data. The structures were solved by direct methods using SHELXS or SIR. Least-square refinements were performed on F^2.[S5,S6]

Table S1. Crystal and structure refinement data for **K1** and **1**–**4**

Identification code	**K1**	**1**	**2**	**3**	**4**
Empirical formula	$C_{46}H_{55}FeKN_4O_6$	$C_{34}H_{31}FeN_4$	$C_{46}H_{55}Cl_2FeKN_4O_6Zn$	$C_{46}H_{55}Cl_2Fe_2KN_4O_6$	$C_{54}H_{71}Cl_4FeKN_4O_8Zn_2$
Formula weight	854.89	551.49	991.16	981.64	1271.64
Temperature/K	123(2) K	123(2)	123(2)	123(2)	123(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/c$	$P2_1/c$	$P2_1/m$
a/Å	10.8231(2)	13.6884(2)	16.4571(2)	16.4365(9)	13.8686(8)
b/Å	21.9105(2)	14.1246(2)	16.5968(2)	16.5146(8)	14.3500(5)
c/Å	20.3007(1)	15.0838(2)	17.0934(2)	17.1501(8)	16.1195(7)
α/°	90.00	90.00	90.00	90.00	90.00
β/°	98.027(1)	113.276(1)	94.918(1)	95.109(5)	114.168(6)
γ/°	90.00	90.00	90.00	90.00	90.00
Volume/Å^3	4766.9(1)	2679(1)	4651.6(1)	4636.8(4)	2926.8(2)
Z	4	4	4	4	2
ρ_{calc}mg/mm^3	1.191	1.367	1.415	1.406	1.443
μ/mm^{-1}	3.699	4.743	5.405	7.295	5.669
F(000)	1808.0	1156.0	2064.0	2048.0	1320.0
Crystal size/mm^3	0.49 × 0.3553 × 0.3271	0.335 × 0.174 × 0.102	0.232 × 0.159 × 0.078	0.38 × 0.143 × 0.039	0.191 × 0.098 × 0.026
2Θ range for data collection	5.96 to 153.44°	7.4 to 147.36°	7.44 to 147.58°	7.44 to 148.36°	17.78 to 133.18°
Index ranges	-13 ≤ h ≤ 13, -27 ≤ k ≤ 27, -25 ≤ l ≤ 25	-16 ≤ h ≤ 15, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18	-20 ≤ h ≤ 20, -17 ≤ k ≤ 20, -21 ≤ l ≤ 20	–20 ≤ h ≤ 19, -18 ≤ k ≤ 20, -21 ≤ l ≤ 21	-14 ≤ h ≤ 16, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19
Reflections collected	96550	14409	27914	19283	15832
Independent reflections	9864 [R(int) = 0.0389]	5200 [R(int) = 0.0238]	9169 [R(int) = 0.0351]	9059 [R(int) = 0.0384]	5331 [R(int) = 0.0517]
Data/restraints/parameters	9864/18/569	5200/0/352	9169/0/551	9059/0/550	5331/25/366
Goodness-of-fit on F^2	1.042	1.043	1.041	1.027	1.018
Final R indexes [I>2σ (I)]	R_1 = 0.0756, wR_2 = 0.2153	R_1 = 0.0341, wR_2 = 0.0959	R_1 = 0.0336, wR_2 = 0.0857	R_1 = 0.0419, wR_2 = 0.1053	R_1 = 0.0654, wR_2 = 0.1678
Final R indexes [all data]	R_1 = 0.0771, wR_2 = 0.2174	R_1 = 0.0359, wR_2 = 0.0976	R_1 = 0.0407, wR_2 = 0.0911	R_1 = 0.0533, wR_2 = 0.1146	R_1 = 0.0883, wR_2 = 0.1864
Largest diff. peak/hole / e Å^{-3}	1.05/–0.56	0.39/–0.39	0.61/–0.39	0.42/–0.48	1.91/–0.55

2. UV-vis spectra of complexes K1 and 1–4 (Figure S1)

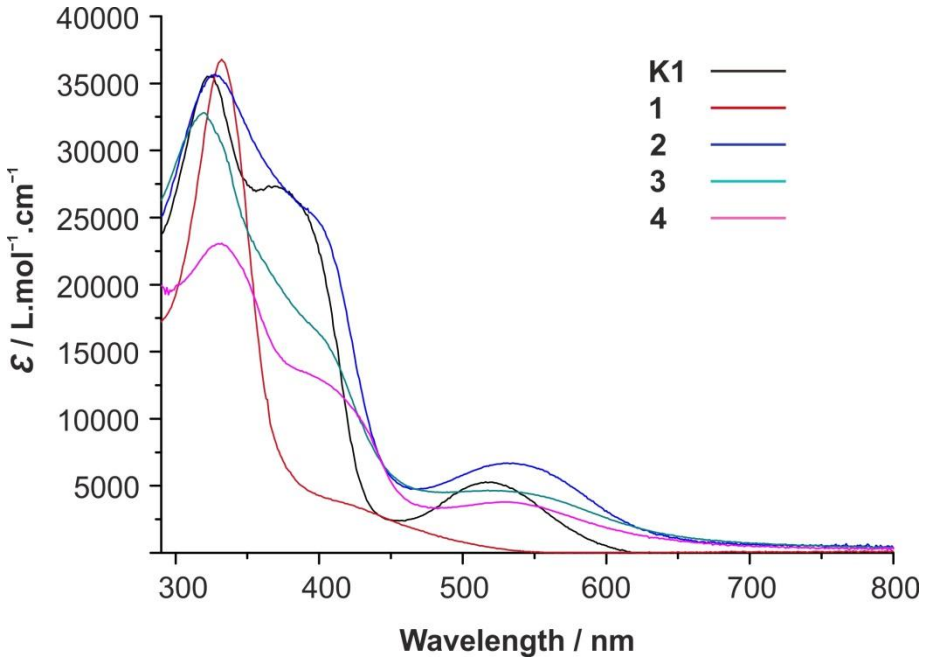


Figure S1: Plots of the UV-vis spectra recorded in THF (of **K1** and **1**–**3**) and 1,2-difluorobenzene (**4**).

3. Cyclic voltammograms of complexes K1 and 2–4 (Figures S2–S5)

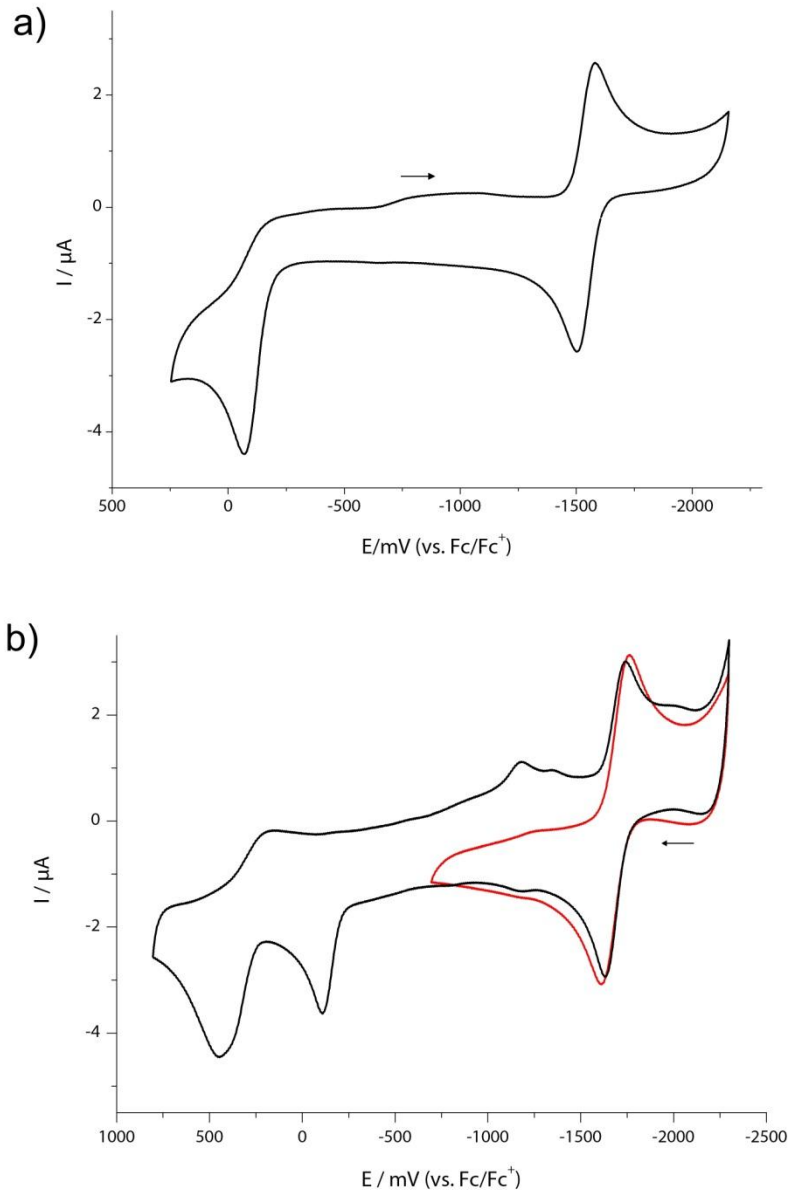


Figure S2: The cyclic voltammograms of **K1** recorded in in CH_3CN/TBAH (a) and 1,2-difluorobenzene (b) with different potential windows. The CV in CH_3CN/TBAH shows a reversible wave at $E_{1/2}$ = –1.57 V and an irreversible redox wave at a peak potential of –0.07 V. The CV in 1,2-difluorobenzene shows a reversible wave at $E_{1/2}$ = –1.69 V and irreversible waves at peak potentials of –0.06 V and +0.47 V. Additional redox process are apparent at –1.1 to –1-4 V vs. Fc/Fc which are not observed when the measurement is performed in a smaller potential window. Conditions: Pt microdisk working electrode, acetonitrile/TBAH, T = 293 K, v = 100 mV s^{-1}; the potentials are referenced to the Fc/Fc^+ couple.

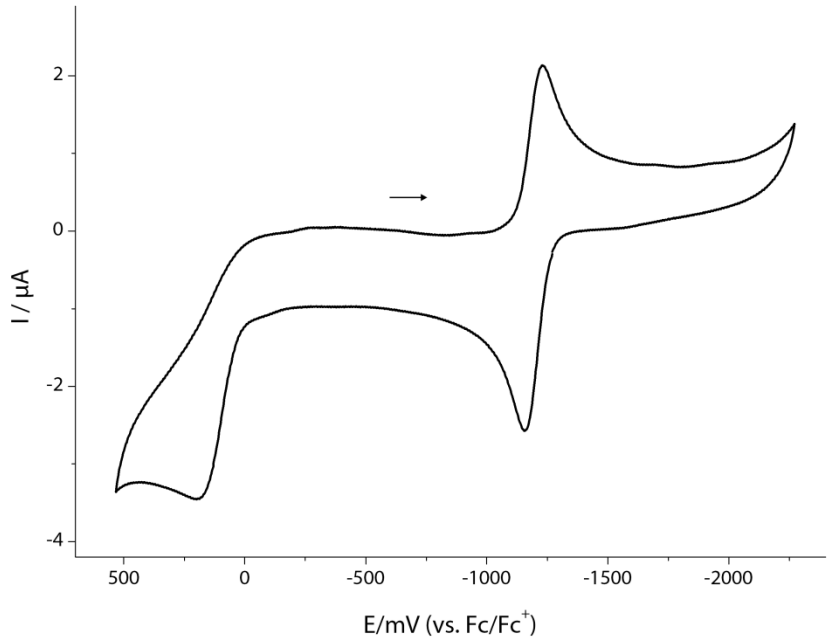


Figure S3: The cyclic voltammogram of compound **2** recorded in CH_3CN/TBAH. Conditions: see Figure S2.

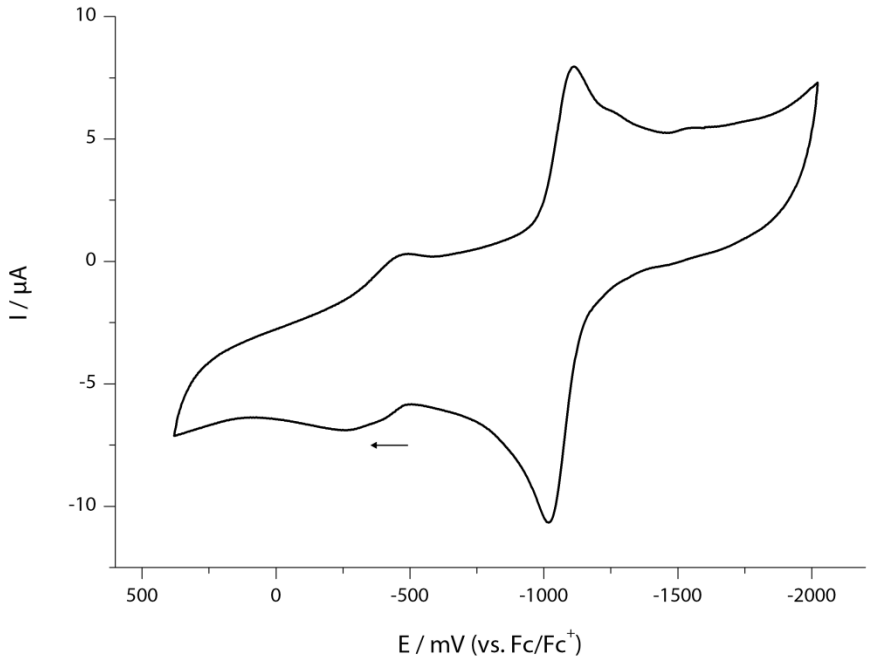


Figure S4: The cyclic voltammogram of compound **3** in CH_3CN/TBAH. Conditions: see Figure S2.

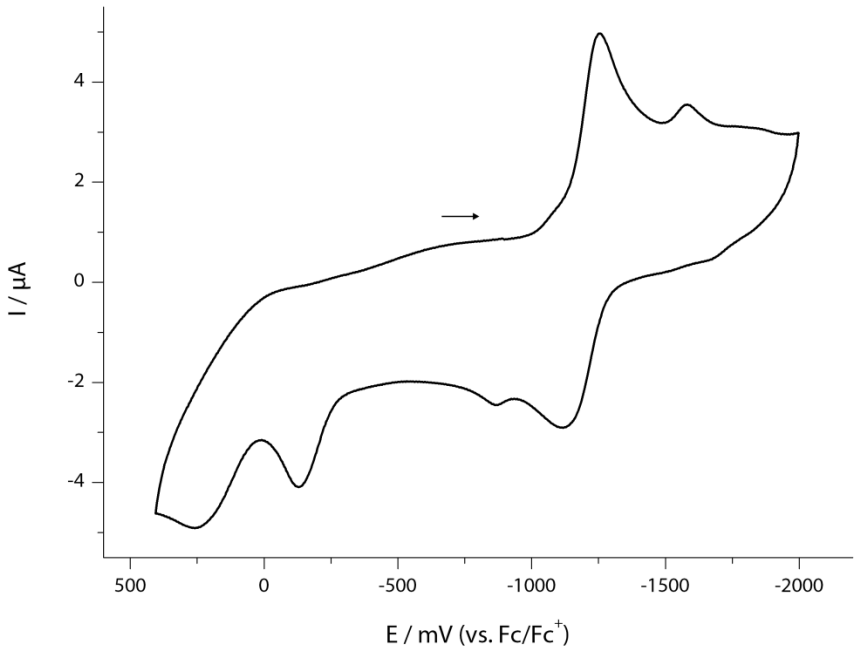


Figure S5: The cyclic voltammogram of compound **4** in CH_3CN/TBAH. Conditions: see Figure S2.

