Electronic Supporting Information

Long-range ferromagnetic coupling through spin polarization in a linear heterotrinuclear iron(III)-copper(II)-iron(III) complex derived from 5-ferrocenyl-2-aminotropone

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contents

1. Synthesis

Synthesis of ligand 2a

To a THF solution (3 mL) of ferrocene (559 mg, 3.01 mmol) was added *t*-butyllithium (3.2 mmol) in pentane at 0°C. After stirring for 30 min, zinc(II) chloride (442 mg, 3.25 mmol) in 3 mL of THF was added to the reaction mixture. Then, after additional stirring for 1 h at 0°C and for 20 min at rt, a mixture of 5-bromo-2-methoxytropone (323 mg, 1.50 mmol) and tetrakis(triphenylphosphine)palladium (182 mg, 0.16 mmol) in 15 mL of THF was added and stirred for 2 h. A standard workup and column chromatography (SiO_2 / hexane:ethyl acetate (2:1)) gave 5-ferrocenyl-2-methoxytropone (388 mg, 1.21 mmol) in 81% yield. Ligand **2a** was quantitatively obtained by overnight reaction of 5-ferrocenyl-2-methoxytropone with ethylamine in THF at 50°C after a short column chromatography (SiO_2 / hexane:ethyl acetate (1:1)); ^{1}H NMR(500 MHz, $CDCl_3$) δ 7.57(d, 1H), 7.44(d, 1H), 7.14(d, 1H), 7.02(s, 1H), 6.50(d, 1H), 4.55(s, 2H), 4.34(s, 2H), 4.09(s, 5H), 3.36(q, 2H), 1.40(t, 3H); ^{13}C NMR(125 MHz, $CDCl_3$) δ 175.9, 153.8, 136.5, 133.8, 133.0, 128.3, 108.9, 88.4, 69.6, 69.3, 66.6, 37.5, 13.8. Anal. Calcd for $C_{19}H_{19}FeNO$: C, 68.49, H, 5.75, N, 4.20. Found: C, 68.26, H, 5.80, N, 4.25.

Synthesis of ligand 2b

Same procedure was applied for the synthesis of **2b** using diethylamine. ^{1}H NMR(500 MHz, $CDCl_3$) δ 7.34(dd, 1H), 7.17(dd, 1H), 6.91(d, 1H), 6.50(s, 1H), 4.52(t, 2H), 4.32(t, 2H), 4.01(s, 5H), 3.53(q, 4H), 1.24(t, 6H); ^{13}C NMR(125 MHz, $CDCl_3$) δ 180.7, 1535.3, 134.6, 134.1, 131.6, 129.7, 114.5, 87.9, 69.6, 69.3, 66.4, 45.9, 12.7. Anal. Calcd for $C_{21}H_{23}FeNO$: C, 69.82, H, 6.42, N, 3.88. Found: C, 69.42, H, 6.40, N, 3.96.

Synthesis of ferrocenium ion $2b^+ClO_4^-$

To a dichloromethane solution (4 mL) of **2b** (20 mg, 0.045 mmol) was added $Fe(ClO_4)_3$ (24 mg, 0.067 mmol) in acetonitrile (6 mL) at -50°C. After stirring for 5 min, volatiles were removed in vacuo and the residue was redissolved in 3 mL of dichloromethane. The solution was filtered and toluene was added for reprecipitation. The precipitate was centrifuged, washed with toluene, and recrystallized from dichloromethane and toluene to give $\mathbf{2b}^+ClO_4^-$ (14 mg, 0.025 mmol, 58%) as dark blue crystals: Anal. Calcd for $C_{21}H_{23}ClFeNO_5$: C, 54.75, H, 5.03, N, 3.04. Found: C, 55.09, H, 5.20, N, 3.26.

Synthesis of copper complex 1

Copper complex **1** was synthesized by the reaction of **2** (63.1 mg, 0.189 mmol) in dichloromethane (5 mL) with copper(II) acetate (17.0 mg, 0.0946 mmol) in methanol (5 mL) in the presence of sodium acetate (34.4 mg, 0.42 mmol) for 1h. The precipitates formed were collected and recrystallized from THF and *iso*-propyl ether to give the pure product (68.1 mg, 0.0936 mmol, 99%) as orange crystals: Anal calcd for $C_{38}H_{36}CuFe_2N_2O_2$: C, 62.70, H, 4.98, N, 3.85; found C, 62.57, H, 5.08, N, 3.85.

Electrochemical oxidation of 1

Single crystals of $\mathbf{1}^{2+}$ $2PF_6^-$ $C_2H_4Cl_2$ were obtained by electrochemical oxidation with a constant current of 1.0 μA from dichloroethane solution (10 mL) of **1** (4.0 mg), few drops of methanol, and tetra-*n*-butylammonium hexafluorophosphate (387 mg) as electrolyte. After a week, a few mg of the product was obtained as black crystals.

2. UV-vis-NIR spectra, ESR spectra, CV and SQUID

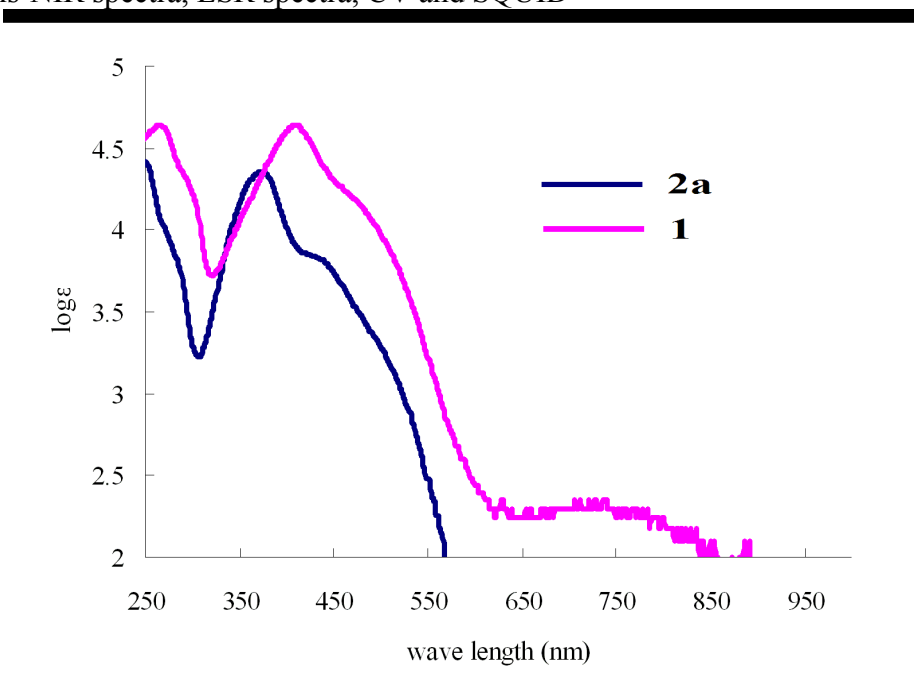


Figure S1. UV-vis spectra of **1** and **2a**.

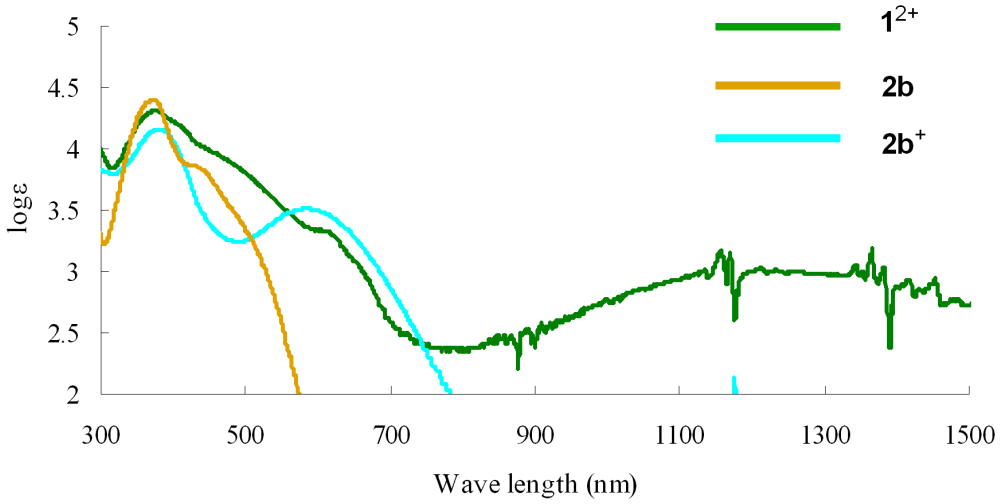


Figure S2. UV-vis-NIR spectra of **1**$^{2+}$, **2b** and **2b**$^{+}$.

