Electronic Supplementary Information

Heterogeneous catalytic properties of unprecedented μ-O-[FeTCPP]$_2$ dimers (H_2TCPP = *meso*-tetra(4-carboxyphenyl) porphyrin): unusual superhyperfine EPR structure

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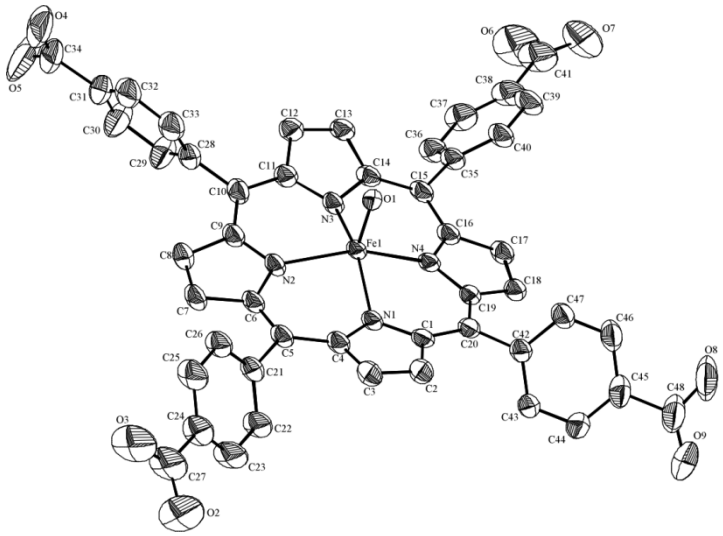

Fig. S1 ORTEP[1] detail of μ-O-[FeTCPP]$_2$·nDMF. The thermal ellipsoids correspond to 50% probability. Hydrogen atoms have been omitted.

[1] Farrugia, L. J., *J. Appl. Crystallogr.* **1997,** *30*, 565.

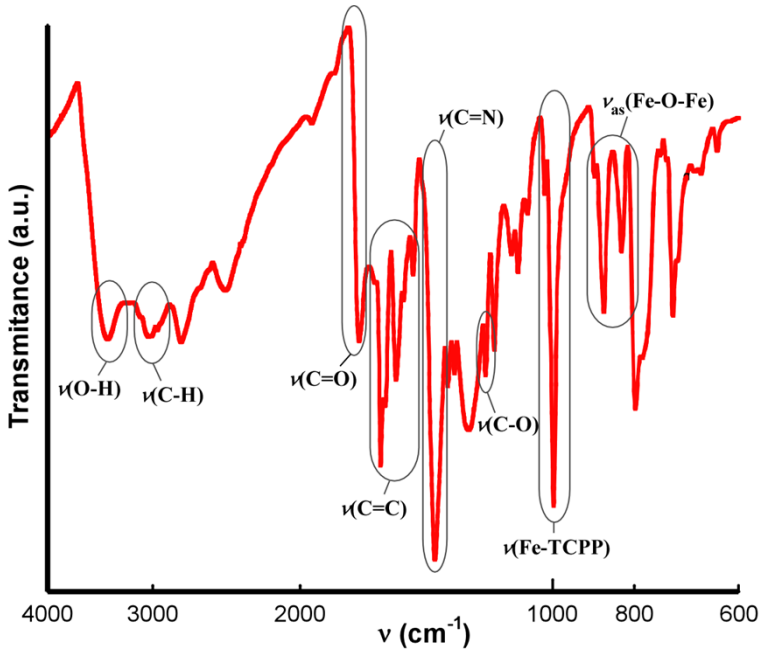

Fig. S2 IR spectra for μ-O-[FeTCPP]$_2$·nDMF.