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4. Crystallographic data for K1 and 1–4

4.1. Crystal and Refinement data of K1

Table S4.1.1 Crystal data and structure refinement for K1

Identification code	**K1**
Empirical formula	$C_{46}H_{55}FeKN_4O_6$
Formula weight	854.89
Temperature/K	123(2) K
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.8231(2)
b/Å	21.9105(2)
c/Å	20.3007(1)
α/°	90.00
β/°	98.027(1)
γ/°	90.00
Volume/Å^3	4766.9(1)
Z	4
ρ_{calc}mg/mm^3	1.191
μ/mm^{-1}	3.699
F(000)	1808.0
Crystal size/mm^3	0.49 × 0.3553 × 0.3271
2Θ range for data collection	5.96 to 153.44°
Index ranges	$-13 \le h \le 13$, $-27 \le k \le 27$, $-25 \le l \le 25$
Reflections collected	96550
Independent reflections	9864 [R(int) = 0.0389]
Data/restraints/parameters	9864/18/569
Goodness-of-fit on F^2	1.042
Final *R* indexes [I>2σ (I)]	R_1 = 0.0756, wR_2 = 0.2153
Final *R* indexes [all data]	R_1 = 0.0771, wR_2 = 0.2174
Largest diff. peak/hole / e Å^{-3}	1.05/-0.56

Table S4.1.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for K1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	2301(3)	2914.8(13)	2851.3(13)	34.1(6)
C2	1022(3)	2734.3(13)	2955.5(15)	38.8(6)
C3	1510(3)	2501.2(13)	3623.9(15)	38.8(6)
C4	2788(3)	2685.4(13)	3532.3(14)	38.5(6)
C5	3259(5)	1246(2)	3009(2)	70.5(13)
C6	3336(4)	1543(2)	2409(3)	76.2(15)
C7	2128(5)	1554.3(16)	2034.1(18)	67.9(13)
C8	1318(4)	1255.6(17)	2418(2)	61.7(10)
C9	2020(5)	1067.3(16)	3007(2)	63.2(11)
C11	2835(3)	3254.9(13)	2344.9(15)	38.8(6)
C12	2086(3)	3428.4(15)	1763.5(16)	44.1(7)
C13	2589(4)	3778.6(18)	1308.4(18)	58.7(9)
C14	3817(4)	3959.4(16)	1415.9(19)	57.8(10)
C15	4528(4)	3764.6(18)	1992(2)	56.9(9)
C21	-219(3)	2715.0(14)	2598.5(16)	42.8(7)
C22	-1178(3)	2476(2)	2917.8(17)	56.8(9)
C23	-2368(4)	2441(2)	2584(2)	66.2(11)
C24	-2635(4)	2642(2)	1941(2)	60.6(9)
C25	-1650(4)	2864(2)	1639(2)	61.9(10)
C31	1060(3)	2359.7(14)	4252.2(15)	42.0(14)
C32	1390(3)	1861.2(13)	4662.7(17)	45.6(11)
C33	791(4)	1759.7(14)	5215.4(16)	54.8(13)
C34	-138(4)	2156.9(17)	5357.6(16)	48.9(19)
C35	-468(3)	2655.4(13)	4947.0(16)	43.0(11)
N3	131(3)	2756.8(11)	4394.3(13)	39.1(9)
C31A	774(2)	2364(2)	4143(2)	25(2)
C32A	-97(3)	1898(3)	4141(3)	54(3)
C33A	-670(3)	1792(3)	4702(3)	63(3)
C34A	-371(4)	2152(3)	5265(3)	58(5)
C35A	500(4)	2619(3)	5267(2)	58(3)
N3A	1072(3)	2724.9(17)	4706(2)	49(2)
C41	3963(2)	2608.4(13)	3957.3(11)	44.3(7)
C42	3922(2)	2361.8(13)	4574.8(11)	41.9(7)

C43	5006(4)	2262(2)	4982.4(18)	57.1(9)
C44	6144(4)	2397(2)	4803.6(19)	63(1)
C45	6189(4)	2646(2)	4181.9(19)	67.1(11)
C101	10(5)	4481(2)	2473(2)	66.9(11)
C102	1229(5)	4804.1(18)	2623(2)	65.3(11)
C103	3142(4)	4771.2(19)	3322(2)	63.6(11)
C104	3892(4)	4386(2)	3833(2)	68.1(11)
C105	3958(5)	3995(3)	4922(3)	77.5(13)
C106	3139(5)	3666(3)	5332(3)	86.6(15)
C107	1494(6)	3838(3)	5958(3)	90.0(16)
C108	365(6)	4247(3)	5922(2)	90.4(17)
C109	-1445(5)	4495(3)	5232(3)	90.2(16)
C110	-2365(5)	4312(3)	4648(3)	72.5(16)
C210	-1960(20)	4006(7)	4730(5)	106(7)
C111	-2520(5)	4351(3)	3476(3)	72.2(15)
C211	-2280(30)	3932(12)	3530(5)	97(7)
C112	-1784(4)	4201(3)	2926(3)	78.7(13)
N1	4061(3)	3420.4(14)	2458.3(15)	53.5(7)
N2	-465(3)	2901.5(16)	1957.0(19)	61.0(8)
N42	5100(4)	2764.8(19)	3760.6(17)	67.5(9)
Fe1	2136.2(4)	2003.84(19)	2910.4(2)	33.47(15)
K1	781.3(8)	3919.7(4)	4081.4(4)	57.4(2)
O1	-670(3)	4539.5(16)	3006.2(16)	74.7(9)
O2	1970(3)	4499.5(11)	3159.0(14)	59.1(7)
O3	3263(3)	4294.9(17)	4390.2(16)	74.8(8)
O4	2217(4)	4074.7(16)	5492.7(17)	84.5(10)
O5	-409(4)	4100.8(14)	5342.1(17)	76.3(9)
O6	-1753(3)	4237.8(18)	4096.6(19)	79.8(9)
C51	4328(8)	1122(3)	3540(4)	162(5)
C61	4451(7)	1836(3)	2160(5)	165(5)
C71	1760(10)	1821(3)	1351(2)	140(4)

Table S4.1.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for K1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	42.7(15)	31.7(13)	28.4(13)	-2.1(10)	6.8(11)	-4.4(11)
C2	49.4(17)	29.4(13)	40.8(15)	0.2(11)	17.0(13)	1.7(11)
C3	50.7(17)	31.2(13)	36.4(14)	-2.3(11)	13.2(12)	-0.2(11)
C4	50.9(17)	35.5(14)	30.4(13)	-6.1(11)	10.2(12)	-3.4(12)
C5	76(3)	51(2)	77(3)	-28(2)	-15(2)	30(2)
C6	73(3)	51(2)	115(4)	-43(2)	51(3)	-12.2(19)
C7	132(4)	34.2(17)	38.1(17)	-9.2(13)	14(2)	6(2)
C8	55(2)	39.0(17)	87(3)	-29.3(18)	-2.2(19)	-0.8(15)
C9	114(4)	28.8(16)	52(2)	-3.9(14)	33(2)	6.4(17)
C11	52.8(17)	29.6(13)	36.9(14)	-5.3(11)	16.5(12)	0.1(12)
C12	53.8(18)	41.9(16)	38.3(15)	4.6(12)	12.6(13)	0.1(13)
C13	85(3)	53(2)	41.3(17)	8.0(15)	18.9(17)	9.8(19)
C14	85(3)	43.8(18)	53(2)	-1.8(15)	39.6(19)	-5.5(17)
C15	61(2)	55(2)	62(2)	-6.5(17)	30.0(18)	-14.3(16)
C21	48.1(17)	37.9(15)	44.3(16)	-7.0(12)	13.3(13)	2.5(12)
C22	47.4(19)	88(3)	35.1(16)	-8.0(16)	7.0(14)	-16.0(18)
C23	49(2)	101(3)	49(2)	-10(2)	7.1(16)	-15(2)
C24	51(2)	80(3)	50(2)	-9.6(18)	3.8(16)	-1.8(18)
C25	61(2)	63(2)	63(2)	11.4(19)	13.7(19)	11.3(18)
C31	53(3)	36(3)	35(2)	-4(2)	-2(2)	-5(2)
C32	56(3)	41(2)	41(2)	6.1(19)	9(2)	2(2)
C33	66(3)	51(3)	49(3)	12(2)	12(2)	1(2)
C34	56(3)	57(5)	36(3)	4(3)	14(3)	-8(3)
C35	47(3)	42(2)	41(2)	-6.8(19)	13(2)	-5.7(19)
N3	49(2)	33.8(18)	36.7(19)	-5.2(14)	13.2(17)	-4.3(15)
C31A	17(4)	30(5)	30(5)	4(4)	4(3)	5(3)
C32A	61(7)	49(6)	54(6)	-5(5)	14(5)	-4(5)
C33A	71(8)	53(7)	72(8)	7(6)	31(6)	-2(6)
C34A	74(10)	53(11)	54(8)	10(8)	33(8)	10(7)
C35A	87(9)	49(6)	42(6)	9(5)	29(6)	18(6)
N3A	78(7)	44(5)	25(4)	-4(3)	13(4)	-1(4)
C41	57.8(19)	42.6(16)	33.1(14)	-10.2(12)	8.3(13)	-0.1(13)
C42	37.3(15)	57.4(18)	30.6(13)	-3.1(12)	3.6(11)	6.4(13)

C43	57(2)	77(3)	36.1(16)	-3.2(16)	2.6(14)	12.2(18)
C44	54(2)	91(3)	43.3(18)	-11.1(19)	4.3(16)	4(2)
C45	66(3)	92(3)	42.8(19)	-11.5(19)	4.9(17)	-7(2)
C101	86(3)	59(2)	56(2)	-0.1(18)	12(2)	6(2)
C102	100(3)	46.1(19)	54(2)	5.4(16)	25(2)	2(2)
C103	66(2)	56(2)	77(3)	-14.6(19)	39(2)	-15.7(18)
C104	51(2)	75(3)	83(3)	-20(2)	28(2)	-6.9(19)
C105	69(3)	89(3)	71(3)	-21(2)	0(2)	16(2)
C106	88(4)	85(3)	84(3)	-1(3)	2(3)	22(3)
C107	114(4)	86(4)	72(3)	14(3)	22(3)	8(3)
C108	150(5)	75(3)	54(2)	-1(2)	44(3)	16(3)
C109	106(4)	88(4)	83(3)	-26(3)	39(3)	8(3)
C110	54(3)	72(4)	98(4)	4(3)	33(3)	14(3)
C210	99(14)	111(15)	113(15)	12(13)	33(12)	66(12)
C111	59(3)	81(4)	75(4)	-22(3)	4(3)	-1(3)
C211	87(13)	99(14)	115(14)	-37(13)	42(11)	-49(12)
C112	62(3)	88(3)	84(3)	-23(3)	1(2)	-3(2)
N1	59.0(18)	52.7(16)	52.5(16)	-1.4(13)	21.0(14)	-10.8(13)
N2	55.2(19)	59.7(19)	70(2)	20.1(16)	16.3(16)	7.2(14)
N42	78(2)	77(2)	47.4(17)	-10.6(16)	8.3(16)	-11.7(19)
Fe1	42.3(3)	28.3(2)	30.5(2)	-3.20(15)	7.33(18)	0.46(16)
K1	60.5(5)	49.1(4)	66.9(5)	15.1(3)	23.6(4)	-5.7(3)
O1	71.7(19)	87(2)	66.5(18)	-26.5(16)	13.9(14)	-3.0(16)
O2	73.8(17)	43.8(13)	65.4(16)	4.1(11)	29.8(13)	-6.9(11)
O3	61.0(17)	98(2)	68.9(18)	-1.0(17)	20.3(14)	10.5(16)
O4	127(3)	67.9(19)	65.0(18)	5.3(15)	36.3(19)	14.3(19)
O5	103(2)	55.5(16)	74(2)	-9.0(14)	27.4(18)	0.8(16)

Table S4.1.4 Bond Lengths for K1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.483(4)	C35	N3	1.3900
C1	C4	1.496(4)	N3	K1	2.741(3)
C1	C11	1.453(4)	C31A	C32A	1.3900
C1	Fe1	2.009(3)	C31A	N3A	1.3900

C2	C3	1.477(4)	C31A	K1	3.410(5)
C2	C21	1.434(5)	C32A	C33A	1.3900
C2	Fe1	2.014(3)	C33A	C34A	1.3900
C2	K1	3.493(3)	C34A	C35A	1.3900
C3	C4	1.477(4)	C35A	N3A	1.3900
C3	C31	1.460(4)	N3A	K1	2.907(4)
C3	C31A	1.438(4)	C41	C42	1.3717
C3	Fe1	2.005(3)	C41	N42	1.389(4)
C3	K1	3.369(3)	C42	C43	1.356(4)
C4	C41	1.444(4)	C43	C44	1.364(6)
C4	Fe1	2.018(3)	C44	C45	1.382(6)
C5	C6	1.395(8)	C45	N42	1.381(6)
C5	C9	1.396(7)	C101	C102	1.491(7)
C5	Fe1	2.051(4)	C101	K1	3.479(4)
C5	C51	1.493(7)	C101	O1	1.397(5)
C6	C7	1.418(7)	C102	O2	1.424(5)
C6	Fe1	2.028(4)	C103	C104	1.487(7)
C6	C61	1.514(7)	C103	O2	1.399(5)
C7	C8	1.413(7)	C104	O3	1.413(5)
C7	Fe1	2.032(3)	C105	C106	1.485(8)
C7	C71	1.506(6)	C105	O3	1.391(6)
C8	C9	1.386(6)	C106	K1	3.385(6)
C8	Fe1	2.055(3)	C106	O4	1.411(6)
C8	C81	1.518(7)	C107	C108	1.508(8)
C9	Fe1	2.067(4)	C107	O4	1.407(7)
C9	C91	1.508(6)	C108	O5	1.384(7)
C11	C12	1.388(5)	C109	C110	1.493(7)
C11	N1	1.364(4)	C109	C210	1.528(10)
C12	C13	1.371(5)	C109	O5	1.408(7)
C13	C14	1.375(6)	C110	O6	1.388(7)
C14	C15	1.374(6)	C210	O6	1.428(10)
C15	N1	1.362(5)	C111	C112	1.495(6)
C21	C22	1.401(5)	C111	O6	1.431(7)
C21	N2	1.355(5)	C211	C112	1.524(10)
C22	C23	1.371(5)	C211	K1	3.35(3)

C23	C24	1.371(6)	C211	O6	1.385(9)
C24	C25	1.390(6)	C112	K1	3.430(5)
C25	N2	1.355(6)	C112	O1	1.406(6)
C31	C32	1.3900	K1	O1	2.849(4)
C31	N3	1.3900	K1	O2	2.729(3)
C31	K1	3.445(3)	K1	O3	2.795(3)
C32	C33	1.3900	K1	O4	3.082(4)
C33	C34	1.3900	K1	O5	3.048(3)

Table S4.1.5 Bond Angles for K1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C4	89.6(2)	C111	C112	K1	89.7(3)
C2	C1	Fe1	68.54(15)	C211	C112	K1	74.0(11)
C4	C1	Fe1	68.51(16)	O1	C112	C111	109.6(4)
C11	C1	C2	135.1(3)	O1	C112	C211	120.4(7)
C11	C1	C4	134.6(3)	O1	C112	K1	54.3(2)
C11	C1	Fe1	126.8(2)	C15	N1	C11	118.5(3)
C1	C2	Fe1	68.19(16)	C25	N2	C21	119.1(3)
C1	C2	K1	92.94(17)	C45	N42	C41	119.3(3)
C3	C2	C1	90.1(2)	C1	Fe1	C2	43.27(12)
C3	C2	Fe1	68.12(16)	C1	Fe1	C4	43.62(11)
C3	C2	K1	72.89(15)	C1	Fe1	C5	138.95(18)
C21	C2	C1	139.7(3)	C1	Fe1	C6	113.36(16)
C21	C2	C3	130.1(3)	C1	Fe1	C7	114.76(14)
C21	C2	Fe1	118.6(2)	C1	Fe1	C8	143.06(16)
C21	C2	K1	101.68(18)	C1	Fe1	C9	177.62(16)
Fe1	C2	K1	136.09(14)	C2	Fe1	C4	62.78(13)
C2	C3	C4	90.6(2)	C2	Fe1	C5	171.68(17)
C2	C3	Fe1	68.76(16)	C2	Fe1	C6	148.0(2)
C2	C3	K1	82.35(16)	C2	Fe1	C7	119.71(16)
C4	C3	Fe1	68.93(16)	C2	Fe1	C8	115.83(15)
C4	C3	K1	92.40(17)	C2	Fe1	C9	137.73(16)
C31	C3	C2	139.1(3)	C3	Fe1	C1	62.93(12)
C31	C3	C4	126.9(3)	C3	Fe1	C2	43.12(12)
C31	C3	Fe1	134.7(2)	C3	Fe1	C4	43.08(12)