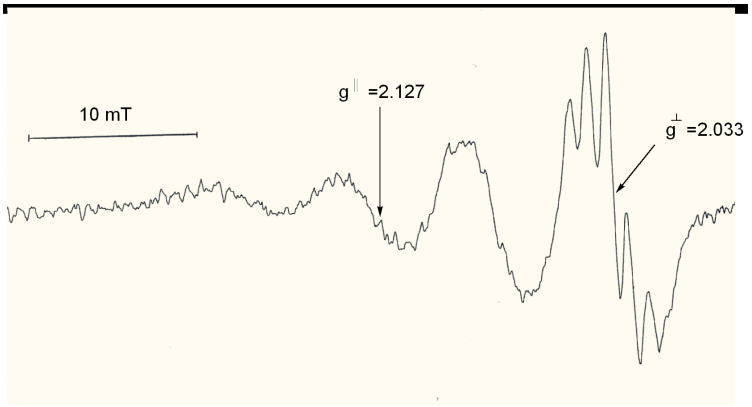


Figure S3. ESR spectra of **1** in THF at rt.

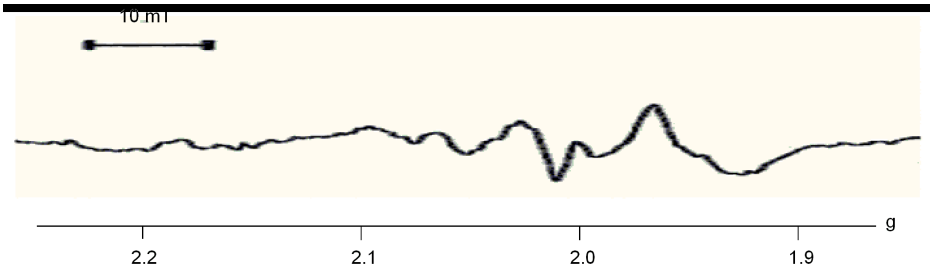


Figure S4. ESR spectra of $\mathbf{1}^{2+}$ in acetonitrile at rt.

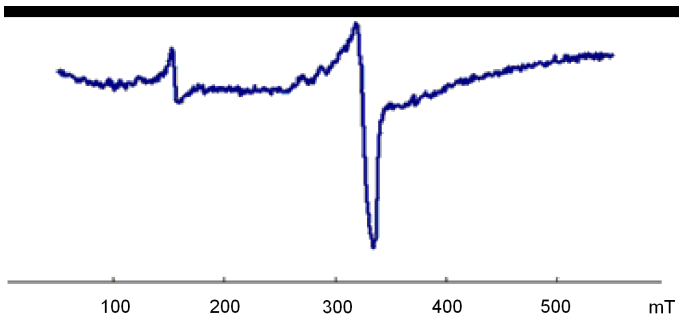


Figure S5. ESR spectra of $\mathbf{2b}^{+}$ ClO_4^- in the solid state at 10 K.

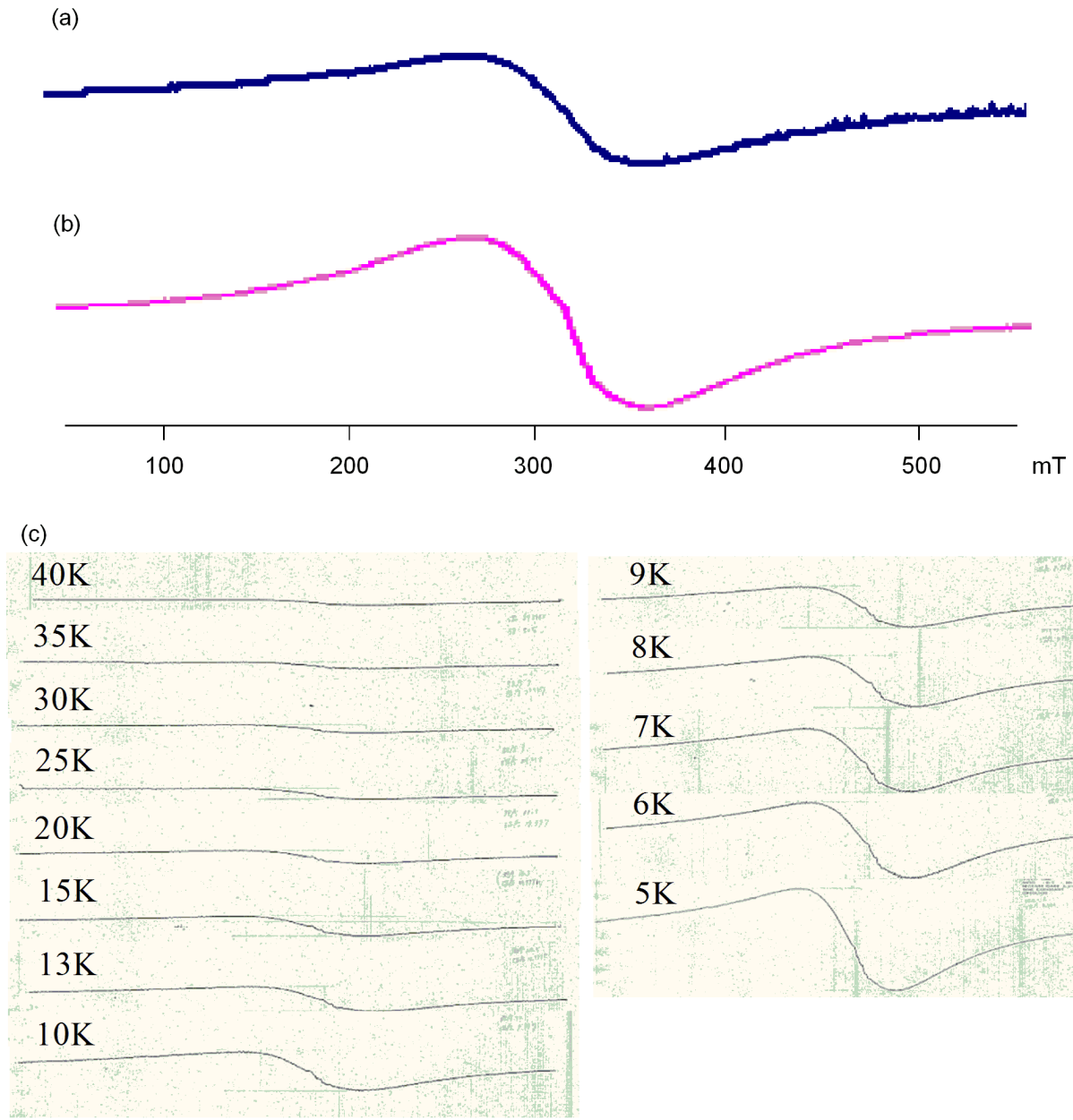


Figure S6. ESR spectra of $\mathbf{1}^{2+}$ $2PF_6^-$ at 7 K in (a) the solid state and (b) a flozen solution of CH_3CN and (c) VT measurements of the solid sample.

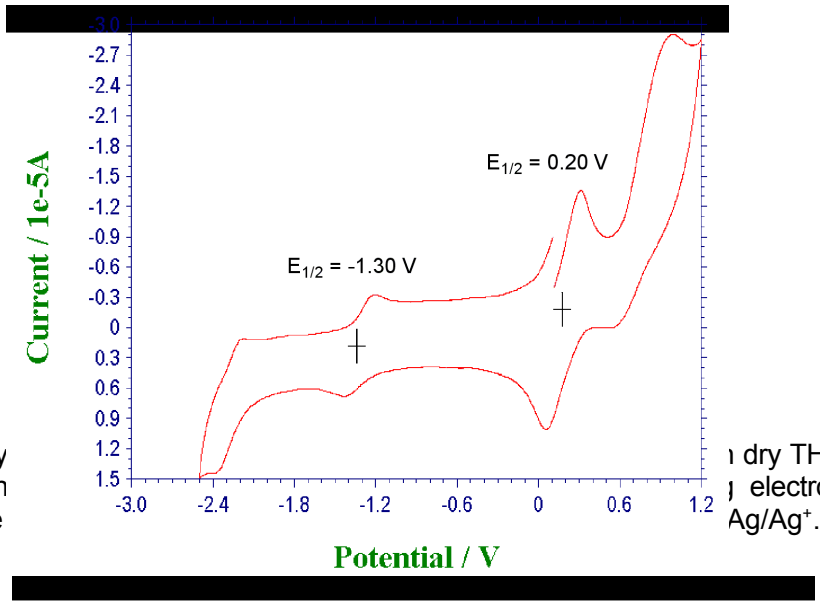


Figure S7. Cy ı dry THF under N_2 at r.t; referen ȷ electrode: glassy carbon. In the Ag/Ag$^+$.