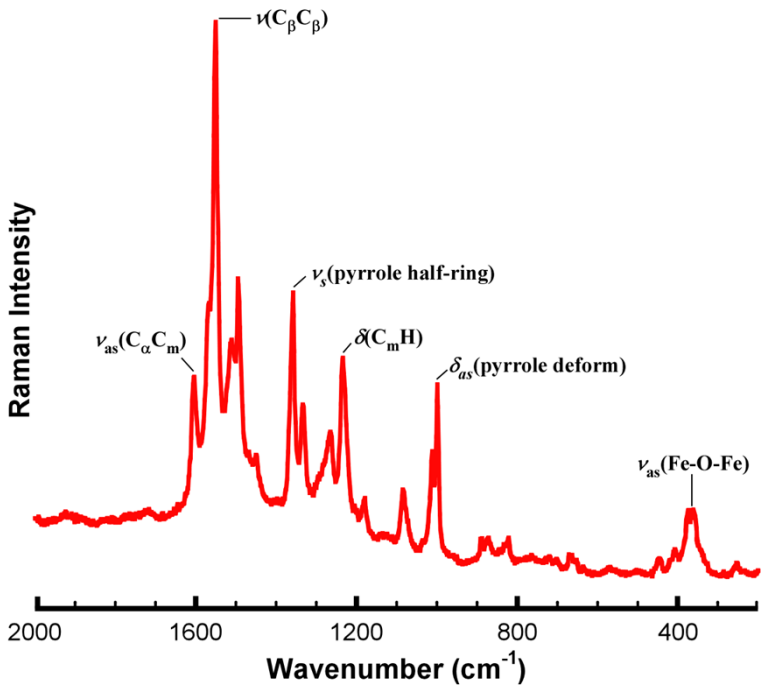

Fig. S3 Raman spectra for μ-O-[FeTCPP]$_2$·nDMF.

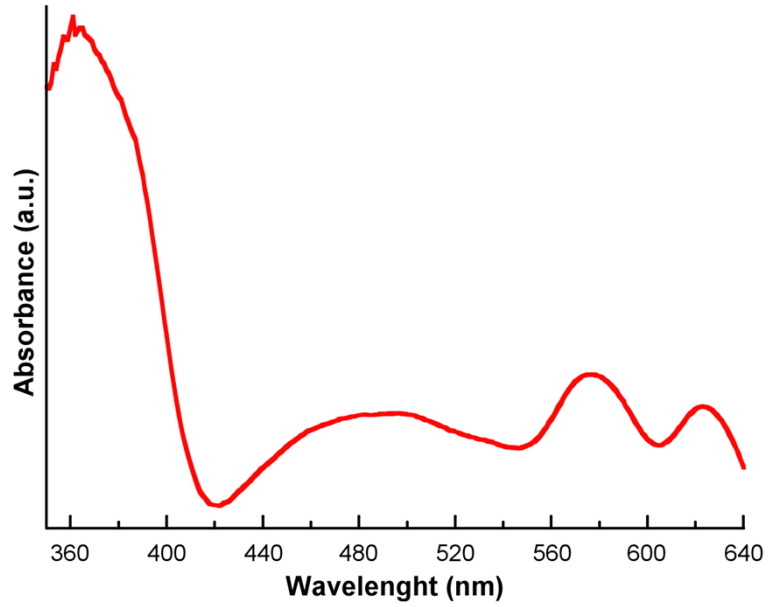

Fig. S4 UV-Visible spectra for μ-O-[FeTCPP]$_2$·nDMF.