C31	C3	K1	80.55(16)	C3	Fe1	C5	128.68(17)
C31A	C3	C2	125.5(3)	C3	Fe1	C6	159.79(19)
C31A	C3	C4	140.6(3)	C3	Fe1	C7	159.27(19)
C31A	C3	C31	14.06(19)	C3	Fe1	C8	128.21(16)
C31A	C3	Fe1	133.9(3)	C3	Fe1	C9	116.11(14)
C31A	C3	K1	79.4(2)	C4	Fe1	C5	112.81(15)
Fe1	C3	K1	144.73(13)	C4	Fe1	C6	119.38(16)
C1	C4	Fe1	67.87(15)	C4	Fe1	C7	149.85(17)
C3	C4	C1	89.6(2)	C4	Fe1	C8	169.63(16)
C3	C4	Fe1	67.99(16)	C4	Fe1	C9	134.11(15)
C41	C4	C1	139.3(3)	C5	Fe1	C8	67.09(17)
C41	C4	C3	130.9(3)	C5	Fe1	C9	39.6(2)
C41	C4	Fe1	119.3(2)	C6	Fe1	C5	40.0(2)
C6	C5	C9	107.6(4)	C6	Fe1	C7	40.9(2)
C6	C5	Fe1	69.1(2)	C6	Fe1	C8	67.74(17)
C6	C5	C51	125.6(7)	C6	Fe1	C9	66.71(18)
C9	C5	Fe1	70.8(2)	C7	Fe1	C5	67.86(18)
C9	C5	C51	126.8(7)	C7	Fe1	C8	40.44(19)
C51	C5	Fe1	127.3(3)	C7	Fe1	C9	66.97(15)
C5	C6	C7	108.3(4)	C8	Fe1	C9	39.31(18)
C5	C6	Fe1	70.9(2)	C3	K1	C31A	24.49(8)
C5	C6	C61	129.5(7)	C3	K1	C106	82.79(11)
C7	C6	Fe1	69.7(2)	N3	K1	C3	44.26(8)
C7	C6	C61	122.1(7)	N3	K1	C31A	20.07(8)
C61	C6	Fe1	123.5(3)	N3	K1	N3A	22.71(9)
C6	C7	Fe1	69.4(2)	N3	K1	C106	82.22(13)
C6	C7	C71	127.3(6)	N3	K1	C211	79.1(4)
C8	C7	C6	107.0(4)	N3	K1	O1	119.26(10)
C8	C7	Fe1	70.6(2)	N3	K1	O3	119.41(10)
C8	C7	C71	125.7(6)	N3	K1	O4	89.96(9)
C71	C7	Fe1	125.9(3)	N3	K1	O5	76.95(8)
C7	C8	Fe1	68.9(2)	N3	K1	O6	86.90(10)
C7	C8	C81	127.9(5)	N3A	K1	C3	43.45(9)
C9	C8	C7	107.8(4)	N3A	K1	C31A	23.8
C9	C8	Fe1	70.8(2)	N3A	K1	C106	60.04(14)

C9	C8	C81	124.3(5)	N3A	K1	C211	101.2(4)
C81	C8	Fe1	127.6(3)	N3A	K1	O4	71.56(11)
C5	C9	Fe1	69.6(2)	N3A	K1	O5	77.51(9)
C5	C9	C91	123.0(6)	C106	K1	C31A	79.29(12)
C8	C9	C5	109.3(4)	C211	K1	C3	100.0(5)
C8	C9	Fe1	69.9(2)	C211	K1	C31A	90.7(5)
C8	C9	C91	127.7(6)	C211	K1	C106	149.3(2)
C91	C9	Fe1	129.2(3)	O1	K1	C3	110.72(9)
C12	C11	C1	120.0(3)	O1	K1	C31A	120.03(9)
N1	C11	C1	119.4(3)	O1	K1	N3A	141.08(11)
N1	C11	C12	120.6(3)	O1	K1	C106	158.44(13)
C13	C12	C11	119.1(3)	O1	K1	C211	47.6(3)
C12	C13	C14	121.4(4)	O1	K1	O4	144.32(9)
C15	C14	C13	117.3(3)	O1	K1	O5	109.19(10)
N1	C15	C14	123.1(4)	O2	K1	C3	95.13(8)
C22	C21	C2	118.6(3)	O2	K1	N3	138.80(8)
N2	C21	C2	121.4(3)	O2	K1	C31A	119.61(9)
N2	C21	C22	119.9(3)	O2	K1	N3A	133.30(8)
C23	C22	C21	119.9(4)	O2	K1	C106	102.29(13)
C24	C23	C22	120.7(4)	O2	K1	C211	107.8(2)
C23	C24	C25	117.4(4)	O2	K1	O1	60.97(9)
N2	C25	C24	123.0(4)	O2	K1	O3	59.12(10)
C3	C31	K1	74.73(16)	O2	K1	O4	111.21(10)
C32	C31	C3	127.0(2)	O2	K1	O5	144.16(9)
C32	C31	N3	120.0	O2	K1	O6	116.27(11)
C32	C31	K1	148.40(14)	O3	K1	C3	94.51(9)
N3	C31	C3	112.8(2)	O3	K1	C31A	107.03(9)
N3	C31	K1	49.00(11)	O3	K1	N3A	97.17(10)
C33	C32	C31	120.0	O3	K1	C106	43.93(13)
C32	C33	C34	120.0	O3	K1	C211	161.5(4)
C33	C34	C35	120.0	O3	K1	O1	116.19(10)
N3	C35	C34	120.0	O3	K1	O4	54.20(10)
C31	N3	K1	108.50(14)	O3	K1	O5	106.20(10)
C35	N3	C31	120.0	O3	K1	O6	145.72(11)
C35	N3	K1	119.96(15)	O4	K1	C3	104.53(9)

C3	C31A	K1	76.2(2)	O4	K1	C31A	94.56(9)
C32A	C31A	C3	126.6(2)	O4	K1	C106	24.64(11)
C32A	C31A	N3A	120.0	O4	K1	C211	131.1(2)
C32A	C31A	K1	137.71(9)	O5	K1	C3	119.62(8)
N3A	C31A	C3	113.3(2)	O5	K1	C31A	95.50(9)
N3A	C31A	K1	57.38(17)	O5	K1	C106	75.77(12)
C31A	C32A	C33A	120.0	O5	K1	C211	76.4(2)
C34A	C33A	C32A	120.0	O5	K1	O4	54.72(10)
C35A	C34A	C33A	120.0	O6	K1	C3	119.60(10)
C34A	C35A	N3A	120.0	O6	K1	C31A	103.77(9)
C31A	N3A	K1	98.9(2)	O6	K1	N3A	105.23(10)
C35A	N3A	C31A	120.0	O6	K1	C106	131.41(13)
C35A	N3A	K1	118.33(14)	O6	K1	C211	24.1(3)
C42	C41	C4	116.99(16)	O6	K1	O1	57.34(10)
C42	C41	N42	120.2(2)	O6	K1	O4	109.02(11)
N42	C41	C4	122.8(3)	O6	K1	O5	55.64(11)
C43	C42	C41	119.0(2)	C101	O1	C112	113.5(3)
C42	C43	C44	122.7(4)	C101	O1	K1	104.8(3)
C43	C44	C45	118.5(4)	C112	O1	K1	102.1(3)
N42	C45	C44	120.3(4)	C102	O2	K1	118.3(2)
C102	C101	K1	83.5(2)	C103	O2	C102	112.1(3)
O1	C101	C102	110.2(4)	C103	O2	K1	122.3(2)
O1	C101	K1	52.3(2)	C104	O3	K1	114.6(3)
O2	C102	C101	108.7(3)	C105	O3	C104	114.8(4)
O2	C103	C104	108.2(3)	C105	O3	K1	115.7(3)
O3	C104	C103	111.2(3)	C106	O4	K1	89.8(3)
O3	C105	C106	111.4(4)	C107	O4	C106	113.5(4)
C105	C106	K1	86.9(3)	C107	O4	K1	109.1(4)
O4	C106	C105	108.5(5)	C108	O5	C109	111.6(4)
O4	C106	K1	65.6(3)	C108	O5	K1	117.9(3)
O4	C107	C108	105.8(4)	C109	O5	K1	111.5(3)
O5	C108	C107	107.1(4)	C110	O6	C210	33.3(9)
C110	C109	C210	31.0(8)	C110	O6	C111	114.0(4)
O5	C109	C110	112.9(4)	C110	O6	K1	127.6(3)
O5	C109	C210	83.2(10)	C210	O6	C111	135.4(10)

O6	C110	C109	109.3(4)	C210	O6	K1	101.2(11)
O6	C210	C109	105.3(8)	C111	O6	K1	118.4(3)
O6	C111	C112	108.4(4)	C211	O6	C110	122.6(9)
C112	C211	K1	80.0(10)	C211	O6	C210	118.6(8)
O6	C211	C112	109.2(8)	C211	O6	C111	39.7(13)
O6	C211	K1	56.6(11)	C211	O6	K1	99.3(14)
C111	C112	C211	36.9(12)				
C2	C1	C4	89.6(2)	C111	C112	K1	89.7(3)

4.2. Crystal and Refinement data of 1

Table S4.2.1 Crystal data and structure refinement for 1

Identification code	**1**
Empirical formula	$C_{34}H_{31}FeN_4$
Formula weight	551.49
Temperature/K	123(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.6884(2)
b/Å	14.1246(2)
c/Å	15.0838(2)
α/°	90.00
β/°	113.276(1)
γ/°	90.00
Volume/Å^3	2679(1)
Z	4
ρ_{calc}mg/mm^3	1.367
μ/mm^{-1}	4.743
F(000)	1156.0
Crystal size/mm^3	0.335 × 0.174 × 0.102
2Θ range for data collection	7.4 to 147.36°
Index ranges	$-16 \le h \le 15$, $-17 \le k \le 17$, $-18 \le l \le 18$
Reflections collected	14409
Independent reflections	5200[R(int) = 0.0238]
Data/restraints/parameters	5200/0/352
Goodness-of-fit on F^2	1.043
Final R indexes [I>2σ (I)]	R_1 = 0.0341, wR_2 = 0.0959
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0976
Largest diff. peak/hole / e Å^{-3}	0.39/–0.39

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Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	1513.4(13)	1746.8(12)	3300.3(11)	19.6(3)
C2	821.3(14)	2500.0(12)	3310.3(13)	22.0(4)
C3	1333.6(16)	3373.2(13)	3274.0(12)	27.8(4)
C4	2332.8(15)	3152.3(14)	3232.8(12)	28.9(4)
C5	2444.9(14)	2152.2(14)	3255.0(12)	23.8(4)
C6	1291.7(16)	710.8(13)	3310.6(14)	30.2(4)
C7	-273.6(15)	2397.6(16)	3294.3(15)	34.2(5)
C8	858(2)	4344.3(16)	3205.2(15)	46.2(6)
C9	3107(2)	3851.8(19)	3138.3(16)	51.9(7)
C10	3372.3(15)	1606.0(18)	3235.1(14)	39.1(5)
C11	3563.1(13)	2712.3(12)	5745.6(12)	18.1(3)
C12	2948.9(12)	1854.5(12)	5746.9(11)	17.7(3)
C13	2086.1(14)	2451.4(11)	5782.0(12)	18.1(3)
C14	2697.5(12)	3308.2(12)	5781.3(11)	18.3(3)
C111	4609.3(12)	2902.5(12)	5732.8(11)	18.7(3)
C115	5710.7(14)	3957.8(14)	5412.6(14)	28.5(4)
C114	6516.3(13)	3298.8(14)	5616.7(13)	27.6(4)
C113	6351.0(14)	2408.5(13)	5910.2(14)	25.8(4)
C121	3173.5(12)	837.4(12)	5869.0(11)	19.0(3)
C125	4033.7(14)	-457.0(13)	5593.1(13)	28.2(4)
C124	3645.4(15)	-1052.4(14)	6102.3(15)	32.8(4)
C123	2997.5(15)	-671.8(14)	6520.2(15)	32.0(4)
C131	1066.8(13)	2230.1(13)	5840.7(12)	20.6(3)
C135	-287.8(14)	1151.2(15)	5531.9(14)	32.1(4)
C134	-835.8(15)	1736.5(17)	5905.4(16)	39.0(5)
C133	-400.1(18)	2604.0(16)	6264.4(18)	37.8(5)
C141	2567.2(13)	4315.7(12)	5931.4(12)	20.2(3)
C145	1434.8(15)	5576.1(14)	5713.8(14)	29.5(4)
C144	2261.7(16)	6191.9(14)	6200.6(15)	33.0(4)
C143	3285.0(16)	5834.3(14)	6579.5(15)	32.0(4)
N1	4774.0(11)	3780.3(11)	5469.0(11)	25.0(3)
C112	5387.9(13)	2200.3(13)	5965.4(12)	22.2(3)
N2	3804.6(11)	468.0(11)	5461.2(10)	23.2(3)

C122	2762.0(13)	283.7(13)	6408.9(12)	24.7(4)
N3	643.7(11)	1378.4(11)	5492.0(11)	24.6(3)
C132	565.7(14)	2864.2(15)	6233.0(14)	27.8(4)
N4	1562.6(11)	4658.5(11)	5575.0(11)	25.3(3)
C142	3441.2(14)	4888.6(13)	6441.7(13)	25.9(4)
Fe1	2252.93(18)	2601.91(18)	4529.00(17)	16.33(9)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	20.1(7)	21.5(9)	16.4(7)	-1.4(6)	6.4(6)	0.7(6)
C2	19.0(8)	27.6(9)	16.3(8)	-1.3(6)	3.6(7)	4.4(6)
C3	39.3(10)	21.7(9)	17.1(8)	2.3(7)	5.6(7)	4.6(8)
C4	35.3(10)	32.7(10)	17.4(8)	1.8(7)	9.1(7)	-9.6(8)
C5	20.5(8)	35.3(10)	16.6(8)	-0.5(7)	8.3(6)	-0.2(7)
C6	36.5(10)	22.5(9)	29.5(9)	-4.1(7)	10.7(8)	-1.7(8)
C7	19.2(9)	56.8(14)	23.6(10)	-4.7(8)	5.4(7)	9.3(8)
C8	75.0(16)	26.3(11)	26.7(10)	4.5(8)	8.9(10)	15.6(11)
C9	68.8(16)	55.5(15)	30.6(11)	0.3(10)	18.8(11)	-35.3(13)
C10	26.2(9)	66.7(16)	29.2(10)	1.7(10)	16.1(8)	10.5(10)
C11	15.3(8)	19.7(8)	17.5(8)	0.0(6)	4.8(6)	2.3(6)
C12	14.9(7)	21.5(8)	16.3(7)	0.8(6)	5.8(6)	1.6(6)
C13	17.0(8)	20.7(8)	17.0(8)	0.1(6)	7.1(6)	1.6(6)
C14	15.4(7)	21.4(8)	17.5(7)	-1.5(6)	6.0(6)	0.8(6)
C111	16.9(7)	20.7(8)	18.2(7)	-2.4(6)	6.7(6)	-0.4(6)
C115	23.8(8)	26.6(9)	37.7(10)	1.6(8)	14.9(7)	-3.4(7)
C114	17.7(8)	36.2(11)	30.5(9)	-2.0(8)	11.5(7)	-2.8(7)
C113	17.9(8)	32.4(10)	26.7(9)	-0.7(7)	8.5(7)	5.5(7)
C121	15.5(7)	19.9(8)	19.1(7)	0.1(6)	4.0(6)	0.6(6)
C125	27.1(9)	22.8(9)	33.4(9)	-2.3(7)	10.5(7)	5.7(7)
C124	32.4(10)	19.9(9)	40.7(11)	3.7(8)	8.5(8)	5.1(8)
C123	29.7(9)	27.1(10)	37.7(10)	9.8(8)	11.7(8)	-0.9(8)
C131	15.8(8)	26.7(9)	19.7(8)	5.1(7)	7.4(6)	2.5(6)
C135	22.5(8)	35.6(11)	38.8(10)	4.5(8)	12.7(8)	-5.1(8)
C134	23.6(9)	47.9(13)	51.8(12)	8.7(10)	21.6(9)	0.2(9)
C133	31.2(11)	46.5(13)	45.6(12)	5.6(9)	25.7(10)	11.8(9)