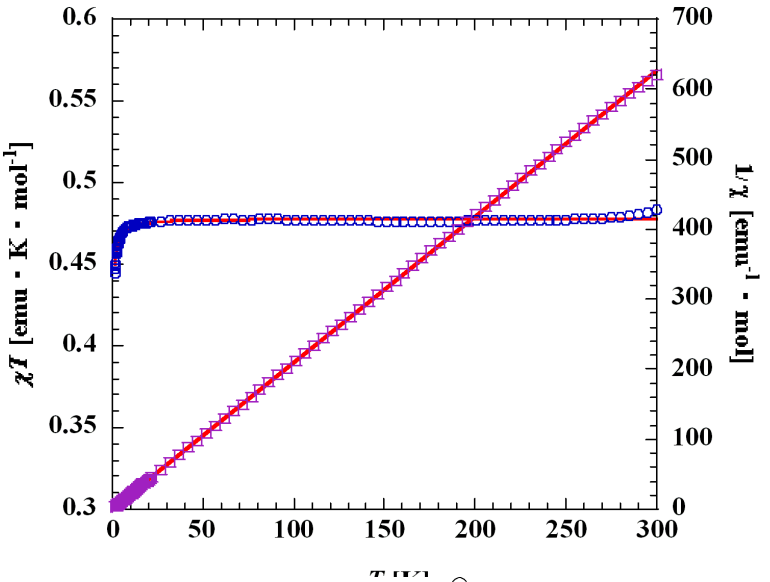
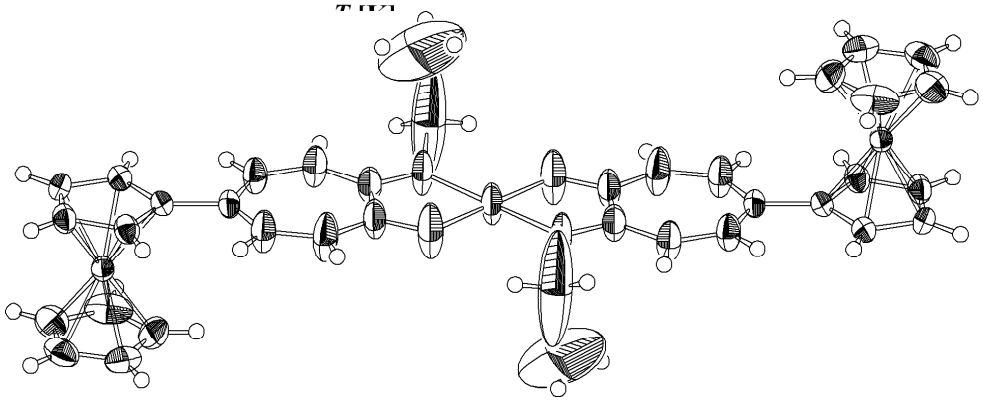


Figure S8. Th $_{M}T$ data; (□) experimental 1

3. X-ray analys

(a



(b)

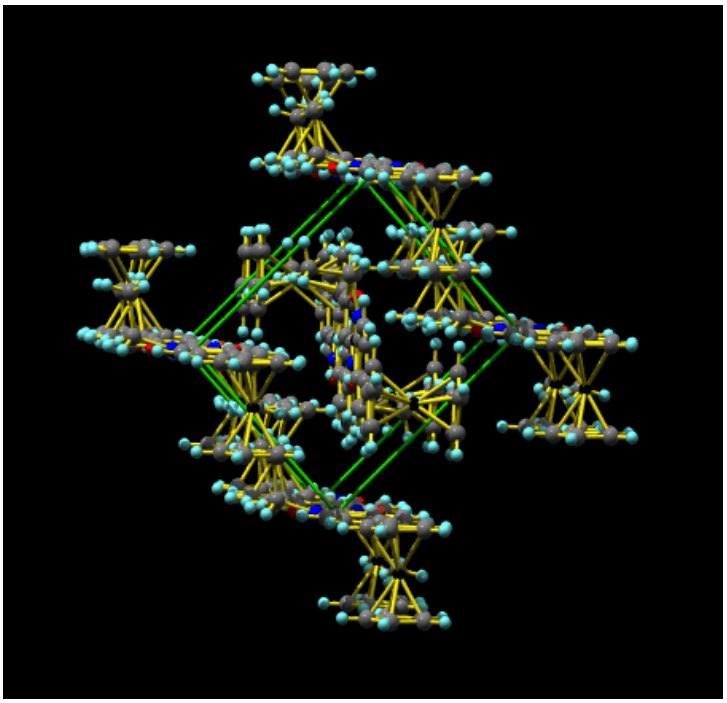


Figure S9. X-ray structure of **1**. (a) ORTEP drawing (50% probability) (b) Packing structure.

Table S1. Crystal data and structure refinement for **1**.

Identification code	**1**	
Empirical formula	C38 H36 Cu Fe2 N2 O2	
Formula weight	727.93	
Temperature	123(2) K	
Wavelength	0.71069 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 20.359(5) Å	α= 90°.
	b = 9.756(9) Å	β= 98.43(3)°.
	c = 8.232(4) Å	γ = 90°.
Volume	1617.4(17) $Å^3$	
Z	2	
Density (calculated)	1.495 Mg/m^3	
Absorption coefficient	1.573 mm^{-1}	
F(000)	750	
Crystal size	0.20 x 0.15 x 0.12 mm^3	

Theta range for data collection	2.91 to 27.52°.
Index ranges	-26<=h<=26, 0<=k<=12, -10<=l<=0
Reflections collected	3997
Independent reflections	3731 [R(int) = 0.0287]
Completeness to theta = 27.52°	99.8 %
Max. and min. transmission	0.8337 and 0.7438
Refinement method	Full-matrix least-squares on F_2
Data / restraints / parameters	3731 / 0 / 205
Goodness-of-fit on F_2	1.164
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1600
R indices (all data)	R1 = 0.0958, wR2 = 0.1799
Largest diff. peak and hole	0.891 and -0.908 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for **1**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	-3796(1)	138(1)	3585(1)	31(1)
Cu(2)	0	0	0	67(1)
C(32)	-3553(2)	2072(4)	2984(5)	38(1)
C(33)	-4248(2)	1972(4)	2944(5)	40(1)
C(5)	-3351(2)	1117(4)	1835(4)	34(1)
C(6)	-2664(2)	895(4)	1473(5)	38(1)
C(7)	-3933(2)	401(4)	1116(4)	38(1)
C(8)	-4485(2)	940(4)	1791(5)	41(1)
C(9)	-4236(3)	-1333(5)	4816(6)	58(1)
C(10)	-3951(3)	-333(5)	5907(6)	54(1)
O(4)	-455(2)	1158(5)	1364(6)	101(2)
C(12)	-3131(2)	-1247(5)	4685(6)	60(1)
N(5)	-883(2)	-628(5)	-726(6)	67(1)
C(14)	-3280(2)	-282(5)	5851(6)	53(1)
C(15)	-1093(2)	959(6)	1235(6)	64(2)

C(16)	-2011(2)	-469(5)	-355(7)	58(1)
C(17)	-2570(2)	-68(4)	286(6)	49(1)
C(18)	-1346(2)	-89(5)	16(6)	54(1)
C(20)	-2151(2)	1685(6)	2297(7)	65(2)
C(21)	-3733(3)	-1901(5)	4035(6)	67(2)
C(22)	-1484(2)	1712(7)	2172(8)	81(2)
C(31)	-1073(5)	-1458(17)	-2450(30)	307(14)
C(34)	-1320(12)	-390(30)	-3990(30)	540(30)

Table S3. Bond lengths [Å] and angles [°] for **1.**.