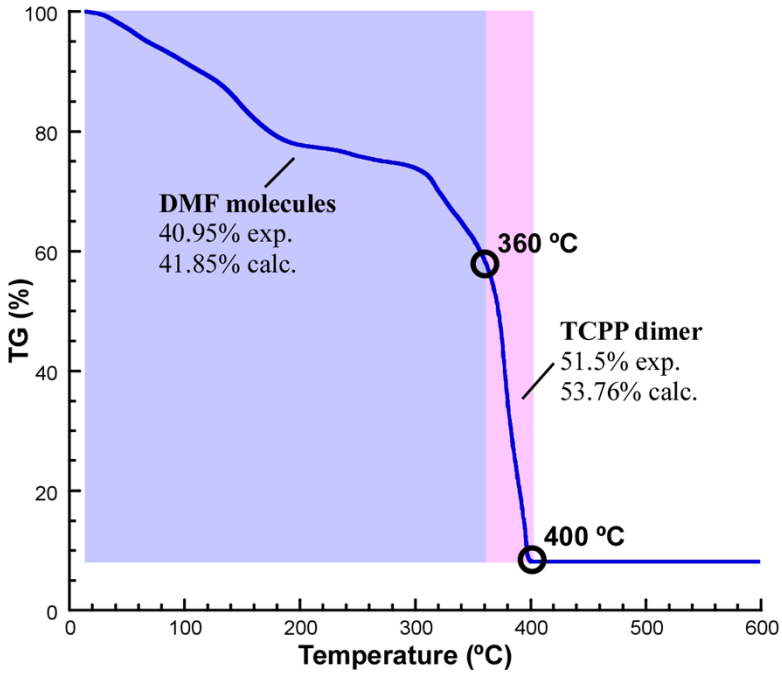

Fig. S5 Thermal analysis for μ-O-[FeTCPP]$_2$·nDMF.

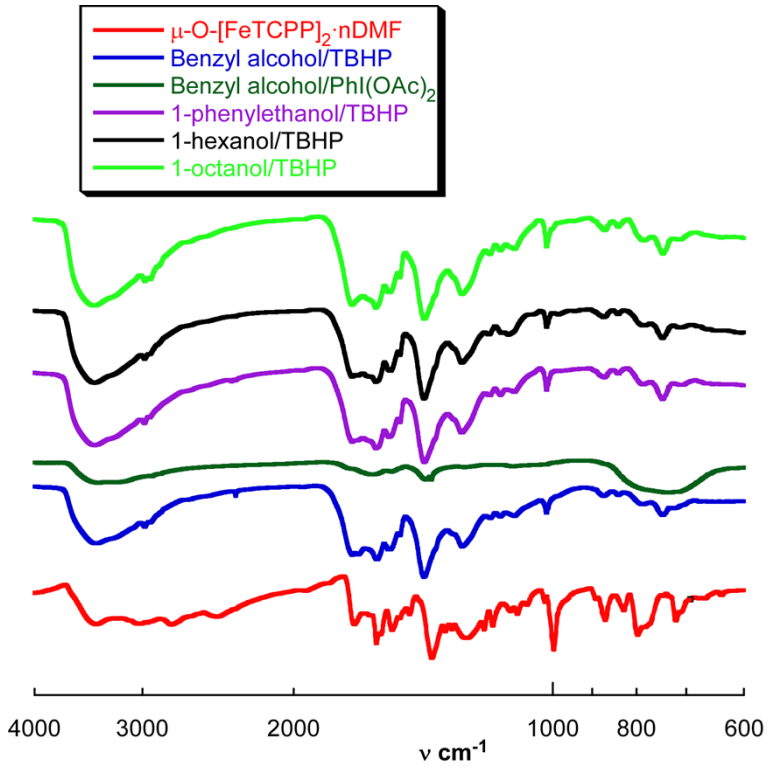

Fig. S6 IR spectrums for the residues of the oxidation of benzyl alcohol, 1-phenylethanol, 1-hexanol, 1-octanol and the original for μ-O-[FeTCPP]$_2$·nDMF.

Table S1 Bond distances (Å) and angles (º) for μ-O-[FeTCPP]$_2$·nDMF.