C141	20.7(8)	20.7(8)	20.5(7)	0.0(6)	9.7(6)	2.5(6)
C145	29.4(9)	26.3(10)	35.8(10)	1.4(8)	15.9(8)	9.9(7)
C144	43.5(11)	19.0(9)	46.7(11)	-1.8(8)	28.7(9)	3.7(8)
C143	34.2(10)	25.6(10)	43.0(11)	-10.9(8)	22.4(9)	-7.9(8)
N1	20.5(7)	22.7(8)	34.0(8)	1.0(6)	13.0(6)	-0.4(6)
C112	19.0(8)	23.4(9)	23.1(8)	0.2(7)	7.2(6)	2.2(7)
N2	21.6(7)	22.4(8)	25.9(7)	-0.5(6)	9.7(6)	2.8(6)
C122	20.8(8)	26.3(9)	26.8(8)	4.7(7)	9.1(7)	2.4(7)
N3	18.6(7)	27.4(8)	28.2(7)	2.8(6)	9.8(6)	-1.4(6)
C132	25.6(9)	30.6(10)	31.0(9)	0.9(8)	15.2(7)	4.3(8)
N4	21.8(7)	25.0(8)	28.1(7)	-0.3(6)	8.9(6)	5.1(6)
C142	22.3(8)	25.0(9)	32.7(9)	-4.6(7)	13.4(7)	0.7(7)
Fe1	15.30(14)	16.60(15)	16.90(15)	0.41(9)	6.16(11)	0.52(9)

Table 4 Bond Lengths for 1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.429(2)	C14	Fe1	2.0063(16)
C1	C5	1.424(2)	C111	N1	1.348(2)
C1	C6	1.496(2)	C111	C112	1.395(2)
C1	Fe1	2.1061(16)	C115	C114	1.382(3)
C2	C3	1.431(3)	C115	N1	1.342(2)
C2	C7	1.496(3)	C114	C113	1.381(3)
C2	Fe1	2.0959(18)	C113	C112	1.385(3)
C3	C4	1.428(3)	C121	N2	1.348(2)
C3	C8	1.504(3)	C121	C122	1.398(2)
C3	Fe1	2.1146(17)	C125	C124	1.379(3)
C4	C5	1.420(3)	C125	N2	1.340(2)
C4	C9	1.496(3)	C124	C123	1.384(3)
C4	Fe1	2.1466(18)	C123	C122	1.382(3)
C5	C10	1.496(3)	C131	N3	1.349(2)
C5	Fe1	2.1365(17)	C131	C132	1.394(3)
C11	C12	1.475(2)	C135	C134	1.378(3)
C11	C14	1.472(2)	C135	N3	1.339(2)
C11	C111	1.465(2)	C134	C133	1.377(3)
C11	Fe1	2.0018(16)	C133	C132	1.391(3)

C12	C13	1.469(2)	C141	N4	1.353(2)
C12	C121	1.465(2)	C141	C142	1.397(2)
C12	Fe1	2.0034(16)	C145	C144	1.386(3)
C13	C14	1.472(2)	C145	N4	1.335(2)
C13	C131	1.466(2)	C144	C143	1.383(3)
C13	Fe1	2.0027(17)	C143	C142	1.381(3)
C14	C141	1.463(2)			

Table 5 Bond Angles for 1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	126.18(16)	N2	C121	C122	121.84(16)
C2	C1	Fe1	69.74(10)	C122	C121	C12	120.58(15)
C5	C1	C2	108.13(16)	N2	C125	C124	123.93(17)
C5	C1	C6	125.68(16)	C125	C124	C123	118.30(18)
C5	C1	Fe1	71.54(10)	C122	C123	C124	119.00(18)
C6	C1	Fe1	125.51(12)	N3	C131	C13	116.03(15)
C1	C2	C3	107.73(16)	N3	C131	C132	122.08(16)
C1	C2	C7	126.30(17)	C132	C131	C13	121.89(17)
C1	C2	Fe1	70.51(10)	N3	C135	C134	123.8(2)
C3	C2	C7	125.85(17)	C133	C134	C135	118.28(18)
C3	C2	Fe1	70.84(10)	C134	C133	C132	119.45(19)
C7	C2	Fe1	127.17(13)	N4	C141	C14	116.98(15)
C2	C3	C8	125.72(19)	N4	C141	C142	121.77(16)
C2	C3	Fe1	69.44(10)	C142	C141	C14	121.24(15)
C4	C3	C2	107.80(16)	N4	C145	C144	124.20(17)
C4	C3	C8	126.3(2)	C143	C144	C145	118.15(17)
C4	C3	Fe1	71.64(10)	C142	C143	C144	118.87(18)
C8	C3	Fe1	128.30(13)	C115	N1	C111	117.78(15)
C3	C4	C9	125.9(2)	C113	C112	C111	118.98(17)
C3	C4	Fe1	69.21(10)	C125	N2	C121	117.66(15)
C5	C4	C3	108.23(15)	C123	C122	C121	119.25(17)
C5	C4	C9	125.8(2)	C135	N3	C131	117.78(16)
C5	C4	Fe1	70.25(9)	C133	C132	C131	118.59(19)
C9	C4	Fe1	128.23(13)	C145	N4	C141	117.43(16)
C1	C5	C10	125.22(19)	C143	C142	C141	119.56(17)

C1	C5	Fe1	69.24(9)	C1	Fe1	C3	66.34(7)
C4	C5	C1	108.11(15)	C1	Fe1	C4	65.54(7)
C4	C5	C10	126.67(18)	C1	Fe1	C5	39.21(7)
C4	C5	Fe1	71.03(10)	C2	Fe1	C1	39.75(6)
C10	C5	Fe1	125.34(12)	C2	Fe1	C3	39.72(7)
C12	C11	Fe1	68.45(9)	C2	Fe1	C4	65.96(7)
C14	C11	C12	90.13(13)	C2	Fe1	C5	66.13(7)
C14	C11	Fe1	68.62(9)	C3	Fe1	C4	39.15(8)
C111	C11	C12	135.35(15)	C3	Fe1	C5	65.74(7)
C111	C11	C14	134.52(16)	C5	Fe1	C4	38.72(8)
C111	C11	Fe1	121.92(12)	C11	Fe1	C1	142.78(7)
C11	C12	Fe1	68.33(9)	C11	Fe1	C2	176.19(7)
C13	C12	C11	89.74(13)	C11	Fe1	C3	141.37(7)
C13	C12	Fe1	68.46(9)	C11	Fe1	C4	117.20(7)
C121	C12	C11	135.56(14)	C11	Fe1	C5	117.62(7)
C121	C12	C13	133.62(15)	C11	Fe1	C12	43.22(7)
C121	C12	Fe1	129.20(12)	C11	Fe1	C13	62.49(7)
C12	C13	C14	90.36(13)	C11	Fe1	C14	43.08(6)
C12	C13	Fe1	68.51(9)	C12	Fe1	C1	113.19(7)
C14	C13	Fe1	68.59(9)	C12	Fe1	C2	135.15(7)
C131	C13	C12	132.66(15)	C12	Fe1	C3	172.53(7)
C131	C13	C14	136.92(15)	C12	Fe1	C4	148.11(7)
C131	C13	Fe1	123.08(12)	C12	Fe1	C5	119.02(7)
C11	C14	C13	89.77(13)	C12	Fe1	C14	62.70(7)
C11	C14	Fe1	68.30(9)	C13	Fe1	C1	125.11(7)
C13	C14	Fe1	68.33(9)	C13	Fe1	C2	113.87(7)
C141	C14	C11	135.34(15)	C13	Fe1	C3	130.55(7)
C141	C14	C13	134.08(15)	C13	Fe1	C4	164.55(7)
C141	C14	Fe1	128.26(12)	C13	Fe1	C5	156.60(7)
N1	C111	C11	116.80(14)	C13	Fe1	C12	43.02(6)
N1	C111	C112	121.85(15)	C13	Fe1	C14	43.07(7)
C112	C111	C11	121.33(16)	C14	Fe1	C1	167.21(7)
N1	C115	C114	123.95(18)	C14	Fe1	C2	133.67(7)
C113	C114	C115	117.87(16)	C14	Fe1	C3	116.01(7)
C114	C113	C112	119.54(17)	C14	Fe1	C4	124.88(7)

N2	C121	C12	117.56(15)	C14	Fe1	C5	153.55(7)

4.3. Crystal and Refinement data of 2

Table S4.3.1 Crystal data and structure refinement for 2

Identification code	**2**
Empirical formula	$C_{46}H_{55}Cl_2FeKN_4O_6Zn$
Formula weight	991.16
Temperature/K	123(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.4571(2)
b/Å	16.5968(2)
c/Å	17.0934(2)
α/°	90.00
β/°	94.918(1)
γ/°	90.00
Volume/Å^3	4651.6(1)
Z	4
ρ_{calc}mg/mm^3	1.415
μ/mm^{-1}	5.405
F(000)	2064.0
Crystal size/mm^3	0.232 × 0.159 × 0.078
2Θ range for data collection	7.44 to 147.58°
Index ranges	$-20 \le h \le 20$, $-17 \le k \le 20$, $-21 \le l \le 20$
Reflections collected	27914
Independent reflections	9169 [R(int) = 0.0351]
Data/restraints/parameters	9169/0/551
Goodness-of-fit on F^2	1.041
Final R indexes [I>2σ (I)]	R_1 = 0.0336, wR_2 = 0.0857
Final R indexes [all data]	R_1 = 0.0407, wR_2 = 0.0911
Largest diff. peak/hole / e Å^{-3}	0.61/–0.39

Table S4.3.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	-4941.0(13)	-312.0(15)	6888.3(14)	32.1(5)
C2	-4497.6(14)	-777.1(14)	6362.4(14)	32.6(5)
C3	-4150.6(13)	-228.7(14)	5834.8(13)	29.7(5)
C4	-4379.4(12)	562.9(13)	6034.3(13)	27.5(4)
C5	-4864.0(12)	522.8(14)	6687.8(14)	29.3(5)
C6	-5454.0(14)	-646.3(17)	7492.7(18)	46.0(7)
C7	-4453.2(17)	-1684.5(15)	6342.8(17)	44.8(6)
C8	-3641.6(16)	-438.4(16)	5173.7(15)	41.1(6)
C9	-4174.1(15)	1310.5(15)	5604.0(14)	36.3(5)
C10	-5250.3(14)	1218.5(16)	7067.6(16)	39.9(6)
C11	-2542.4(11)	-242.0(12)	7281.8(12)	20.7(4)
C12	-2723.9(11)	619.7(12)	7429.6(12)	20.2(4)
C13	-3258.7(11)	377.2(12)	8041.5(12)	21.9(4)
C14	-3070.7(12)	-478.1(12)	7897.5(12)	21.1(4)
C15	530.5(19)	-2224.9(16)	6829.8(17)	50.2(7)
C16	-147.6(18)	-2201.3(18)	7351.5(19)	52.1(7)
C17	-461.5(15)	-1862.9(17)	8622(2)	50.3(7)
C18	-83.4(17)	-1772.6(15)	9439.9(18)	45.9(7)
C19	936.5(19)	-1052.8(17)	10193.7(15)	46.8(7)
C20	1351.3(19)	-255.4(17)	10258.1(15)	45.5(6)
C21	2250.5(19)	591.9(19)	9649.2(19)	55.7(8)
C22	2752.1(17)	666.8(19)	8964(2)	53.7(8)
C23	2667.7(19)	839.1(19)	7592(2)	58.5(8)
C24	2156(2)	620.0(18)	6861(2)	57.2(8)
C25	1645(2)	-506(2)	6128.7(17)	58.8(8)
C26	1438(2)	-1373(2)	6213.2(17)	57.6(8)
C111	-2134.8(11)	-716.6(12)	6729.4(12)	21.0(4)
C112	-2321.6(13)	-1542.3(13)	6610.3(13)	26.7(4)
C113	-1958.9(13)	-1973.5(13)	6052.5(13)	28.7(4)
C114	-1399.4(13)	-1598.6(14)	5600.1(13)	29.8(5)
C115	-1210.9(13)	-808.8(13)	5756.3(12)	27.1(4)
C121	-2584.3(11)	1395.8(12)	7091.3(11)	20.2(4)
C122	-3090.9(12)	2058.2(13)	7234.3(13)	25.6(4)

C123	-2960.6(13)	2794.1(13)	6897.6(13)	28.1(4)
C124	-2340.8(13)	2883.3(13)	6403.3(13)	28.4(4)
C125	-1854.5(12)	2226.6(13)	6291.0(13)	25.2(4)
C131	-3547.0(12)	807.2(12)	8707.6(12)	24.1(4)
C133	-3396.2(15)	1890.3(14)	9637.2(14)	35.0(5)
C134	-4064.8(15)	1599.3(15)	9982.8(15)	38.2(5)
C135	-4445.1(16)	923.8(16)	9663.8(17)	42.7(6)
C141	-3143.4(12)	-1198.6(12)	8376.3(12)	21.9(4)
C142	-3813.9(13)	-1312.0(13)	8811.0(13)	28.0(4)
C143	-3836.6(14)	-1975.8(14)	9289.3(14)	34.1(5)
C144	-3203.5(15)	-2527.0(14)	9323.4(15)	35.7(5)
C145	-2566.2(14)	-2380.7(13)	8873.5(15)	34.1(5)
N1	-1558.1(10)	-374.5(10)	6311.1(10)	22.0(3)
N2	-1956.8(10)	1502.6(10)	6636(1)	21.0(3)
N3	-4244(5)	546(3)	8985(4)	27.8(7)
C132	-3157(8)	1485(6)	9034(10)	27.8(7)
C137	-4140(10)	491(6)	9144(10)	27.8(7)
N3A	-3077(13)	1494(10)	8950(18)	27.8(7)
N4	-2519.9(11)	-1733.6(11)	8401.7(11)	28.1(4)
O1	827.6(13)	-1429.2(11)	6748.5(10)	46.9(5)
O2	169.5(9)	-1965.8(10)	8115(1)	36.6(4)
O3	421.1(11)	-1076.3(10)	9482.9(10)	37.8(4)
O4	1837.8(11)	-160.7(10)	9614.1(10)	38.5(4)
O5	2237.5(10)	669.6(11)	8264.4(12)	44.8(4)
O6	2024.5(12)	-225.6(12)	6861.7(11)	48.4(5)
Cl1	-189.0(3)	1058.2(3)	5743.0(3)	34.39(13)
Cl2	-430.5(3)	589.0(3)	7856.2(3)	33.27(12)
K1	1030.5(3)	-521.2(3)	8109.2(3)	29.01(11)
Fe1	-3741.41(18)	11.86(18)	6999.10(19)	20.44(8)
Zn1	-1043.33(15)	689.97(16)	6634.26(15)	21.28(8)

Table S4.3.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	21.6(9)	35.7(12)	37.9(13)	9.6(10)	-3.2(9)	-4.7(9)
C2	31.2(10)	28.4(11)	35.6(13)	2.3(9)	-12.8(10)	-5.1(9)