Fe(1)-C(21)	2.024(5)
Fe(1)-C(7)	2.027(4)
Fe(1)-C(32)	2.030(4)
Fe(1)-C(12)	2.030(4)
Fe(1)-C(10)	2.035(4)
Fe(1)-C(9)	2.038(4)
Fe(1)-C(8)	2.039(4)
Fe(1)-C(14)	2.043(4)
Fe(1)-C(33)	2.045(4)
Fe(1)-C(5)	2.047(4)
Cu(2)-N(5)	1.910(4)
Cu(2)-N(5)#1	1.910(4)
Cu(2)-O(4)#1	1.924(4)
Cu(2)-O(4)	1.924(4)
C(32)-C(33)	1.414(5)
C(32)-C(5)	1.430(5)
C(33)-C(8)	1.418(6)
C(5)-C(7)	1.428(5)
C(5)-C(6)	1.488(5)
C(6)-C(17)	1.389(6)
C(6)-C(20)	1.392(6)
C(7)-C(8)	1.426(5)
C(9)-C(10)	1.393(7)
C(9)-C(21)	1.400(7)

C(10)-C(14)	1.374(7)
O(4)-C(15)	1.301(5)
C(12)-C(14)	1.409(7)
C(12)-C(21)	1.416(7)
N(5)-C(18)	1.308(5)
N(5)-C(31)	1.630(14)
C(15)-C(22)	1.396(7)
C(15)-C(18)	1.472(6)
C(16)-C(17)	1.380(6)
C(16)-C(18)	1.393(6)
C(20)-C(22)	1.376(6)
C(31)-C(34)	1.66(3)

C(21)-Fe(1)-C(7)	107.65(18)
C(21)-Fe(1)-C(32)	161.3(2)
C(7)-Fe(1)-C(32)	68.95(16)
C(21)-Fe(1)-C(12)	40.9(2)
C(7)-Fe(1)-C(12)	121.10(19)
C(32)-Fe(1)-C(12)	123.89(19)
C(21)-Fe(1)-C(10)	67.69(19)
C(7)-Fe(1)-C(10)	162.31(19)
C(32)-Fe(1)-C(10)	121.06(18)
C(12)-Fe(1)-C(10)	67.4(2)
C(21)-Fe(1)-C(9)	40.3(2)
C(7)-Fe(1)-C(9)	125.56(19)
C(32)-Fe(1)-C(9)	156.34(19)
C(12)-Fe(1)-C(9)	67.8(2)
C(10)-Fe(1)-C(9)	40.0(2)
C(21)-Fe(1)-C(8)	121.9(2)
C(7)-Fe(1)-C(8)	41.05(15)
C(32)-Fe(1)-C(8)	68.46(16)
C(12)-Fe(1)-C(8)	157.2(2)
C(10)-Fe(1)-C(8)	125.58(18)
C(9)-Fe(1)-C(8)	108.93(19)
C(21)-Fe(1)-C(14)	68.0(2)
C(7)-Fe(1)-C(14)	156.59(18)

C(32)-Fe(1)-C(14)	107.34(18)
C(12)-Fe(1)-C(14)	40.5(2)
C(10)-Fe(1)-C(14)	39.4(2)
C(9)-Fe(1)-C(14)	67.0(2)
C(8)-Fe(1)-C(14)	160.97(19)
C(21)-Fe(1)-C(33)	157.0(2)
C(7)-Fe(1)-C(33)	68.91(16)
C(32)-Fe(1)-C(33)	40.60(15)
C(12)-Fe(1)-C(33)	160.6(2)
C(10)-Fe(1)-C(33)	108.29(17)
C(9)-Fe(1)-C(33)	121.99(19)
C(8)-Fe(1)-C(33)	40.65(16)
C(14)-Fe(1)-C(33)	124.22(18)
C(21)-Fe(1)-C(5)	124.40(19)
C(7)-Fe(1)-C(5)	41.03(15)
C(32)-Fe(1)-C(5)	41.07(14)
C(12)-Fe(1)-C(5)	106.86(18)
C(10)-Fe(1)-C(5)	155.79(19)
C(9)-Fe(1)-C(5)	161.88(19)
C(8)-Fe(1)-C(5)	68.88(15)
C(14)-Fe(1)-C(5)	120.99(18)
C(33)-Fe(1)-C(5)	68.86(15)
N(5)-Cu(2)-N(5)#1	180.0
N(5)-Cu(2)-O(4)#1	98.09(16)
N(5)#1-Cu(2)-O(4)#1	81.91(16)
N(5)-Cu(2)-O(4)	81.91(16)
N(5)#1-Cu(2)-O(4)	98.09(16)
O(4)#1-Cu(2)-O(4)	180.0
C(33)-C(32)-C(5)	108.9(3)
C(33)-C(32)-Fe(1)	70.3(2)
C(5)-C(32)-Fe(1)	70.1(2)
C(32)-C(33)-C(8)	107.8(3)
C(32)-C(33)-Fe(1)	69.1(2)
C(8)-C(33)-Fe(1)	69.4(2)
C(7)-C(5)-C(32)	106.9(3)
C(7)-C(5)-C(6)	126.4(3)

C(32)-C(5)-C(6)	126.7(3)
C(7)-C(5)-Fe(1)	68.7(2)
C(32)-C(5)-Fe(1)	68.8(2)
C(6)-C(5)-Fe(1)	126.8(3)
C(17)-C(6)-C(20)	123.1(4)
C(17)-C(6)-C(5)	118.0(3)
C(20)-C(6)-C(5)	118.8(4)
C(8)-C(7)-C(5)	108.2(3)
C(8)-C(7)-Fe(1)	69.9(2)
C(5)-C(7)-Fe(1)	70.2(2)
C(33)-C(8)-C(7)	108.2(3)
C(33)-C(8)-Fe(1)	69.9(2)
C(7)-C(8)-Fe(1)	69.0(2)
C(10)-C(9)-C(21)	108.1(4)
C(10)-C(9)-Fe(1)	69.9(3)
C(21)-C(9)-Fe(1)	69.3(3)
C(14)-C(10)-C(9)	109.0(4)
C(14)-C(10)-Fe(1)	70.6(3)
C(9)-C(10)-Fe(1)	70.1(3)
C(15)-O(4)-Cu(2)	115.1(3)
C(14)-C(12)-C(21)	107.3(4)
C(14)-C(12)-Fe(1)	70.3(3)
C(21)-C(12)-Fe(1)	69.3(3)
C(18)-N(5)-C(31)	120.8(5)
C(18)-N(5)-Cu(2)	115.8(3)
C(31)-N(5)-Cu(2)	121.6(4)
C(10)-C(14)-C(12)	108.2(4)
C(10)-C(14)-Fe(1)	70.0(3)
C(12)-C(14)-Fe(1)	69.2(3)
O(4)-C(15)-C(22)	121.3(5)
O(4)-C(15)-C(18)	113.9(4)
C(22)-C(15)-C(18)	124.8(4)
C(17)-C(16)-C(18)	132.1(4)
C(16)-C(17)-C(6)	131.8(4)
N(5)-C(18)-C(16)	122.3(4)
N(5)-C(18)-C(15)	113.2(4)