C3	31.3(10)	30.9(11)	25.0(11)	-0.8(9)	-8.7(9)	-0.7(9)
C4	23.5(9)	29.3(11)	28.4(11)	4.1(8)	-5.4(8)	-1.4(8)
C5	18.2(9)	34.0(12)	34.7(12)	7.6(9)	-2.8(8)	0.2(8)
C6	23.2(10)	56.8(17)	58.1(18)	23.3(13)	3.3(11)	-8.6(11)
C7	49.4(14)	29.0(13)	52.2(16)	1.9(11)	-18.3(13)	-10.4(11)
C8	48.2(14)	44.4(14)	29.3(13)	-5.7(10)	-5.2(11)	4.7(11)
C9	37.8(12)	36.4(13)	32.9(13)	11.9(10)	-7.4(10)	-3(1)
C10	23.5(10)	46.8(15)	49.3(15)	4.7(12)	2.1(10)	8.8(10)
C11	19.7(8)	20.4(9)	21.9(10)	1.6(7)	1.4(7)	0.1(7)
C12	17.9(8)	22.9(10)	19.7(10)	-1.8(7)	1.4(7)	-0.5(7)
C13	21.0(8)	21.2(10)	23.7(10)	0.2(8)	3.4(8)	-0.4(7)
C14	21.8(9)	20.2(10)	21.2(10)	-0.1(7)	1.7(8)	1.9(7)
C15	70.7(19)	37.0(14)	39.0(15)	-9.0(11)	-18.0(14)	7.7(13)
C16	46.9(14)	42.3(15)	62.5(19)	-4.7(13)	-22.5(14)	-2.7(12)
C17	28.9(11)	33.7(14)	90(2)	-1.3(14)	12.6(13)	-0.2(10)
C18	48.1(14)	29.2(13)	65.5(19)	5.1(12)	33.5(14)	2.5(11)
C19	74.7(19)	41.0(14)	26.5(13)	4.8(10)	16.0(13)	12.2(13)
C20	66.4(17)	42.0(14)	28.5(13)	-7.0(11)	5.8(12)	14.2(13)
C21	56.4(17)	54.1(18)	55.3(19)	-21.2(14)	-2.6(15)	-13.5(14)
C22	36.8(13)	48.5(17)	75(2)	-14.8(15)	1.8(14)	-12.4(12)
C23	50.1(16)	46.5(17)	83(2)	10.1(15)	32.4(17)	-4.4(13)
C24	66.9(19)	49.0(17)	60(2)	19.2(14)	31.2(16)	4.8(14)
C25	79(2)	69(2)	30.6(14)	11.6(13)	17.8(15)	18.0(17)
C26	84(2)	60.3(19)	28.7(14)	-2.2(12)	8.4(14)	24.8(17)
C111	21.3(8)	22.3(10)	18.8(10)	-0.3(7)	-1.4(7)	1.7(7)
C112	29.9(10)	24(1)	26.0(11)	-2.1(8)	1.5(9)	-1.0(8)
C113	33.6(10)	22.1(10)	29.5(11)	-6.5(8)	-1.9(9)	1.9(8)
C114	34.2(11)	31.0(11)	24.4(11)	-8.8(8)	3.0(9)	5.7(9)
C115	28.7(10)	31.4(11)	21.5(10)	-2.5(8)	3.8(8)	3.8(8)
C121	20.5(8)	20.9(9)	18.7(9)	-1.6(7)	-1.0(7)	-0.6(7)
C122	25.0(9)	25.8(10)	26.2(11)	-0.5(8)	3.7(8)	2.5(8)
C123	29.8(10)	19.7(10)	34.2(12)	-0.6(8)	-0.5(9)	3.8(8)
C124	30.9(10)	20(1)	33.6(12)	5.2(8)	-1.7(9)	-2.6(8)
C125	25.2(9)	25.3(10)	25.2(11)	3.1(8)	2.4(8)	-2.5(8)
C131	24.9(9)	22.3(10)	25.4(11)	0.3(8)	3.1(8)	3.0(8)

C133	42.0(12)	29.7(12)	32.9(13)	-7.8(9)	1.5(10)	1.1(10)
C134	44.0(13)	39.1(13)	32.9(13)	-11.1(10)	12.0(11)	7.2(11)
C135	41.9(13)	41.6(14)	47.8(16)	-8.6(12)	23.3(12)	0.3(11)
C141	25.5(9)	19.1(9)	20.7(10)	0.2(7)	0.4(8)	-1.1(7)
C142	26.6(10)	27.2(11)	30.8(12)	3.5(9)	5.6(9)	-0.6(8)
C143	33.6(11)	34.1(12)	35.2(13)	7.9(10)	6.3(10)	-5.4(9)
C144	40.3(12)	29.1(12)	36.9(13)	13.1(10)	-0.7(10)	-4.4(10)
C145	35.0(11)	24.8(11)	42.1(14)	6.3(9)	0.8(10)	4.5(9)
N1	23.3(8)	22.6(8)	20.4(8)	-1.6(6)	2.9(7)	1.5(6)
N2	21.4(7)	20.4(8)	21.1(8)	1.0(6)	1.3(6)	-0.3(6)
N3	30(2)	30.3(8)	23(3)	-2.8(11)	6.2(9)	1.3(8)
C132	30(2)	30.3(8)	23(3)	-2.8(11)	6.2(9)	1.3(8)
C137	30(2)	30.3(8)	23(3)	-2.8(11)	6.2(9)	1.3(8)
N3A	30(2)	30.3(8)	23(3)	-2.8(11)	6.2(9)	1.3(8)
N4	29.7(9)	24.2(9)	30.6(10)	2.9(7)	3.5(8)	2.7(7)
O1	70.9(12)	38.3(10)	30.9(9)	-2.2(7)	0.3(9)	11.8(9)
O2	28.1(7)	35.0(9)	45.4(10)	0.1(7)	-3.8(7)	1.2(7)
O3	47.8(9)	28.1(8)	39.4(10)	5.0(7)	15.4(8)	1.7(7)
O4	46.8(9)	36.5(9)	31.6(9)	-7.4(7)	0.3(7)	3.9(8)
O5	32.0(8)	44.6(11)	59.4(12)	2.9(9)	13.3(8)	-3.8(7)
O6	60.1(11)	45.3(11)	41.9(11)	12.1(8)	17.4(9)	7.5(9)
Cl1	39.7(3)	29.9(3)	36.6(3)	0.3(2)	21.1(2)	-1.3(2)
Cl2	34.8(3)	39.4(3)	24.5(3)	-2.9(2)	-4.0(2)	9.2(2)
K1	29.8(2)	29.5(2)	28.0(2)	1.61(18)	3.68(18)	1.79(17)
Fe1	19.34(14)	19.33(16)	22.35(17)	1.85(12)	0.12(12)	-0.89(11)
Zn1	21.64(13)	22.30(14)	20.37(14)	-0.37(10)	4.49(10)	0.97(10)

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Table S4.3.4 Bond Lengths for 2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.431(4)	C24	K1	3.499(3)
C1	C5	1.435(3)	C25	C26	1.489(5)
C1	C6	1.496(3)	C25	O6	1.429(4)
C1	Fe1	2.039(2)	C26	O1	1.418(4)
C2	C3	1.434(3)	C111	C112	1.415(3)
C2	C7	1.508(3)	C111	N1	1.361(3)

C2	Fe1	2.053(2)	C112	C113	1.369(3)
C3	C4	1.416(3)	C113	C114	1.398(3)
C3	C8	1.504(3)	C114	C115	1.368(3)
C3	Fe1	2.084(2)	C115	N1	1.356(3)
C4	C5	1.429(3)	C121	C122	1.414(3)
C4	C9	1.496(3)	C121	N2	1.357(3)
C4	Fe1	2.088(2)	C122	C123	1.375(3)
C5	C10	1.493(3)	C123	C124	1.387(3)
C5	Fe1	2.061(2)	C124	C125	1.375(3)
C11	C12	1.487(3)	C124	K1[1]	3.471(2)
C11	C14	1.474(3)	C125	N2	1.355(3)
C11	C111	1.439(3)	C131	N3	1.350(11)
C11	Fe1	2.0350(18)	C131	C132	1.389(11)
C12	C13	1.479(3)	C131	C137	1.38(2)
C12	C121	1.438(3)	C131	N3A	1.419(17)
C12	Fe1	2.0376(19)	C133	C134	1.380(4)
C13	C14	1.478(3)	C133	C132	1.319(10)
C13	C131	1.457(3)	C134	C135	1.374(4)
C13	Fe1	1.983(2)	C135	C137	1.28(2)
C14	C141	1.460(3)	C141	C142	1.395(3)
C14	Fe1	1.987(2)	C141	N4	1.355(3)
C15	C16	1.488(5)	C142	C143	1.374(3)
C15	O1	1.419(3)	C143	C144	1.384(3)
C16	O2	1.418(3)	C144	C145	1.374(3)
C17	C18	1.489(5)	C145	N4	1.349(3)
C17	O2	1.419(3)	N1	Zn1	2.0158(17)
C17	K1	3.482(3)	N2	Zn1	2.0198(16)
C18	O3	1.421(3)	O1	K1	2.7676(19)
C19	C20	1.489(4)	O2	K1	2.7855(17)
C19	O3	1.421(3)	O3	K1	2.7878(17)
C20	O4	1.424(3)	O4	K1	2.8557(18)
C21	C22	1.494(5)	O5	K1	2.7986(18)
C21	O4	1.420(3)	O6	K1	2.8395(19)
C22	O5	1.406(4)	Cl1	Zn1	2.2447(6)
C23	C24	1.491(5)	Cl2	K1	3.0306(7)

C23	O5	1.428(4)	Cl2	Zn1	2.2465(6)
C24	O6	1.420(4)	K1	C124[2]	3.471(2)

[1]-X,1/2+Y,3/2-Z; [2]-X,-1/2+Y,3/2-Z

Table S4.3.5 Bond Angles for 2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C5	108.1(2)	C125	N2	Zn1	118.11(13)
C2	C1	C6	125.6(2)	C131	C132	C133	124.6(5)
C2	C1	Fe1	70.06(12)	C135	C137	C131	120.0(9)
C5	C1	C6	126.1(2)	C145	N4	C141	117.35(19)
C5	C1	Fe1	70.32(12)	C15	O1	K1	116.24(15)
C6	C1	Fe1	129.27(17)	C26	O1	C15	113.1(2)
C1	C2	C3	107.7(2)	C26	O1	K1	117.74(18)
C1	C2	C7	125.5(2)	C16	O2	C17	111.4(2)
C1	C2	Fe1	69.00(13)	C16	O2	K1	112.39(16)
C3	C2	C7	126.7(2)	C17	O2	K1	107.32(14)
C3	C2	Fe1	70.89(12)	C18	O3	K1	118.42(15)
C7	C2	Fe1	128.33(16)	C19	O3	C18	111.7(2)
C2	C3	C8	127.1(2)	C19	O3	K1	118.66(15)
C2	C3	Fe1	68.57(12)	C20	O4	K1	115.09(15)
C4	C3	C2	108.0(2)	C21	O4	C20	111.3(2)
C4	C3	C8	124.9(2)	C21	O4	K1	113.96(16)
C4	C3	Fe1	70.32(12)	C22	O5	C23	112.4(2)
C8	C3	Fe1	127.35(16)	C22	O5	K1	116.70(16)
C3	C4	C5	108.83(19)	C23	O5	K1	117.37(18)
C3	C4	C9	125.1(2)	C24	O6	C25	112.1(2)
C3	C4	Fe1	69.99(12)	C24	O6	K1	105.57(16)
C5	C4	C9	126.0(2)	C25	O6	K1	111.46(17)
C5	C4	Fe1	68.82(12)	Zn1	Cl2	K1	117.74(2)
C9	C4	Fe1	129.20(15)	C17	K1	C24	157.08(8)
C1	C5	C10	126.4(2)	C124[2]	K1	C17	83.61(6)
C1	C5	Fe1	68.70(12)	C124[2]	K1	C24	102.06(7)
C4	C5	C1	107.3(2)	O1	K1	C17	80.01(7)
C4	C5	C10	126.2(2)	O1	K1	C24	79.30(7)
C4	C5	Fe1	70.91(12)	O1	K1	C124[2]	79.28(5)

C10	C5	Fe1	127.71(16)	O1	K1	O2	60.63(6)
C12	C11	Fe1	68.68(10)	O1	K1	O3	120.12(6)
C14	C11	C12	89.71(15)	O1	K1	O4	152.18(6)
C14	C11	Fe1	66.76(10)	O1	K1	O5	119.85(6)
C111	C11	C12	138.56(18)	O1	K1	O6	59.91(6)
C111	C11	C14	131.26(18)	O1	K1	Cl2	100.03(4)
C111	C11	Fe1	117.03(14)	O2	K1	C17	22.89(6)
C11	C12	Fe1	68.49(10)	O2	K1	C24	139.82(7)
C13	C12	C11	89.93(15)	O2	K1	$C124^2$	69.40(5)
C13	C12	Fe1	66.44(10)	O2	K1	O3	59.52(5)
C121	C12	C11	138.73(18)	O2	K1	O4	112.00(5)
C121	C12	C13	130.77(18)	O2	K1	O5	164.73(5)
C121	C12	Fe1	116.93(13)	O2	K1	O6	118.52(6)
C12	C13	Fe1	70.40(11)	O2	K1	Cl2	97.26(4)
C14	C13	C12	89.88(15)	O3	K1	C17	42.64(7)
C14	C13	Fe1	68.29(11)	O3	K1	C24	160.01(7)
C131	C13	C12	132.26(18)	O3	K1	$C124^2$	78.85(5)
C131	C13	C14	133.42(18)	O3	K1	O4	58.91(5)
C131	C13	Fe1	136.04(14)	O3	K1	O5	117.20(6)
C11	C14	C13	90.47(15)	O3	K1	O6	164.09(6)
C11	C14	Fe1	70.25(11)	O3	K1	Cl2	89.02(4)
C13	C14	Fe1	67.99(11)	O4	K1	C17	101.01(7)
C141	C14	C11	134.39(18)	O4	K1	C24	101.89(7)
C141	C14	C13	131.69(18)	O4	K1	$C124^2$	73.27(5)
C141	C14	Fe1	134.58(14)	O4	K1	Cl2	107.66(4)
O1	C15	C16	108.5(2)	O5	K1	C17	159.70(7)
O2	C16	C15	108.9(2)	O5	K1	C24	42.87(7)
C18	C17	K1	85.70(14)	O5	K1	$C124^2$	95.43(5)
O2	C17	C18	108.5(2)	O5	K1	O4	59.67(6)
O2	C17	K1	49.79(11)	O5	K1	O6	59.95(6)
O3	C18	C17	109.0(2)	O5	K1	Cl2	97.59(4)
O3	C19	C20	108.9(2)	O6	K1	C17	139.79(7)
O4	C20	C19	109.0(2)	O6	K1	C24	23.01(7)
O4	C21	C22	109.5(2)	O6	K1	$C124^2$	85.76(6)
O5	C22	C21	109.5(2)	O6	K1	O4	112.75(6)

O5	C23	C24	110.0(2)	O6	K1	Cl2	106.79(4)
C23	C24	K1	84.93(16)	Cl2	K1	C17	81.77(5)
O6	C24	C23	108.4(3)	Cl2	K1	C24	92.22(6)
O6	C24	K1	51.42(12)	Cl2	K1	C124^{2}	165.25(4)
O6	C25	C26	108.4(2)	C1	Fe1	C2	40.95(10)
O1	C26	C25	107.9(2)	C1	Fe1	C3	68.28(9)
C112	C111	C11	121.11(18)	C1	Fe1	C4	67.97(9)
N1	C111	C11	120.12(18)	C1	Fe1	C5	40.99(9)
N1	C111	C112	118.76(18)	C2	Fe1	C3	40.55(9)
C113	C112	C111	120.3(2)	C2	Fe1	C4	67.66(9)
C112	C113	C114	120.0(2)	C2	Fe1	C5	68.68(9)
C115	C114	C113	117.9(2)	C3	Fe1	C4	39.69(9)
N1	C115	C114	122.9(2)	C5	Fe1	C3	67.87(9)
C122	C121	C12	120.67(18)	C5	Fe1	C4	40.28(9)
N2	C121	C12	120.20(17)	C11	Fe1	C1	151.50(9)
N2	C121	C122	119.13(18)	C11	Fe1	C2	121.68(9)
C123	C122	C121	120.2(2)	C11	Fe1	C3	114.48(9)
C122	C123	C124	119.9(2)	C11	Fe1	C4	133.61(8)
C123	C124	K1^{1}	114.17(14)	C11	Fe1	C5	167.44(9)
C125	C124	C123	117.87(19)	C11	Fe1	C12	42.83(8)
C125	C124	K1^{1}	106.32(13)	C12	Fe1	C1	157.39(9)
N2	C125	C124	123.1(2)	C12	Fe1	C2	161.65(9)
C13	C131	N3A	114.5(5)	C12	Fe1	C3	128.90(9)
N3	C131	C13	117.4(3)	C12	Fe1	C4	114.22(8)
N3	C131	C137	13.4(4)	C12	Fe1	C5	125.47(9)
N3	C131	N3A	127.9(6)	C13	Fe1	C1	118.31(9)
C132	C131	C13	122.7(3)	C13	Fe1	C2	148.14(9)
C132	C131	N3	119.8(3)	C13	Fe1	C3	171.31(9)
C132	C131	C137	114.5(8)	C13	Fe1	C4	135.34(9)
C132	C131	N3A	8.2(9)	C13	Fe1	C5	112.80(9)
C137	C131	C13	121.9(6)	C13	Fe1	C11	62.88(8)
C137	C131	N3A	122.7(6)	C13	Fe1	C12	43.15(8)
C132	C133	C134	117.3(4)	C13	Fe1	C14	43.72(8)
C135	C134	C133	117.9(2)	C14	Fe1	C1	115.67(9)
C137	C135	C134	122.8(8)	C14	Fe1	C2	114.84(9)

C142	C141	C14	121.04(18)	C14	Fe1	C3	140.56(9)
N4	C141	C14	117.17(18)	C14	Fe1	C4	176.36(8)
N4	C141	C142	121.74(19)	C14	Fe1	C5	142.59(9)
C143	C142	C141	119.2(2)	C14	Fe1	C11	42.99(8)
C142	C143	C144	119.8(2)	C14	Fe1	C12	62.52(8)
C145	C144	C143	117.9(2)	N1	Zn1	N2	106.87(7)
N4	C145	C144	124.1(2)	N1	Zn1	Cl1	109.00(5)
C111	N1	Zn1	121.16(13)	N1	Zn1	Cl2	109.52(5)
C115	N1	C111	120.03(18)	N2	Zn1	Cl1	109.19(5)
C115	N1	Zn1	117.73(14)	N2	Zn1	Cl2	108.86(5)
C121	N2	Zn1	121.11(13)	Cl1	Zn1	Cl2	113.20(2)
C125	N2	C121	119.63(17)				

[1]-X,1/2+Y,3/2-Z; [2]-X,-1/2+Y,3/2-Z

4.4. Crystal and Refinement data of 3

Table S4.4.1 Crystal data and structure refinement for 3

Identification code	**3**
Empirical formula	$C_{46}H_{55}Cl_2Fe_2KN_4O_6$
Formula weight	981.64
Temperature/K	123(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.4365(9)
b/Å	16.5146(8)
c/Å	17.1501(8)
α/°	90.00
β/°	95.109(5)
γ/°	90.00
Volume/Å^3	4636.8(4)
Z	4
ρ_{calc}mg/mm^3	1.406
μ/mm^{-1}	7.295
F(000)	2048.0
Crystal size/mm^3	0.38 × 0.143 × 0.039
2Θ range for data collection	7.44 to 148.36°
Index ranges	$-20 \le h \le 19$, $-18 \le k \le 20$, $-21 \le l \le 21$
Reflections collected	19283
Independent reflections	9059 [R(int) = 0.0384]
Data/restraints/parameters	9059/0/550
Goodness-of-fit on F^2	1.027
Final R indexes [I>2σ (I)]	R_1 = 0.0419, wR_2 = 0.1053
Final R indexes [all data]	R_1 = 0.0533, wR_2 = 0.1146
Largest diff. peak/hole / e Å^{-3}	0.42/–0.48

Table S4.4.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 3. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C1	618.6(15)	556.3(17)	1023.8(15)	28.1(5)
C2	133.9(14)	517.8(17)	1674.4(16)	28.9(5)
C3	58.8(16)	-322.2(19)	1876.2(17)	34.0(6)
C4	505.7(17)	-787.6(17)	1354.8(17)	33.4(6)
C5	850.5(16)	-242.0(18)	832.0(15)	30.7(6)
C6	820.2(18)	1305.6(19)	597.1(17)	36.9(6)
C7	-252.2(17)	1212(2)	2051.1(19)	40.2(7)
C8	-448.6(18)	-658(2)	2479(2)	48.2(8)
C9	559(2)	-1694.1(19)	1339(2)	45.8(8)
C10	1363(2)	-446(2)	176.3(17)	41.9(7)
C11	2270.4(13)	622.3(15)	2417.1(13)	20.1(5)
C12	2457.7(14)	-241.2(15)	2279.1(13)	20.5(4)
C13	1927.9(14)	-477.1(15)	2888.8(14)	21.9(5)
C14	1739.6(14)	381.3(15)	3029.6(14)	21.4(5)
C111	2405.4(13)	1397.5(15)	2076.3(13)	20.3(4)
C112	1898.9(15)	2068.8(16)	2216.9(15)	26.5(5)
C113	2020.1(16)	2801.1(16)	1874.4(16)	29.3(5)
C114	2639.5(16)	2885.1(16)	1372.2(15)	28.1(5)
C115	3122.2(15)	2230.1(16)	1267.8(15)	27.6(5)
C121	2860.2(14)	-721.0(15)	1724.6(13)	21.5(5)
C122	2678.4(15)	-1549.1(16)	1617.2(15)	26.7(5)
C123	3040.3(16)	-1985.6(17)	1061.8(15)	30.0(5)
C124	3591.0(17)	-1607.0(18)	607.2(16)	31.9(6)
C125	3772.3(16)	-806.4(17)	750.1(15)	28.9(5)
C131	1863.8(14)	-1199.7(15)	3368.8(14)	22.1(5)
C132	1188.5(15)	-1316.7(16)	3791.9(15)	27.6(5)
C133	1172.0(17)	-1982.6(18)	4270.3(17)	34.8(6)
C134	1805.3(19)	-2525.5(18)	4318.5(18)	36.8(6)
C135	2448.0(18)	-2376.2(17)	3876.0(17)	34.1(6)
C141	1446.3(15)	814.8(16)	3692.4(14)	24.1(5)
C143	543(2)	929(2)	4633(2)	43.3(7)
C144	916.5(19)	1609.4(19)	4950.2(17)	38.9(7)

C145	1587.1(19)	1900.2(18)	4604.9(17)	35.6(6)
C146	1856.7(16)	1499.3(16)	3977.9(15)	27.8(5)
C200	4866(2)	-2171(2)	2341(2)	57.8(10)
C201	5534(3)	-2203(2)	1828(2)	57.9(10)
C202	6457(3)	-1351(3)	1230(2)	65.8(12)
C203	6677(3)	-489(3)	1151(2)	67.0(12)
C204	7188(3)	634(2)	1897(3)	64.4(11)
C205	7697(2)	843(2)	2631(3)	67.0(12)
C206	7775(2)	663(3)	4000(3)	62.5(11)
C207	7263(3)	589(3)	4671(3)	61.9(10)
C208	6359(3)	-262(2)	5267.3(18)	51.6(9)
C209	5942(3)	-1062(2)	5193.2(18)	52.9(9)
C210	4928(2)	-1768(2)	4430(2)	52.7(9)
C211	4553(2)	-1849(2)	3615(3)	59.2(11)
N1	3029.5(12)	1505.4(13)	1620.0(12)	22.0(4)
N2	3430.9(12)	-370.7(13)	1306.3(12)	23.4(4)
N3	2491.2(14)	-1726.9(14)	3405.6(13)	30.0(5)
N4	782.6(15)	529.7(15)	4012.8(15)	36.8(5)
O1	5180.2(12)	-1955.4(13)	3106.8(13)	41.1(5)
O2	5843.0(17)	-1404.9(15)	1758.2(13)	52.5(6)
O3	7050.8(17)	-211.2(16)	1888.8(15)	53.8(6)
O4	7265.6(13)	672.2(14)	3293.6(16)	48.8(6)
O5	6853.8(15)	-167.3(14)	4631.0(13)	42.3(5)
O6	5436.3(14)	-1077.1(13)	4479.1(13)	41.7(5)
Cl1	4838.2(4)	1068.2(4)	732.2(4)	39.45(17)
Cl2	4626.0(4)	604.6(5)	2879.5(4)	39.45(17)
K1	6071.2(3)	-528.4(4)	3129.1(3)	30.61(13)
Fe1	1257.3(2)	8.5(2)	1991.6(2)	20.43(10)
Fe2	3989.7(2)	698.9(2)	1653.3(2)	21.79(10)

Table S4.4.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	20.2(11)	31.3(13)	31.2(12)	6.4(11)	-5.9(9)	-2.1(10)
C2	14.2(10)	35.3(14)	36.5(13)	6.3(11)	-1.0(9)	1.4(10)
C3	18.7(11)	37.0(15)	44.9(15)	11.1(13)	-5.2(10)	-8.7(11)

C4	27.4(12)	29.2(14)	40.7(14)	2.5(12)	-12.6(11)	-4.7(11)
C5	26.7(12)	34.5(14)	28.8(12)	-0.4(11)	-8.3(10)	-2.4(11)
C6	34.3(14)	37.8(16)	36.8(14)	11.6(12)	-6.3(11)	-5.4(12)
C7	21.4(12)	47.4(18)	51.8(17)	4.5(14)	3.1(11)	10.0(12)
C8	20.2(12)	61(2)	63(2)	23.7(18)	1.5(13)	-9.9(14)
C9	47.1(17)	28.6(15)	57.2(19)	3.7(14)	-21.1(15)	-9.9(14)
C10	43.0(16)	48.4(18)	32.9(14)	-6.6(13)	-3.9(12)	6.6(15)
C11	13.5(9)	23.1(12)	23.8(11)	-1.6(9)	1.6(8)	-0.9(9)
C12	17.1(10)	20.4(11)	23.7(11)	1.6(9)	0.1(8)	1.4(9)
C13	15.9(10)	23.7(12)	26.3(11)	-0.7(10)	3.0(9)	1.6(9)
C14	17.6(10)	21.7(12)	25.3(11)	1.0(9)	4.0(9)	-0.8(9)
C111	15.4(9)	21.4(11)	23.7(11)	-1.8(9)	-0.8(8)	0.1(9)
C112	21.9(11)	25.9(13)	31.8(12)	-0.3(10)	3.6(9)	2(1)
C113	26.5(12)	23.0(12)	38.0(13)	-0.4(11)	-0.1(10)	3.2(10)
C114	28.1(12)	22.0(12)	33.5(13)	4.7(10)	-0.8(10)	-2.3(10)
C115	22.5(11)	28.1(13)	31.9(12)	3.9(11)	1.6(9)	-2.5(10)
C121	16.4(10)	25.2(12)	22.6(11)	0.2(9)	0.4(8)	2.3(9)
C122	25.6(11)	25.4(13)	28.9(12)	-0.7(10)	0.8(9)	-0.8(10)
C123	30.5(12)	25.3(13)	33.3(13)	-9.0(11)	-2.2(10)	4.1(11)
C124	31.7(13)	33.7(14)	30.4(12)	-9.0(11)	2.9(10)	4.7(12)
C125	25.5(11)	33.5(14)	27.8(12)	-2.0(11)	3.2(10)	5.1(11)
C131	19.5(10)	20.7(11)	25.6(11)	-1.2(9)	-0.5(9)	-1.5(9)
C132	23.4(11)	27.4(13)	32.3(12)	5.4(11)	4.4(10)	0.7(10)
C133	28.7(13)	34.3(15)	41.9(15)	8.3(13)	5.0(11)	-6.5(12)
C134	40.4(15)	27.9(14)	41.5(15)	12.6(12)	-0.3(12)	-2.1(12)
C135	31.9(13)	25.5(13)	44.3(15)	7.6(12)	0.8(11)	3.6(11)
C141	20.7(10)	24.6(12)	27.2(11)	-0.5(10)	3.6(9)	4(1)
C143	40.0(15)	40.8(17)	52.3(18)	-7.2(15)	21.8(14)	2.0(14)
C144	40.3(15)	40.4(16)	37.3(14)	-10.0(13)	11.1(12)	8.1(13)
C145	38.8(15)	32.9(14)	35.0(14)	-8.5(12)	2.1(12)	0.8(12)
C146	26.8(12)	27.2(13)	29.6(12)	-1.2(11)	3.9(10)	-0.7(11)
C200	44.6(18)	44.5(19)	78(3)	-9.3(18)	-27.8(18)	-0.4(16)
C201	74(3)	42.7(19)	52(2)	-13.4(16)	-22.0(19)	9.4(19)
C202	90(3)	74(3)	34.1(16)	-3.7(18)	9.5(18)	29(3)
C203	88(3)	81(3)	34.2(16)	13.0(19)	19.3(18)	23(3)

C204	65(2)	53(2)	81(3)	24(2)	37(2)	9(2)
C205	49(2)	46(2)	113(4)	12(2)	44(2)	-4.0(17)
C206	33.8(17)	55(2)	97(3)	-22(2)	-0.2(18)	-11.0(16)
C207	57(2)	54(2)	72(2)	-25(2)	-4.7(19)	-9.9(19)
C208	76(2)	47.5(19)	30.9(14)	-6.7(14)	5.5(15)	19.5(19)
C209	85(3)	45.9(19)	30.8(15)	7.7(14)	22.4(16)	18.6(19)
C210	49.7(19)	31.7(16)	83(3)	3.8(17)	40.9(19)	3.7(15)
C211	26.0(14)	33.7(17)	120(4)	0(2)	19.7(18)	2.7(13)
N1	16.9(8)	22(1)	26.9(10)	0.6(8)	2.1(7)	-1.2(8)
N2	22.5(9)	24.4(10)	23.8(9)	-1.8(8)	4.8(8)	2.2(8)
N3	25.9(10)	26.9(11)	37.0(12)	3.6(9)	2.5(9)	3.9(9)
N4	33.0(12)	32.1(12)	47.8(14)	-8.6(11)	17(1)	-2.7(10)
O1	25.3(9)	38.5(11)	58.3(13)	-1.3(10)	-2.7(9)	1.9(9)
O2	73.8(17)	47.4(13)	34.9(11)	-3.8(10)	-2.9(11)	15.5(13)
O3	59.3(15)	52.9(14)	52.2(13)	16.6(12)	21.4(11)	11.2(13)
O4	29.9(10)	45.1(13)	73.6(16)	4.9(12)	16.3(11)	-1.8(10)
O5	49.6(12)	37.7(11)	38.2(11)	-7.8(9)	-3.1(9)	5.6(10)
O6	50.4(12)	30.7(10)	46.5(11)	5.5(9)	18.7(10)	4.5(10)
Cl1	43.3(4)	32.8(3)	46.3(4)	0.5(3)	26.9(3)	-0.8(3)
Cl2	34.2(3)	53.4(4)	29.5(3)	-3.5(3)	-4.5(2)	12.7(3)
K1	26.9(3)	32.8(3)	32.4(3)	1.8(2)	4.0(2)	0.6(2)
Fe1	14.75(16)	20.50(19)	25.62(19)	2.23(14)	-0.53(13)	-0.76(14)
Fe2	16.72(17)	24.2(2)	24.76(19)	-0.22(15)	3.82(13)	1.15(14)

Table S4.4.4 Bond Lengths for 3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.429(4)	C132	C133	1.374(4)
C1	C5	1.419(4)	C133	C134	1.371(4)
C1	C6	1.490(4)	C134	C135	1.377(4)
C1	Fe1	2.089(2)	C135	N3	1.347(4)
C2	C3	1.438(4)	C141	C146	1.383(4)
C2	C7	1.486(4)	C141	N4	1.349(3)
C2	Fe1	2.058(2)	C143	C144	1.369(5)
C3	C4	1.431(4)	C143	N4	1.341(4)
C3	C8	1.492(4)	C144	C145	1.383(4)