C(16)-C(18)-C(15)	124.5(4)
C(22)-C(20)-C(6)	130.7(4)
C(9)-C(21)-C(12)	107.4(4)
C(9)-C(21)-Fe(1)	70.4(3)
C(12)-C(21)-Fe(1)	69.8(3)
C(20)-C(22)-C(15)	132.8(5)
N(5)-C(31)-C(34)	111.2(15)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$)for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	28(1)	32(1)	33(1)	1(1)	6(1)	0(1)
Cu(2)	26(1)	109(1)	68(1)	-33(1)	16(1)	-8(1)
C(32)	37(2)	33(2)	45(2)	3(2)	13(2)	-1(1)
C(33)	35(2)	40(2)	47(2)	6(2)	15(2)	7(2)
C(5)	29(2)	43(2)	32(2)	5(1)	9(1)	1(1)
C(6)	24(2)	51(2)	38(2)	-1(2)	8(2)	-2(1)
C(7)	32(2)	52(2)	31(2)	0(2)	7(2)	0(2)
C(8)	25(2)	57(2)	41(2)	7(2)	4(2)	7(2)
C(9)	58(3)	53(3)	63(3)	20(2)	12(2)	-12(2)
C(10)	73(3)	49(2)	45(2)	13(2)	21(2)	8(2)
O(4)	39(2)	155(4)	115(3)	-75(3)	28(2)	-19(2)
C(12)	47(3)	67(3)	67(3)	22(2)	9(2)	23(2)
N(5)	26(2)	97(3)	81(3)	-46(3)	18(2)	-8(2)
C(14)	60(3)	54(2)	42(2)	9(2)	-6(2)	-1(2)
C(15)	28(2)	104(4)	61(3)	-29(3)	14(2)	-9(2)
C(16)	32(2)	71(3)	74(3)	-30(3)	14(2)	-4(2)
C(17)	31(2)	57(2)	61(3)	-17(2)	12(2)	-10(2)
C(18)	31(2)	76(3)	58(3)	-17(2)	13(2)	-2(2)

C(20)	32(2)	95(4)	71(3)	-40(3)	13(2)	-8(2)
C(21)	120(5)	30(2)	48(3)	1(2)	3(3)	6(2)
C(22)	31(2)	121(5)	93(4)	-61(4)	14(2)	-15(3)
C(31)	88(7)	320(20)	530(30)	-340(20)	121(12)	-66(9)
C(34)	280(30)	1040(100)	250(30)	160(40)	-120(20)	-20(30)

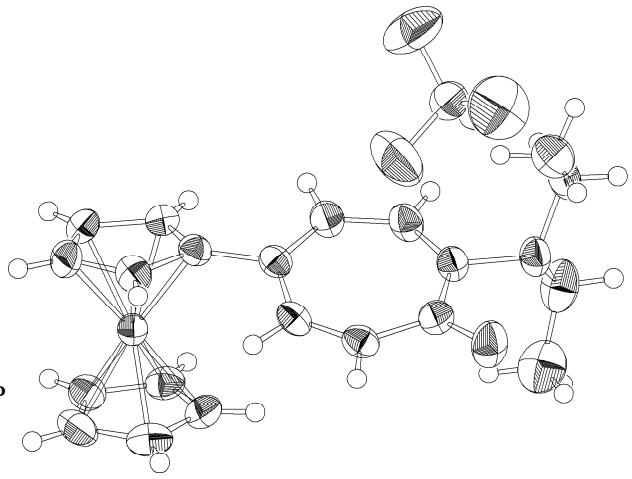


Figure S10. ORTEP ClO_4^-.

Table S5. Crystal data and structure refinement for $\mathbf{2b}^{+}\,ClO_4^{-}$.

Identification code	$\mathbf{2b}^{+}\,ClO_4^{-}$	
Empirical formula	C21 H23 Cl Fe N O5	
Formula weight	460.70	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 7.6219(6) Å	α= 90°.
	b = 24.8096(18) Å	β= 92.7620(10)°.
	c = 10.8126(8) Å	γ = 90°.
Volume	2042.2(3) Å3	
Z	4	
Density (calculated)	1.498 Mg/m3	
Absorption coefficient	0.902 mm-1	
F(000)	956	
Crystal size	? x ? x ? mm3	
Theta range for data collection	2.06 to 23.27°.	
Index ranges	-8<=h<=8, -27<=k<=23, -12<=l<=11	
Reflections collected	9107	
Independent reflections	2941 [R(int) = 0.0140]	
Completeness to theta = 23.27°	99.9 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	2941 / 0 / 264	
Goodness-of-fit on F2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0836	
R indices (all data)	R1 = 0.0339, wR2 = 0.0856	
Largest diff. peak and hole	0.551 and -0.242 e.Å-3	

Table S6. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for $\mathbf{2b}^{+}\,ClO_4^{-}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)

Fe(1)	625(1)	209(1)	2517(1)	34(1)
Cl(2)	3674(1)	1347(1)	8683(1)	51(1)
C(1)	-2057(3)	242(1)	2354(3)	47(1)
N(1)	6551(3)	2305(1)	5139(2)	45(1)
C(10)	3125(3)	242(1)	3255(2)	37(1)
O(1)	6901(3)	2294(1)	2774(2)	61(1)
C(14)	5851(3)	1828(1)	4447(2)	38(1)
C(2)	-1354(4)	274(1)	1172(3)	53(1)
C(11)	4029(3)	759(1)	3470(2)	35(1)
C(15)	6083(3)	1895(1)	3124(2)	39(1)
C(12)	4374(3)	933(1)	4656(2)	42(1)
C(8)	1993(3)	-23(1)	4086(2)	40(1)
C(6)	1924(4)	-506(1)	2279(3)	49(1)
C(17)	4458(3)	1054(1)	2381(2)	39(1)
C(9)	3060(3)	-68(1)	2128(2)	43(1)
C(3)	-1389(3)	681(1)	3062(2)	45(1)
C(16)	5316(3)	1521(1)	2239(2)	40(1)
C(7)	1258(3)	-480(1)	3470(3)	47(1)
O(3)	4165(4)	859(1)	9276(2)	97(1)
C(13)	5141(3)	1421(1)	5076(2)	44(1)
C(5)	-274(4)	981(1)	2322(3)	48(1)
O(2)	2854(4)	1670(1)	9557(2)	98(1)
C(4)	-249(4)	729(1)	1152(3)	53(1)
O(5)	5147(4)	1627(2)	8281(3)	117(1)
O(4)	2594(5)	1249(2)	7634(3)	129(1)
C(20)	8054(4)	2170(1)	6054(3)	62(1)
C(18)	5100(4)	2620(1)	5736(3)	63(1)
C(21)	9611(4)	1961(1)	5415(4)	76(1)
C(19)	3792(4)	2832(2)	4788(4)	79(1)

Table S7. Bond lengths [Å] and angles [°] for $\mathbf{2b}^{+}\,ClO_4^{-}$.

Fe(1)-C(8)	2.031(2)
Fe(1)-C(10)	2.032(2)

Fe(1)-C(3)	2.039(2)
Fe(1)-C(5)	2.041(3)
Fe(1)-C(9)	2.043(2)
Fe(1)-C(7)	2.044(2)
Fe(1)-C(1)	2.045(3)
Fe(1)-C(4)	2.047(3)
Fe(1)-C(2)	2.050(3)
Fe(1)-C(6)	2.055(2)
Cl(2)-O(4)	1.391(3)
Cl(2)-O(5)	1.407(3)
Cl(2)-O(2)	1.408(2)
Cl(2)-O(3)	1.413(2)
C(1)-C(2)	1.411(4)
C(1)-C(3)	1.412(4)
N(1)-C(14)	1.485(3)
N(1)-C(20)	1.514(4)
N(1)-C(18)	1.523(4)
C(10)-C(8)	1.435(3)
C(10)-C(9)	1.440(3)
C(10)-C(11)	1.469(3)
O(1)-C(15)	1.240(3)
C(14)-C(13)	1.346(3)
C(14)-C(15)	1.459(3)
C(2)-C(4)	1.410(4)
C(11)-C(12)	1.367(3)
C(11)-C(17)	1.437(3)
C(15)-C(16)	1.436(4)
C(12)-C(13)	1.410(3)
C(8)-C(7)	1.418(4)
C(6)-C(9)	1.403(4)
C(6)-C(7)	1.408(4)
C(17)-C(16)	1.344(4)
C(3)-C(5)	1.408(4)
C(5)-C(4)	1.411(4)
C(20)-C(21)	1.494(5)
C(18)-C(19)	1.491(5)