C3	Fe1	2.037(3)	C145	C146	1.370(4)
C4	C5	1.424(4)	C200	C201	1.468(6)
C4	C9	1.500(4)	C200	O1	1.413(4)
C4	Fe1	2.051(3)	C201	O2	1.421(5)
C5	C10	1.502(4)	C202	C203	1.478(7)
C5	Fe1	2.082(3)	C202	O2	1.418(5)
C11	C12	1.482(3)	C203	O3	1.432(5)
C11	C14	1.479(3)	C204	C205	1.488(7)
C11	C111	1.433(3)	C204	O3	1.415(5)
C11	Fe1	2.029(2)	C204	K1	3.495(4)
C12	C13	1.472(3)	C205	O4	1.421(5)
C12	C121	1.443(3)	C206	C207	1.490(6)
C12	Fe1	2.033(2)	C206	O4	1.410(5)
C13	C14	1.476(3)	C207	O5	1.417(5)
C13	C131	1.459(3)	C208	C209	1.489(6)
C13	Fe1	1.981(2)	C208	O5	1.426(4)
C14	C141	1.461(3)	C209	O6	1.418(4)
C14	Fe1	1.981(2)	C210	C211	1.483(6)
C111	C112	1.420(3)	C210	O6	1.412(4)
C111	N1	1.356(3)	C211	O1	1.418(4)
C112	C113	1.367(4)	C211	K1	3.471(4)
C113	C114	1.398(4)	N1	Fe2	2.062(2)
C114	C115	1.363(4)	N2	Fe2	2.054(2)
C114	K1[1]	3.430(3)	O1	K1	2.773(2)
C115	N1	1.355(3)	O2	K1	2.758(2)
C121	C122	1.408(4)	O3	K1	2.829(2)
C121	N2	1.360(3)	O4	K1	2.787(2)
C122	C123	1.372(4)	O5	K1	2.838(2)
C123	C124	1.394(4)	O6	K1	2.775(2)
C124	C125	1.373(4)	Cl1	Fe2	2.2814(7)
C125	N2	1.356(3)	Cl2	K1	3.0243(9)
C131	C132	1.393(3)	Cl2	Fe2	2.2690(7)
C131	N3	1.347(3)	K1	C114[2]	3.430(3)

[1]1-X,1/2+Y,1/2-Z; [2]1-X,-1/2+Y,1/2-Z

Table S4.4.5 Bond Angles for 3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C6	125.8(3)	C143	N4	C141	117.2(3)
C2	C1	Fe1	68.65(14)	C200	O1	C211	112.1(3)
C5	C1	C2	108.6(2)	C200	O1	K1	112.1(2)
C5	C1	C6	125.6(3)	C211	O1	K1	107.35(19)
C5	C1	Fe1	69.85(14)	C201	O2	C202	113.1(3)
C6	C1	Fe1	129.19(18)	C201	O2	K1	115.9(2)
C1	C2	C3	107.3(3)	C202	O2	K1	117.4(2)
C1	C2	C7	126.5(3)	C203	O3	K1	112.1(2)
C1	C2	Fe1	71.04(14)	C204	O3	C203	112.3(3)
C3	C2	C7	126.2(3)	C204	O3	K1	106.0(2)
C3	C2	Fe1	68.66(14)	C205	O4	K1	117.2(2)
C7	C2	Fe1	127.5(2)	C206	O4	C205	112.9(3)
C2	C3	C8	126.2(3)	C206	O4	K1	116.0(2)
C2	C3	Fe1	70.23(14)	C207	O5	C208	111.1(3)
C4	C3	C2	107.9(2)	C207	O5	K1	113.8(2)
C4	C3	C8	125.7(3)	C208	O5	K1	115.4(2)
C4	C3	Fe1	70.05(15)	C209	O6	K1	118.7(2)
C8	C3	Fe1	128.9(2)	C210	O6	C209	111.3(3)
C3	C4	C9	125.6(3)	C210	O6	K1	118.6(2)
C3	C4	Fe1	68.98(15)	Fe2	Cl2	K1	117.72(3)
C5	C4	C3	108.0(2)	$C114^2$	K1	C204	102.97(8)
C5	C4	C9	126.4(3)	$C114^2$	K1	C211	84.34(7)
C5	C4	Fe1	71.04(15)	C211	K1	C204	156.63(12)
C9	C4	Fe1	128.05(19)	O1	K1	$C114^2$	70.62(6)
C1	C5	C4	108.2(3)	O1	K1	C204	139.80(10)
C1	C5	C10	124.2(3)	O1	K1	C211	22.95(8)
C1	C5	Fe1	70.38(15)	O1	K1	O3	118.84(8)
C4	C5	C10	127.6(3)	O1	K1	O4	166.52(7)
C4	C5	Fe1	68.67(15)	O1	K1	O5	112.78(7)
C10	C5	Fe1	127.28(19)	O1	K1	O6	59.78(7)
C12	C11	Fe1	68.74(12)	O1	K1	Cl2	96.70(5)
C14	C11	C12	89.92(19)	O2	K1	$C114^2$	81.13(7)

C14	C11	Fe1	66.66(13)	O2	K1	C204	79.16(10)
C111	C11	C12	138.8(2)	O2	K1	C211	80.13(10)
C111	C11	C14	130.8(2)	O2	K1	O1	60.70(8)
C111	C11	Fe1	116.85(16)	O2	K1	O3	59.97(9)
C11	C12	Fe1	68.45(12)	O2	K1	O4	120.06(8)
C13	C12	C11	89.82(19)	O2	K1	O5	154.19(7)
C13	C12	Fe1	66.62(12)	O2	K1	O6	120.47(8)
C121	C12	C11	138.4(2)	O2	K1	Cl2	99.12(6)
C121	C12	C13	131.1(2)	O3	K1	$C114^{2}$	87.05(7)
C121	C12	Fe1	116.34(16)	O3	K1	C204	22.89(9)
C12	C13	Fe1	70.38(13)	O3	K1	C211	140.03(10)
C14	C13	C12	90.45(19)	O3	K1	O5	113.66(8)
C14	C13	Fe1	68.15(13)	O3	K1	Cl2	105.75(6)
C131	C13	C12	134.0(2)	O4	K1	$C114^{2}$	95.98(7)
C131	C13	C14	131.8(2)	O4	K1	C204	42.87(10)
C131	C13	Fe1	134.94(17)	O4	K1	C211	159.68(10)
C11	C14	Fe1	70.09(13)	O4	K1	O3	60.09(8)
C13	C14	C11	89.81(18)	O4	K1	O5	60.02(8)
C13	C14	Fe1	68.12(13)	O4	K1	Cl2	96.40(5)
C141	C14	C11	132.6(2)	O5	K1	$C114^{2}$	73.39(6)
C141	C14	C13	133.4(2)	O5	K1	C204	102.31(10)
C141	C14	Fe1	135.89(17)	O5	K1	C211	101.05(9)
C112	C111	C11	120.9(2)	O5	K1	Cl2	106.57(5)
N1	C111	C11	120.4(2)	O6	K1	$C114^{2}$	79.19(7)
N1	C111	C112	118.7(2)	O6	K1	C204	160.17(10)
C113	C112	C111	120.5(2)	O6	K1	C211	42.50(9)
C112	C113	C114	119.7(2)	O6	K1	O3	165.79(7)
C113	C114	$K1^{1}$	112.95(18)	O6	K1	O4	117.50(8)
C115	C114	C113	117.8(2)	O6	K1	O5	59.01(7)
C115	C114	$K1^{1}$	106.56(17)	O6	K1	Cl2	88.34(5)
N1	C115	C114	123.5(2)	Cl2	K1	$C114^{2}$	165.46(5)
C122	C121	C12	121.0(2)	Cl2	K1	C204	91.30(7)
N2	C121	C12	119.5(2)	Cl2	K1	C211	81.40(6)
N2	C121	C122	119.5(2)	C2	Fe1	C1	40.30(11)
C123	C122	C121	120.1(2)	C2	Fe1	C5	67.94(11)

C122	C123	C124	119.7(3)	C3	Fe1	C1	68.02(11)
C125	C124	C123	118.3(2)	C3	Fe1	C2	41.11(11)
N2	C125	C124	122.7(3)	C3	Fe1	C4	40.97(13)
C132	C131	C13	120.6(2)	C3	Fe1	C5	68.18(12)
N3	C131	C13	117.5(2)	C4	Fe1	C1	67.57(11)
N3	C131	C132	121.9(2)	C4	Fe1	C2	68.75(11)
C133	C132	C131	118.8(2)	C4	Fe1	C5	40.29(11)
C134	C133	C132	120.3(3)	C5	Fe1	C1	39.78(11)
C133	C134	C135	117.7(3)	C11	Fe1	C1	114.05(10)
N3	C135	C134	123.8(3)	C11	Fe1	C2	125.40(11)
C146	C141	C14	119.4(2)	C11	Fe1	C3	157.61(12)
N4	C141	C14	118.7(2)	C11	Fe1	C4	161.42(11)
N4	C141	C146	121.8(2)	C11	Fe1	C5	128.77(10)
N4	C143	C144	124.5(3)	C11	Fe1	C12	42.81(9)
C143	C144	C145	117.4(3)	C12	Fe1	C1	133.52(10)
C146	C145	C144	119.6(3)	C12	Fe1	C2	167.35(11)
C145	C146	C141	119.4(3)	C12	Fe1	C3	151.47(11)
O1	C200	C201	109.6(3)	C12	Fe1	C4	121.64(11)
O2	C201	C200	108.1(3)	C12	Fe1	C5	114.43(10)
O2	C202	C203	108.2(3)	C13	Fe1	C1	176.29(10)
O3	C203	C202	108.4(3)	C13	Fe1	C2	142.66(10)
C205	C204	K1	84.4(2)	C13	Fe1	C3	115.68(11)
O3	C204	C205	108.3(3)	C13	Fe1	C4	114.91(11)
O3	C204	K1	51.06(16)	C13	Fe1	C5	140.41(11)
O4	C205	C204	110.4(3)	C13	Fe1	C11	62.67(10)
O4	C206	C207	109.3(3)	C13	Fe1	C12	43.00(9)
O5	C207	C206	109.5(3)	C13	Fe1	C14	43.73(10)
O5	C208	C209	108.7(3)	C14	Fe1	C1	135.38(11)
O6	C209	C208	108.6(3)	C14	Fe1	C2	112.85(11)
O6	C210	C211	108.9(3)	C14	Fe1	C3	118.48(11)
C210	C211	K1	85.53(19)	C14	Fe1	C4	148.37(11)
O1	C211	C210	109.1(3)	C14	Fe1	C5	171.34(11)
O1	C211	K1	49.69(15)	C14	Fe1	C11	43.25(9)
C111	N1	C115	119.6(2)	C14	Fe1	C12	62.81(9)
C111	N1	Fe2	121.03(16)	N1	Fe2	Cl1	108.76(6)

C115	N1	Fe2	117.81(16)	N1	Fe2	Cl2	111.01(6)
C121	N2	Fe2	121.63(16)	N2	Fe2	N1	103.06(8)
C125	N2	C121	119.6(2)	N2	Fe2	Cl1	108.32(6)
C125	N2	Fe2	117.25(17)	N2	Fe2	Cl2	111.52(6)
C135	N3	C131	117.5(2)	Cl2	Fe2	Cl1	113.60(3)

[1]1-X,1/2+Y,1/2-Z; [2]1-X,-1/2+Y,1/2-Z

4.5. Crystal and Refinement data of 4

Table S4.5.1 Crystal data and structure refinement for 4

Identification code	**4**
Empirical formula	$C_{54}H_{71}Cl_4FeKN_4O_8Zn_2$
Formula weight	1271.64
Temperature/K	123(2)
Crystal system	monoclinic
Space group	$P2_1/m$
a/Å	13.8686(8)
b/Å	14.3500(5)
c/Å	16.1195(7)
α/°	90.00
β/°	114.168(6)
γ/°	90.00
Volume/Å^3	2926.8(2)
Z	2
ρ_{calc}mg/mm^3	1.443
μ/mm^{-1}	5.669
F(000)	1320.0
Crystal size/mm^3	0.191 × 0.098 × 0.026
2Θ range for data collection	17.78 to 133.18°
Index ranges	$-14 \le h \le 16$, $-17 \le k \le 17$, $-19 \le l \le 19$
Reflections collected	15832
Independent reflections	5331 [R(int) = 0.0517]
Data/restraints/parameters	5331/25/366
Goodness-of-fit on F^2	1.018
Final R indexes [I>2σ (I)]	R_1 = 0.0654, wR_2 = 0.1678
Final R indexes [all data]	R_1 = 0.0883, wR_2 = 0.1864
Largest diff. peak/hole / e Å^{-3}	1.91/–0.55

Table S4.5.2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O4	161(7)	3326(6)	4066(6)	57(2)
C400	856(13)	3399(12)	3636(11)	86(5)
C401	834(12)	2456(16)	3197(11)	110(6)
C402	-320(14)	2254(15)	2833(13)	129(9)
C403	-676(13)	2859(18)	3408(16)	163(12)
C1	6254(4)	2994(4)	10115(4)	42.1(13)
C2	5467(4)	3309(4)	9263(4)	39.8(12)

C3	4988(6)	2500	8726(5)	40.2(17)
C4	6897(5)	3596(5)	10919(4)	53.9(16)
C5	5134(5)	4301(5)	8989(5)	52.2(15)
C6	4056(7)	2500	7828(6)	51(2)
C7	7926(4)	3010(3)	9046(3)	27.3(10)
C8	7071(4)	3019(3)	8122(3)	29.1(10)
C71	8466(4)	3747(3)	9688(3)	28.7(10)
C72	7987(4)	4609(3)	9675(3)	35.0(11)
C73	8523(4)	5288(4)	10293(4)	43.7(13)
C74	9529(5)	5112(4)	10938(4)	48.0(15)
C75	9957(4)	4263(4)	10939(3)	38.3(12)
C81	6658(4)	3774(4)	7469(3)	31.6(11)
C82	7228(5)	4610(4)	7599(3)	37.9(12)
C83	6787(5)	5376(4)	7053(4)	47.1(14)
C84	5795(5)	5301(4)	6358(4)	45.3(14)
C85	5310(5)	4442(4)	6212(3)	42.3(13)
N1	9462(3)	3594(3)	10313(3)	28.3(8)
N2	5711(3)	3691(3)	6744(3)	35.1(10)
Cl1	11849.5(15)	2500	11436.4(14)	45.0(5)
Cl2	10454.9(17)	2500	8875.1(12)	38.9(4)
Cl3	5621.4(17)	2500	4930.2(12)	41.4(4)
Cl4	3309.8(18)	2500	5462.4(17)	69.3(7)
Fe1	6565.8(9)	2500	9027.6(7)	29.2(3)
Zn1	10315.3(7)	2500	10209.5(6)	29.1(2)
Zn2	5063.3(8)	2500	6075.9(6)	37.0(3)
K1	0	5000	5000	52.7(5)
O1	1786(6)	5906(6)	4983(5)	67.9(19)
O2	-116(5)	5914(5)	3421(4)	50.7(15)
O3	-1940(5)	5213(4)	3552(4)	47.6(14)
C201	1751(8)	6176(7)	4159(6)	48(2)
C202	653(11)	6503(11)	3515(10)	86(4)
C203	-1139(10)	6212(9)	2867(8)	66(3)
C204	-1972(12)	5577(11)	2775(10)	75(4)
C205	-2794(12)	4705(11)	3551(10)	81(4)
C206	2747(9)	5589(9)	5593(7)	57(3)

O11	2179(10)	5375(8)	5821(8)	40(3)
O12	1012(10)	5931(8)	4062(8)	44(3)
O13	-1079(9)	5199(8)	3113(7)	39(2)
C221	2600(17)	6046(16)	5462(14)	51(5)
C222	2159(16)	5798(15)	4413(13)	51(5)
C223	589(13)	5823(12)	3166(11)	37(3)
C224	-714(12)	5913(10)	2771(9)	27(3)
C225	-2124(14)	5272(13)	2796(11)	29(4)
C226	-2616(14)	4496(12)	3249(11)	34(3)
O5	5053(18)	2500	2366(12)	203(8)
C301	4163(8)	3037(10)	954(7)	131(6)
C302	4891(13)	3306(8)	1839(7)	127(5)

Table S4.5.3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O4	58(6)	52(5)	56(5)	0(4)	18(5)	-7(4)
C400	94(13)	85(12)	75(10)	3(9)	31(10)	12(10)
C401	112(12)	129(14)	83(9)	-50(17)	33(9)	20(20)
C402	146(16)	150(20)	83(11)	-17(13)	38(12)	30(17)
C403	200(20)	160(30)	120(17)	-18(16)	47(18)	50(20)
C1	33(3)	61(3)	32(3)	-8(2)	13(2)	1(3)
C2	29(3)	52(3)	38(3)	-5(2)	13(2)	6(2)
C3	34(4)	50(4)	37(4)	0	14(3)	0
C4	43(3)	78(4)	38(3)	-16(3)	15(3)	-4(3)
C5	42(3)	57(4)	57(4)	-2(3)	18(3)	16(3)
C6	33(4)	69(6)	44(4)	0	6(4)	0
C7	26(2)	28(2)	27(2)	-0.2(19)	10.0(19)	3(2)
C8	25(2)	30(3)	28(2)	-3.2(19)	6.5(19)	-2(2)
C71	27(2)	31(2)	25(2)	0.5(19)	6.6(19)	-1(2)
C72	30(3)	32(2)	36(3)	1(2)	6(2)	3(2)
C73	35(3)	34(3)	49(3)	-6(2)	5(3)	5(2)
C74	39(3)	33(3)	53(3)	-16(3)	0(3)	0(2)
C75	32(3)	37(3)	32(2)	-4(2)	-1(2)	3(2)
C81	29(3)	37(3)	24(2)	2(2)	7(2)	7(2)
C82	40(3)	37(3)	31(2)	6(2)	9(2)	-2(2)

C83	57(4)	39(3)	36(3)	5(2)	9(3)	-1(3)
C84	57(4)	39(3)	34(3)	10(2)	13(3)	10(3)
C85	42(3)	46(3)	28(2)	4(2)	4(2)	10(3)
N1	26(2)	28.5(19)	25.8(18)	-0.5(16)	6.1(16)	-2.4(17)
N2	34(2)	39(2)	24.8(19)	-3.9(17)	4.4(18)	3.3(19)
Cl1	27.9(9)	45.1(10)	48.6(10)	0	1.9(8)	0
Cl2	56.7(12)	28.7(8)	37.7(9)	0	26.0(9)	0
Cl3	52.0(12)	37.8(9)	31.8(8)	0	14.5(8)	0
Cl4	30.8(11)	107(2)	52.5(12)	0	-0.4(9)	0
Fe1	23.5(6)	35.0(6)	24.8(5)	0	5.6(4)	0
Zn1	26.0(5)	29.8(5)	29.0(5)	0	8.5(4)	0
Zn2	30.4(5)	42.2(5)	29.2(5)	0	2.8(4)	0
K1	37.0(9)	78.6(13)	34.3(8)	14.6(9)	6.3(7)	-10.8(9)
O5	270(20)	189(18)	148(14)	0	82(15)	0
C301	76(6)	228(16)	105(7)	80(9)	54(6)	54(8)
C302	211(15)	81(7)	77(6)	-7(5)	49(8)	37(8)

Table S4.5.4 Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O4	C400	1.402(9)	Fe1	$C2^1$	2.071(6)
O4	C403	1.383(10)	Fe1	$C7^1$	2.013(5)
O4	K1	2.892(9)	Fe1	$C8^1$	2.004(5)
C400	C401	1.522(10)	Zn1	$N1^1$	2.013(4)
C401	C402	1.491(10)	Zn2	$N2^1$	2.023(4)
C402	C403	1.493(9)	K1	$O1^2$	2.807(8)
C1	$C1^1$	1.417(13)	K1	O1	2.807(8)
C1	C2	1.434(8)	K1	O2	2.808(6)
C1	C4	1.508(8)	K1	$O2^2$	2.808(6)
C1	Fe1	2.094(5)	K1	$O3^2$	2.764(6)
C2	C3	1.438(7)	K1	O3	2.764(6)
C2	C5	1.506(9)	K1	$O11^2$	2.811(12)
C2	Fe1	2.071(6)	K1	O11	2.811(12)
C3	$C2^1$	1.438(7)	K1	$O12^2$	2.789(13)
C3	C6	1.494(11)	K1	O12	2.789(13)
C3	Fe1	2.037(8)	K1	$O13^2$	2.801(11)
C7	$C7^1$	1.464(9)	K1	O13	2.801(11)

C7	C8	1.476(6)	O1	C201	1.366(12)
C7	C71	1.454(7)	O1	C206	1.370(13)
C7	Fe1	2.013(5)	O2	C202	1.320(15)
C8	C8[1]	1.490(10)	O2	C203	1.399(13)
C8	C81	1.454(7)	O3	C204	1.341(15)
C8	Fe1	2.004(5)	O3	C205	1.391(15)
C71	C72	1.400(7)	C201	C202	1.524(17)
C71	N1	1.354(6)	C203	C204	1.430(19)
C72	C73	1.374(8)	C205	C206[2]	1.418(18)
C73	C74	1.380(8)	C206	C205[2]	1.418(18)
C74	C75	1.356(8)	O11	C221	1.37(2)
C75	N1	1.357(6)	O11	C226[2]	1.38(2)
C81	C82	1.404(8)	O12	C222	1.47(2)
C81	N2	1.359(6)	O12	C223	1.33(2)
C82	C83	1.385(8)	O13	C224	1.356(18)
C83	C84	1.377(8)	O13	C225	1.33(2)
C84	C85	1.378(9)	C221	C222	1.58(3)
C85	N2	1.349(7)	C223	C224	1.66(2)
N1	Zn1	2.013(4)	C225	C226	1.63(2)
N2	Zn2	2.023(4)	C226	O11[2]	1.38(2)
Cl1	Zn1	2.234(2)	O5	C302[1]	1.398(13)
Cl2	Zn1	2.2371(19)	O5	C302	1.398(13)
Cl3	Zn2	2.276(2)	C301	C301[1]	1.54(3)
Cl4	Zn2	2.219(2)	C301	C302	1.423(15)
Fe1	C1[1]	2.094(5)			

[1]+X,1/2-Y,+Z; [2]-X,1-Y,1-Z

Table S4.5.5 Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C400	O4	K1	114.2(8)	N2	Zn2	Cl4	113.83(13)
C403	O4	C400	100.8(14)	N2[1]	Zn2	Cl4	113.83(13)
C403	O4	K1	125.6(10)	Cl4	Zn2	Cl3	108.25(9)
O4	C400	C401	106.1(11)	O1	K1	O1[2]	180.0
C402	C401	C400	99.7(8)	O1[2]	K1	O2	120.1(2)
C401	C402	C403	102.6(6)	O1	K1	O2	59.9(2)
O4	C403	C402	111.8(11)	O1	K1	O2[2]	120.1(2)

C1[1]	C1	C2	108.4(3)	O1[2]	K1	O2[2]	59.9(2)
C1[1]	C1	C4	125.0(4)	O1	K1	O11	29.9(3)
C1[1]	C1	Fe1	70.22(18)	O1[2]	K1	O11	150.1(3)
C2	C1	C4	126.4(6)	O1	K1	O11[2]	150.1(3)
C2	C1	Fe1	69.0(3)	O1[2]	K1	O11[2]	29.9(3)
C4	C1	Fe1	131.3(4)	O2	K1	O2[2]	180.000(1)
C1	C2	C3	107.8(5)	O2[2]	K1	O11	90.6(3)
C1	C2	C5	127.0(5)	O2	K1	O11[2]	90.6(3)
C1	C2	Fe1	70.7(3)	O2	K1	O11	89.4(3)
C3	C2	C5	125.2(5)	O2[2]	K1	O11[2]	89.4(3)
C3	C2	Fe1	68.3(4)	O3[2]	K1	O1	60.1(2)
C5	C2	Fe1	129.5(4)	O3	K1	O1	119.9(2)
C2	C3	C2[1]	107.7(7)	O3	K1	O1[2]	60.1(2)
C2	C3	C6	125.9(3)	O3[2]	K1	O1[2]	119.9(2)
C2[1]	C3	C6	125.9(3)	O3[2]	K1	O2[2]	60.53(19)
C2	C3	Fe1	70.8(4)	O3	K1	O2[2]	119.47(19)
C2[1]	C3	Fe1	70.8(4)	O3[2]	K1	O2	119.47(19)
C6	C3	Fe1	130.5(6)	O3	K1	O2	60.53(19)
C7[1]	C7	C8	90.5(3)	O3	K1	O3[2]	180.000(1)
C7[1]	C7	Fe1	68.67(13)	O3[2]	K1	O11	30.3(3)
C8	C7	Fe1	68.2(3)	O3[2]	K1	O11[2]	149.7(3)
C71	C7	C7[1]	136.6(3)	O3	K1	O11	149.7(3)
C71	C7	C8	132.7(4)	O3	K1	O11[2]	30.3(3)
C71	C7	Fe1	118.7(3)	O3[2]	K1	O12	88.8(3)
C7	C8	C8[1]	89.5(3)	O3	K1	O12	91.2(3)
C7	C8	Fe1	68.7(3)	O3[2]	K1	O12[2]	91.2(3)
C8[1]	C8	Fe1	68.18(14)	O3	K1	O12[2]	88.8(3)
C81	C8	C7	130.7(4)	O3	K1	O13[2]	146.2(3)
C81	C8	C8[1]	138.1(3)	O3[2]	K1	O13	146.2(3)
C81	C8	Fe1	130.7(4)	O3	K1	O13	33.8(3)
C72	C71	C7	121.9(4)	O3[2]	K1	O13[2]	33.8(3)
N1	C71	C7	118.9(4)	O11[2]	K1	O11	180.0(3)
N1	C71	C72	119.2(4)	O12	K1	O1[2]	150.3(3)
C73	C72	C71	120.3(5)	O12[2]	K1	O1[2]	29.7(3)
C72	C73	C74	119.7(5)	O12	K1	O1	29.7(3)

C75	C74	C73	118.2(5)	O12^{2}	K1	O1	150.3(3)
C74	C75	N1	123.2(5)	O12^{2}	K1	O2^{2}	30.7(3)
C82	C81	C8	119.8(4)	O12	K1	O2	30.7(3)
N2	C81	C8	120.8(5)	O12^{2}	K1	O2	149.3(3)
N2	C81	C82	119.4(5)	O12	K1	O2^{2}	149.3(3)
C83	C82	C81	120.5(5)	O12^{2}	K1	O11	121.3(4)
C84	C83	C82	119.3(6)	O12	K1	O11	58.7(4)
C83	C84	C85	117.7(5)	O12^{2}	K1	O11^{2}	58.7(4)
N2	C85	C84	124.1(5)	O12	K1	O11^{2}	121.3(3)
C71	N1	C75	119.3(4)	O12	K1	O12^{2}	180.000(1)
C71	N1	Zn1	121.3(3)	O12^{2}	K1	O13^{2}	61.7(3)
C75	N1	Zn1	118.5(3)	O12	K1	O13^{2}	118.3(3)
C81	N2	Zn2	126.4(3)	O12	K1	O13	61.7(3)
C85	N2	C81	118.6(5)	O12^{2}	K1	O13	118.3(3)
C85	N2	Zn2	111.0(3)	O13	K1	O1	91.4(3)
C1	Fe1	C1^{1}	39.6(4)	O13^{2}	K1	O1	88.6(3)
C2	Fe1	C1^{1}	67.4(2)	O13^{2}	K1	O1^{2}	91.4(3)
C2^{1}	Fe1	C1^{1}	40.3(2)	O13	K1	O1^{2}	88.6(3)
C2	Fe1	C1	40.3(2)	O13^{2}	K1	O2	147.0(3)
C2^{1}	Fe1	C1	67.4(2)	O13^{2}	K1	O2^{2}	33.0(3)
C2	Fe1	C2^{1}	68.2(3)	O13	K1	O2^{2}	147.0(3)
C3	Fe1	C1	68.3(3)	O13	K1	O2	33.0(3)
C3	Fe1	C1^{1}	68.3(3)	O13^{2}	K1	O11	61.0(3)
C3	Fe1	C2	41.0(2)	O13	K1	O11	119.0(3)
C3	Fe1	C2^{1}	41.0(2)	O13	K1	O11^{2}	61.0(3)
C7^{1}	Fe1	C1	128.7(2)	O13^{2}	K1	O11^{2}	119.0(3)
C7	Fe1	C1	112.2(2)	O13	K1	O13^{2}	180.000(2)
C7^{1}	Fe1	C1^{1}	112.2(2)	C201	O1	K1	117.4(6)
C7	Fe1	C1^{1}	128.7(2)	C201	O1	C206	115.4(9)
C7^{1}	Fe1	C2	163.2(2)	C206	O1	K1	116.3(7)
C7	Fe1	C2	123.3(2)	C202	O2	K1	116.8(7)
C7^{1}	Fe1	C2^{1}	123.3(2)	C202	O2	C203	116.0(9)
C7	Fe1	C2^{1}	163.2(2)	C203	O2	K1	112.9(6)
C7^{1}	Fe1	C3	155.77(17)	C204	O3	K1	118.7(8)
C7	Fe1	C3	155.77(17)	C204	O3	C205	120.1(10)

C7[1]	Fe1	C7	42.7(3)	C205	O3	K1	118.5(7)
C8	Fe1	C1	137.6(2)	O1	C201	C202	112.2(10)
C8[1]	Fe1	C1	171.8(2)	O2	C202	C201	114.6(11)
C8	Fe1	C1[1]	171.8(2)	O2	C203	C204	115.9(11)
C8[1]	Fe1	C1[1]	137.6(2)	O3	C204	C203	115.8(12)
C8[1]	Fe1	C2	147.7(2)	O3	C205	C206[2]	117.1(12)
C8	Fe1	C2[1]	147.7(2)	O1	C206	C205[2]	116.2(11)
C8	Fe1	C2	115.4(2)	C221	O11	K1	119.8(11)
C8[1]	Fe1	C2[1]	115.4(2)	C221	O11	C226[2]	106.9(13)
C8[1]	Fe1	C3	119.2(2)	C226[2]	O11	K1	116.5(10)
C8	Fe1	C3	119.2(2)	C222	O12	K1	115.8(10)
C8	Fe1	C7	43.12(18)	C223	O12	K1	116.0(10)
C8[1]	Fe1	C7	62.64(19)	C223	O12	C222	109.3(14)
C8[1]	Fe1	C7[1]	43.12(18)	C224	O13	K1	113.3(9)
C8	Fe1	C7[1]	62.64(19)	C225	O13	K1	116.0(9)
C8[1]	Fe1	C8	43.6(3)	C225	O13	C224	108.4(13)
N1[1]	Zn1	N1	102.5(2)	O11	C221	C222	104.4(16)
N1[1]	Zn1	Cl1	107.80(12)	O12	C222	C221	105.5(16)
N1	Zn1	Cl1	107.80(12)	O12	C223	C224	109.5(13)
N1[1]	Zn1	Cl2	111.39(12)	O13	C224	C223	108.4(12)
N1	Zn1	Cl2	111.39(12)	O13	C225	C226	111.5(14)
Cl1	Zn1	Cl2	115.16(9)	O11[2]	C226	C225	108.5(13)
N2	Zn2	N2[1]	115.2(2)	C302[1]	O5	C302	111.7(15)
N2	Zn2	Cl3	101.97(13)	C302	C301	C301[1]	105.7(7)
N2[1]	Zn2	Cl3	101.97(13)	O5	C302	C301	104.8(13)

[1]+X,1/2-Y,+Z; [2]-X,1-Y,1-Z

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