C(8)-Fe(1)-C(10)	41.35(10)
C(8)-Fe(1)-C(3)	106.53(10)
C(10)-Fe(1)-C(3)	124.62(10)
C(8)-Fe(1)-C(5)	120.57(11)
C(10)-Fe(1)-C(5)	107.87(10)
C(3)-Fe(1)-C(5)	40.37(11)
C(8)-Fe(1)-C(9)	68.96(10)
C(10)-Fe(1)-C(9)	41.39(10)
C(3)-Fe(1)-C(9)	163.14(11)
C(5)-Fe(1)-C(9)	126.81(11)
C(8)-Fe(1)-C(7)	40.72(10)
C(10)-Fe(1)-C(7)	68.96(10)
C(3)-Fe(1)-C(7)	119.84(11)
C(5)-Fe(1)-C(7)	155.19(11)
C(9)-Fe(1)-C(7)	68.04(11)
C(8)-Fe(1)-C(1)	123.66(11)
C(10)-Fe(1)-C(1)	161.27(11)
C(3)-Fe(1)-C(1)	40.44(11)
C(5)-Fe(1)-C(1)	67.94(11)
C(9)-Fe(1)-C(1)	155.55(11)
C(7)-Fe(1)-C(1)	106.74(11)
C(8)-Fe(1)-C(4)	156.45(11)
C(10)-Fe(1)-C(4)	121.61(11)
C(3)-Fe(1)-C(4)	67.89(11)
C(5)-Fe(1)-C(4)	40.39(11)
C(9)-Fe(1)-C(4)	109.37(11)
C(7)-Fe(1)-C(4)	162.19(12)
C(1)-Fe(1)-C(4)	67.89(12)
C(8)-Fe(1)-C(2)	160.91(11)
C(10)-Fe(1)-C(2)	156.84(11)
C(3)-Fe(1)-C(2)	67.78(11)
C(5)-Fe(1)-C(2)	67.75(11)
C(9)-Fe(1)-C(2)	121.70(11)
C(7)-Fe(1)-C(2)	124.83(11)
C(1)-Fe(1)-C(2)	40.31(12)

C(4)-Fe(1)-C(2)	40.25(12)
C(8)-Fe(1)-C(6)	68.19(11)
C(10)-Fe(1)-C(6)	68.61(10)
C(3)-Fe(1)-C(6)	154.92(11)
C(5)-Fe(1)-C(6)	163.50(12)
C(9)-Fe(1)-C(6)	40.06(11)
C(7)-Fe(1)-C(6)	40.19(11)
C(1)-Fe(1)-C(6)	120.63(11)
C(4)-Fe(1)-C(6)	126.59(11)
C(2)-Fe(1)-C(6)	108.75(11)
O(4)-Cl(2)-O(5)	106.5(2)
O(4)-Cl(2)-O(2)	112.5(2)
O(5)-Cl(2)-O(2)	108.2(2)
O(4)-Cl(2)-O(3)	110.7(2)
O(5)-Cl(2)-O(3)	111.5(2)
O(2)-Cl(2)-O(3)	107.48(15)
C(2)-C(1)-C(3)	107.8(2)
C(2)-C(1)-Fe(1)	70.04(15)
C(3)-C(1)-Fe(1)	69.57(14)
C(14)-N(1)-C(20)	113.3(2)
C(14)-N(1)-C(18)	111.8(2)
C(20)-N(1)-C(18)	112.3(2)
C(8)-C(10)-C(9)	106.7(2)
C(8)-C(10)-C(11)	126.3(2)
C(9)-C(10)-C(11)	126.7(2)
C(8)-C(10)-Fe(1)	69.31(13)
C(9)-C(10)-Fe(1)	69.71(14)
C(11)-C(10)-Fe(1)	121.39(16)
C(13)-C(14)-C(15)	130.6(2)
C(13)-C(14)-N(1)	119.1(2)
C(15)-C(14)-N(1)	110.3(2)
C(4)-C(2)-C(1)	108.2(2)
C(4)-C(2)-Fe(1)	69.75(15)
C(1)-C(2)-Fe(1)	69.64(15)
C(12)-C(11)-C(17)	124.5(2)
C(12)-C(11)-C(10)	119.5(2)

C(17)-C(11)-C(10)	116.0(2)
O(1)-C(15)-C(16)	120.5(2)
O(1)-C(15)-C(14)	118.4(2)
C(16)-C(15)-C(14)	121.0(2)
C(11)-C(12)-C(13)	129.2(2)
C(7)-C(8)-C(10)	108.0(2)
C(7)-C(8)-Fe(1)	70.11(14)
C(10)-C(8)-Fe(1)	69.34(13)
C(9)-C(6)-C(7)	108.8(2)
C(9)-C(6)-Fe(1)	69.51(14)
C(7)-C(6)-Fe(1)	69.48(14)
C(16)-C(17)-C(11)	131.6(2)
C(6)-C(9)-C(10)	108.2(2)
C(6)-C(9)-Fe(1)	70.43(15)
C(10)-C(9)-Fe(1)	68.90(13)
C(5)-C(3)-C(1)	108.1(2)
C(5)-C(3)-Fe(1)	69.87(15)
C(1)-C(3)-Fe(1)	69.99(14)
C(17)-C(16)-C(15)	131.7(2)
C(6)-C(7)-C(8)	108.3(2)
C(6)-C(7)-Fe(1)	70.33(15)
C(8)-C(7)-Fe(1)	69.17(14)
C(14)-C(13)-C(12)	130.7(2)
C(3)-C(5)-C(4)	108.1(2)
C(3)-C(5)-Fe(1)	69.76(14)
C(4)-C(5)-Fe(1)	70.04(15)
C(2)-C(4)-C(5)	107.9(3)
C(2)-C(4)-Fe(1)	70.00(16)
C(5)-C(4)-Fe(1)	69.57(15)
C(21)-C(20)-N(1)	111.6(2)
C(19)-C(18)-N(1)	111.4(2)

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters (Å2x 103)for $\mathbf{2b}^{+}\ ClO_4^{-}$. The anisotropic

displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	34(1)	32(1)	36(1)	-2(1)	0(1)	0(1)
Cl(2)	66(1)	47(1)	39(1)	-2(1)	7(1)	3(1)
C(1)	32(1)	50(2)	60(2)	1(1)	-2(1)	0(1)
N(1)	55(1)	41(1)	37(1)	-8(1)	4(1)	-10(1)
C(10)	33(1)	38(1)	39(1)	-2(1)	-3(1)	2(1)
O(1)	86(2)	53(1)	43(1)	2(1)	13(1)	-26(1)
C(14)	40(1)	39(1)	35(1)	-3(1)	2(1)	-5(1)
C(2)	49(2)	65(2)	45(2)	-8(1)	-14(1)	7(1)
C(11)	29(1)	40(1)	37(1)	-1(1)	0(1)	0(1)
C(15)	40(1)	41(1)	37(1)	2(1)	5(1)	0(1)
C(12)	48(1)	46(2)	33(1)	3(1)	3(1)	-11(1)
C(8)	45(1)	36(1)	38(1)	4(1)	-4(1)	1(1)
C(6)	54(2)	32(1)	59(2)	-13(1)	-7(1)	8(1)
C(17)	37(1)	51(2)	30(1)	-4(1)	-1(1)	-2(1)
C(9)	38(1)	46(2)	45(2)	-9(1)	3(1)	7(1)
C(3)	45(1)	45(2)	45(2)	0(1)	4(1)	12(1)
C(16)	41(1)	49(2)	29(1)	3(1)	2(1)	-1(1)
C(7)	52(2)	31(1)	58(2)	7(1)	-7(1)	-3(1)
O(3)	155(3)	63(2)	73(2)	9(1)	25(2)	43(2)
C(13)	52(2)	50(2)	29(1)	-1(1)	3(1)	-11(1)
C(5)	50(2)	36(1)	57(2)	5(1)	-4(1)	5(1)
O(2)	151(3)	77(2)	68(2)	8(1)	36(2)	57(2)
C(4)	56(2)	60(2)	44(2)	14(1)	3(1)	10(1)
O(5)	96(2)	140(3)	118(2)	21(2)	26(2)	-33(2)
O(4)	161(3)	138(3)	83(2)	-2(2)	-51(2)	-39(2)
C(20)	76(2)	58(2)	51(2)	1(1)	-15(2)	-26(2)
C(18)	79(2)	54(2)	59(2)	-16(2)	28(2)	-9(2)
C(21)	61(2)	70(2)	94(3)	4(2)	-21(2)	-7(2)
C(19)	63(2)	73(2)	101(3)	-13(2)	22(2)	10(2)

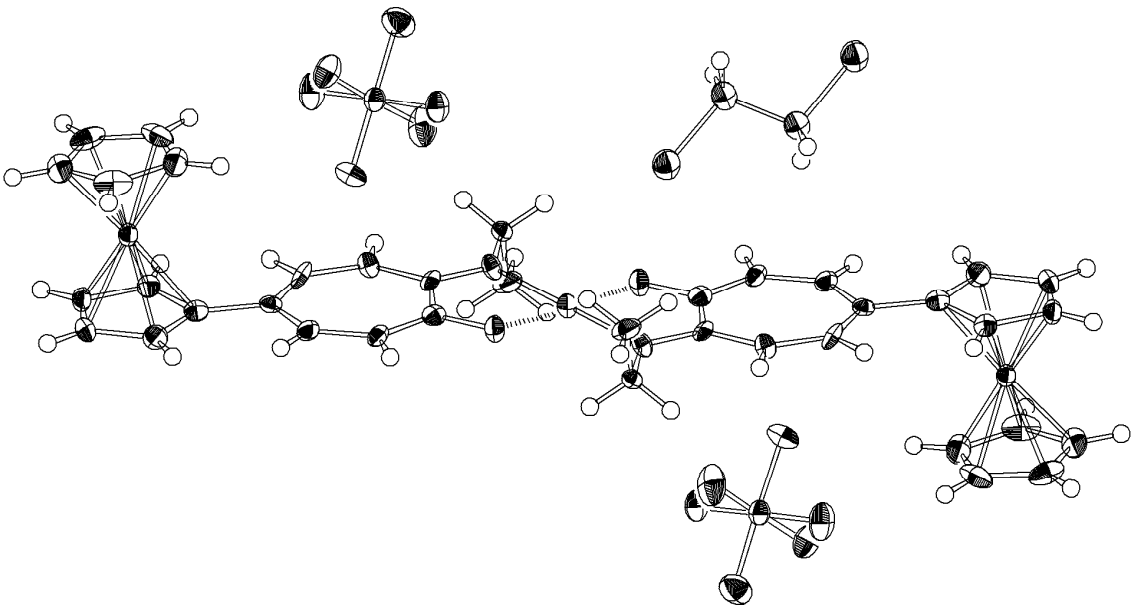


Figure S11. ORTEP drawing (50% probability) showing X-ray structure of $\mathbf{1}^{2+}$ $2PF_6^-$ $C_2H_4Cl_2$.

Table S9. Crystal data and structure refinement for $\mathbf{1}^{2+}$ $2PF_6^-$ $C_2H_4Cl_2$.

Identification code		
Empirical formula	C40 H40 Cl2 Cu F12 Fe2 N2 O2 P2	
Formula weight	1116.82	
Temperature	120(2) K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.197(10) Å	α= 84.50(8)°.
	b = 10.402(16) Å	β= 68.16(7)°.
	c = 10.513(10) Å	γ = 84.28(8)°.
Volume	1028(2) Å3	
Z	1	
Density (calculated)	1.804 Mg/m3	

Absorption coefficient	1.512 mm^{-1}
F(000)	563
Crystal size	0.18 x 0.08 x 0.04 mm^3
Theta range for data collection	1.97 to 27.50°.
Index ranges	-10<=h<=13, -13<=k<=12, -13<=l<=13
Reflections collected	7444
Independent reflections	3263 [R(int) = 0.0539]
Completeness to theta = 27.50°	69.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.7878
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3263 / 0 / 286
Goodness-of-fit on F^2	0.964
Final R indices [I>2sigma(I)]	R1 = 0.0630, wR2 = 0.1461
R indices (all data)	R1 = 0.1027, wR2 = 0.1652
Largest diff. peak and hole	1.673 and -0.598 $e.Å^{-3}$

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for $\mathbf{1}^{2+}\,2PF_6^-\,C_2H_4Cl_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu	5000	5000	5000	21(1)
Fe	2633(1)	-2513(1)	9405(1)	19(1)
Cl	-587(2)	2036(2)	5175(3)	35(1)
P	2328(2)	2647(2)	10561(2)	22(1)
F(1)	3435(5)	3639(4)	10550(5)	29(1)
F(2)	1198(6)	1667(4)	10601(6)	38(1)
F(3)	1076(6)	3559(5)	11537(6)	42(2)
F(4)	3574(6)	1738(5)	9603(6)	44(2)
F(5)	2143(7)	3437(5)	9243(6)	47(2)
F(6)	2492(6)	1871(4)	11887(5)	35(1)
N	3366(7)	3979(5)	5625(7)	20(2)

O	5845(6)	3463(5)	5633(6)	24(1)
C(1)	5054(9)	2497(7)	6027(8)	20(2)
C(2)	3596(8)	2763(7)	6000(8)	17(2)
C(3)	2622(9)	1800(6)	6323(8)	20(2)
C(4)	2684(9)	517(7)	6729(9)	22(2)
C(5)	3766(8)	-311(7)	6975(8)	17(2)
C(6)	5075(9)	108(7)	6817(9)	23(2)
C(7)	5636(9)	1309(7)	6401(8)	20(2)
C(8)	2010(8)	4477(7)	5545(8)	17(2)
C(9)	2002(10)	4369(8)	4114(9)	30(2)
C(10)	3519(9)	-1682(7)	7322(8)	20(2)
C(11)	2259(9)	-2302(7)	7574(8)	20(2)
C(12)	2445(10)	-3617(7)	7965(8)	24(2)
C(13)	3795(9)	-3842(7)	8037(9)	24(2)
C(14)	4477(9)	-2663(7)	7649(9)	25(2)
C(15)	1953(12)	-3408(8)	11384(9)	34(2)
C(16)	3034(10)	-2622(9)	11238(10)	32(2)
C(17)	2591(12)	-1326(8)	10909(9)	35(2)
C(18)	1259(11)	-1381(8)	10880(10)	36(3)
C(19)	845(10)	-2633(9)	11165(9)	33(2)
C(20)	392(9)	560(7)	4525(10)	27(2)

Table S11. Bond lengths [Å] and angles [°] for $\mathbf{1}^{2+}2PF_6^-\ C_2H_4Cl_2$.

Cu-O#1	1.921(6)
Cu-O	1.921(6)
Cu-N#1	1.934(7)
Cu-N	1.934(7)
Fe-C(18)	2.039(9)
Fe-C(13)	2.042(8)
Fe-C(12)	2.059(8)
Fe-C(19)	2.063(9)
Fe-C(17)	2.083(9)
Fe-C(11)	2.085(8)
Fe-C(15)	2.088(10)

Fe-C(14)	2.094(9)
Fe-C(16)	2.105(9)
Fe-C(10)	2.164(9)
Cl-C(20)	1.791(8)
P-F(4)	1.586(5)
P-F(6)	1.598(6)
P-F(3)	1.598(6)
P-F(1)	1.600(5)
P-F(2)	1.601(6)
P-F(5)	1.605(6)
N-C(2)	1.313(9)
N-C(8)	1.457(10)
O-C(1)	1.291(10)
C(1)-C(7)	1.403(11)
C(1)-C(2)	1.495(12)
C(2)-C(3)	1.411(11)
C(3)-C(4)	1.365(11)
C(4)-C(5)	1.415(11)
C(5)-C(6)	1.392(12)
C(5)-C(10)	1.461(11)
C(6)-C(7)	1.389(11)
C(8)-C(9)	1.523(12)
C(10)-C(11)	1.420(12)
C(10)-C(14)	1.449(11)
C(11)-C(12)	1.405(11)
C(12)-C(13)	1.402(13)
C(13)-C(14)	1.420(12)
C(15)-C(16)	1.392(14)
C(15)-C(19)	1.399(14)
C(16)-C(17)	1.430(13)
C(17)-C(18)	1.378(15)
C(18)-C(19)	1.379(14)
C(20)-C(20)#2	1.537(18)

O#1-Cu-O	180.0(3)
O#1-Cu-N#1	82.2(3)

O-Cu-N#1	97.8(3)
O#1-Cu-N	97.8(3)
O-Cu-N	82.2(3)
N#1-Cu-N	179.998(1)
C(18)-Fe-C(13)	171.7(4)
C(18)-Fe-C(12)	134.7(4)
C(13)-Fe-C(12)	40.0(3)
C(18)-Fe-C(19)	39.3(4)
C(13)-Fe-C(19)	132.6(4)
C(12)-Fe-C(19)	109.1(4)
C(18)-Fe-C(17)	39.0(4)
C(13)-Fe-C(17)	146.3(4)
C(12)-Fe-C(17)	173.7(4)
C(19)-Fe-C(17)	66.3(4)
C(18)-Fe-C(11)	113.1(4)
C(13)-Fe-C(11)	66.9(3)
C(12)-Fe-C(11)	39.6(3)
C(19)-Fe-C(11)	115.1(4)
C(17)-Fe-C(11)	137.3(3)
C(18)-Fe-C(15)	65.6(4)
C(13)-Fe-C(15)	109.1(3)
C(12)-Fe-C(15)	113.3(4)
C(19)-Fe-C(15)	39.4(4)
C(17)-Fe-C(15)	66.2(4)
C(11)-Fe-C(15)	143.7(4)
C(18)-Fe-C(14)	148.1(4)
C(13)-Fe-C(14)	40.1(3)
C(12)-Fe-C(14)	66.8(4)
C(19)-Fe-C(14)	172.3(3)
C(17)-Fe-C(14)	118.3(4)
C(11)-Fe-C(14)	66.3(3)
C(15)-Fe-C(14)	135.1(4)
C(18)-Fe-C(16)	65.5(4)
C(13)-Fe-C(16)	114.9(4)
C(12)-Fe-C(16)	143.3(3)
C(19)-Fe-C(16)	65.8(4)

C(17)-Fe-C(16)	39.9(4)
C(11)-Fe-C(16)	177.0(3)
C(15)-Fe-C(16)	38.8(4)
C(14)-Fe-C(16)	113.2(4)
C(18)-Fe-C(10)	118.7(3)
C(13)-Fe-C(10)	67.0(3)
C(12)-Fe-C(10)	66.3(3)
C(19)-Fe-C(10)	145.8(4)
C(17)-Fe-C(10)	114.8(3)
C(11)-Fe-C(10)	39.0(3)
C(15)-Fe-C(10)	174.8(4)
C(14)-Fe-C(10)	39.8(3)
C(16)-Fe-C(10)	138.8(4)
F(4)-P-F(6)	90.0(3)
F(4)-P-F(3)	179.6(4)
F(6)-P-F(3)	89.6(3)
F(4)-P-F(1)	90.7(3)
F(6)-P-F(1)	90.3(3)
F(3)-P-F(1)	89.1(3)
F(4)-P-F(2)	90.4(3)
F(6)-P-F(2)	89.3(3)
F(3)-P-F(2)	89.7(3)
F(1)-P-F(2)	178.8(3)
F(4)-P-F(5)	90.8(3)
F(6)-P-F(5)	179.2(3)
F(3)-P-F(5)	89.6(3)
F(1)-P-F(5)	89.9(3)
F(2)-P-F(5)	90.5(3)
C(2)-N-C(8)	121.8(7)
C(2)-N-Cu	115.4(5)
C(8)-N-Cu	122.5(5)
C(1)-O-Cu	114.7(5)
O-C(1)-C(7)	118.1(7)
O-C(1)-C(2)	115.5(7)
C(7)-C(1)-C(2)	126.4(7)
N-C(2)-C(3)	125.5(7)

N-C(2)-C(1)	111.6(7)
C(3)-C(2)-C(1)	122.9(6)
C(4)-C(3)-C(2)	132.9(8)
C(3)-C(4)-C(5)	131.9(8)
C(6)-C(5)-C(4)	123.0(7)
C(6)-C(5)-C(10)	118.9(7)
C(4)-C(5)-C(10)	118.0(7)
C(7)-C(6)-C(5)	131.5(7)
C(6)-C(7)-C(1)	131.3(8)
N-C(8)-C(9)	111.0(6)
C(11)-C(10)-C(14)	105.6(7)
C(11)-C(10)-C(5)	128.1(7)
C(14)-C(10)-C(5)	125.9(8)
C(11)-C(10)-Fe	67.5(4)
C(14)-C(10)-Fe	67.5(5)
C(5)-C(10)-Fe	123.7(5)
C(12)-C(11)-C(10)	109.7(7)
C(12)-C(11)-Fe	69.2(5)
C(10)-C(11)-Fe	73.5(4)
C(13)-C(12)-C(11)	108.3(7)
C(13)-C(12)-Fe	69.4(5)
C(11)-C(12)-Fe	71.2(4)
C(12)-C(13)-C(14)	108.1(7)
C(12)-C(13)-Fe	70.6(5)
C(14)-C(13)-Fe	71.9(5)
C(13)-C(14)-C(10)	108.2(8)
C(13)-C(14)-Fe	68.0(5)
C(10)-C(14)-Fe	72.7(5)
C(16)-C(15)-C(19)	108.4(8)
C(16)-C(15)-Fe	71.2(5)
C(19)-C(15)-Fe	69.3(5)
C(15)-C(16)-C(17)	107.7(8)
C(15)-C(16)-Fe	70.0(5)
C(17)-C(16)-Fe	69.2(5)
C(18)-C(17)-C(16)	106.0(8)
C(18)-C(17)-Fe	68.7(5)

C(16)-C(17)-Fe	70.8(5)
C(17)-C(18)-C(19)	110.7(8)
C(17)-C(18)-Fe	72.2(5)
C(19)-C(18)-Fe	71.3(5)
C(18)-C(19)-C(15)	107.1(9)
C(18)-C(19)-Fe	69.4(6)
C(15)-C(19)-Fe	71.3(5)
C(20)#2-C(20)-Cl	107.3(8)

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

Table S12. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $\mathbf{1}^{2+}2PF_6^-\ C_2H_4Cl_2$. The anisotropic
displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cu	22(1)	16(1)	25(1)	1(1)	-9(1)	-3(1)
Fe	22(1)	16(1)	18(1)	1(1)	-7(1)	-2(1)
Cl	27(1)	32(1)	45(2)	0(1)	-12(1)	-3(1)
P	22(1)	20(1)	25(1)	-1(1)	-9(1)	-5(1)
F(1)	27(3)	26(2)	40(3)	-1(2)	-17(2)	-11(2)
F(2)	34(3)	33(3)	55(4)	4(2)	-25(3)	-15(2)
F(3)	26(3)	40(3)	57(4)	-15(3)	-9(3)	1(2)
F(4)	46(4)	32(3)	40(4)	-17(3)	-1(3)	5(3)
F(5)	73(4)	36(3)	44(4)	14(2)	-38(3)	-8(3)
F(6)	38(3)	38(3)	32(3)	10(2)	-16(3)	-10(2)
N	21(4)	15(3)	29(4)	-4(3)	-15(3)	0(3)
O	23(3)	17(3)	33(4)	1(2)	-11(3)	-4(2)
C(1)	22(4)	24(4)	15(4)	-5(3)	-7(4)	-4(3)
C(2)	22(4)	20(4)	7(4)	4(3)	-5(3)	-5(3)
C(3)	20(4)	17(4)	26(5)	-1(3)	-14(4)	1(3)
C(4)	20(4)	26(4)	19(5)	10(3)	-6(4)	-14(3)

C(5)	15(4)	20(4)	16(4)	-7(3)	-4(3)	-1(3)
C(6)	16(4)	21(4)	24(5)	2(3)	0(4)	1(3)
C(7)	22(4)	22(4)	14(4)	2(3)	-5(4)	-8(3)
C(8)	17(4)	17(3)	17(4)	-3(3)	-7(3)	-1(3)
C(9)	26(5)	36(5)	19(5)	5(4)	-1(4)	5(4)
C(10)	28(5)	24(4)	11(4)	-2(3)	-9(4)	-2(4)
C(11)	27(5)	22(4)	13(4)	-1(3)	-11(4)	-3(4)
C(12)	38(5)	16(4)	17(5)	1(3)	-8(4)	-7(4)
C(13)	26(5)	15(4)	29(5)	-2(3)	-7(4)	2(3)
C(14)	22(4)	25(4)	27(5)	1(4)	-8(4)	1(4)
C(15)	60(7)	26(4)	15(5)	4(4)	-16(5)	-5(5)
C(16)	23(5)	60(6)	24(5)	-12(4)	-19(4)	4(5)
C(17)	57(7)	29(5)	20(5)	-3(4)	-12(5)	-17(4)
C(18)	51(7)	31(5)	23(5)	-9(4)	-13(5)	20(5)
C(19)	20(5)	59(6)	21(5)	-9(4)	-4(4)	-16(4)
C(20)	20(4)	27(4)	39(6)	-3(4)	-14(4)	-2(4)