Distances

Fe(1)-O(1)	1.7597(4)	C(40)-C(39)	1.390(4)
Fe(1)-N(1)	2.077(2)	C(40)-H(40)	0.9500
Fe(1)-N(4)	2.083(2)	C(37)-C(38)	1.376(6)
Fe(1)-N(2)	2.084(2)	C(37)-C(36)	1.386(4)
Fe(1)-N(3)	2.087(2)	C(37)-H(37)	0.9500
O(1)-Fe(1)^{i}	1.7597(4)	C(7)-C(8)	1.348(4)
N(4)-C(19)	1.370(4)	C(7)-H(7)	0.9500
N(4)-C(16)	1.374(3)	C(13)-C(12)	1.354(4)
N(2)-C(9)	1.368(4)	C(13)-H(13)	0.9500
N(2)-C(6)	1.376(3)	C(12)-H(12)	0.9500
N(1)-C(1)	1.366(4)	C(2)-C(3)	1.343(4)
N(1)-C(4)	1.376(3)	C(2)-H(2)	0.9500
N(3)-C(11)	1.365(4)	C(3)-H(3)	0.9500
N(3)-C(14)	1.376(3)	C(28)-C(29)	1.374(5)
O(8)-C(48)	1.284(6)	C(28)-C(33)	1.407(5)
O(3)-C(27)	1.217(6)	C(8)-H(8)	0.9500
O(7)-C(41)	1.260(7)	C(35)-C(36)	1.399(5)
O(9)-C(48)	1.220(6)	C(33)-C(32)	1.365(5)
C(16)-C(15)	1.407(4)	C(33)-H(33)	0.9500
C(16)-C(17)	1.440(4)	C(26)-C(25)	1.374(4)
C(6)-C(5)	1.383(4)	C(26)-C(21)	1.406(4)
C(6)-C(7)	1.441(4)	C(26)-H(26)	0.9500
O(6)-C(41)	1.248(7)	C(21)-C(22)	1.381(5)
C(20)-C(1)	1.397(4)	C(36)-H(36)	0.9500
C(20)-C(19)	1.421(4)	C(24)-C(23)	1.371(5)
C(20)-C(42)	1.476(4)	C(24)-C(25)	1.395(6)
C(19)-C(18)	1.427(4)	C(24)-C(27)	1.504(4)
C(1)-C(2)	1.452(4)	C(22)-C(23)	1.396(4)
C(9)-C(10)	1.396(4)	C(22)-H(22)	0.9500
C(9)-C(8)	1.446(4)	C(23)-H(23)	0.9500
C(11)-C(10)	1.407(4)	C(44)-C(45)	1.380(5)
C(11)-C(12)	1.430(4)	C(44)-H(44)	0.9500
C(17)-C(18)	1.350(4)	C(46)-C(45)	1.410(5)
C(17)-H(17)	0.9500	C(46)-H(46)	0.9500
C(15)-C(14)	1.403(4)	C(45)-C(48)	1.502(5)
C(15)-C(35)	1.498(3)	C(39)-C(38)	1.390(6)
C(4)-C(5)	1.410(4)	C(39)-H(39)	0.9500

C(4)-C(3)	1.439(4)	C(38)-C(41)	1.514(5)
C(43)-C(44)	1.384(4)	C(29)-C(30)	1.389(5)
C(43)-C(42)	1.398(4)	C(29)-H(29)	0.9500
C(43)-H(43)	0.9500	C(25)-H(25)	0.9500
C(10)-C(28)	1.489(4)	C(32)-C(31)	1.357(6)
C(42)-C(47)	1.401(4)	C(32)-H(32)	0.9500
C(14)-C(13)	1.429(4)	C(31)-C(30)	1.407(6)
C(5)-C(21)	1.498(4)	C(31)-C(34)	1.494(5)
C(18)-H(18)	0.9500	C(30)-H(30)	0.9500
C(47)-C(46)	1.377(5)	C(27)-O(2)	1.283(6)
C(47)-H(47)	0.9500	C(34)-O(5)	1.187(7)
C(40)-C(35)	1.384(4)	C(34)-O(4)	1.285(7)

Angles

O(1)-Fe(1)-N(1)	102.84(7)	C(12)-C(13)-H(13)	126.4
O(1)-Fe(1)-N(4)	103.42(9)	C(14)-C(13)-H(13)	126.4
N(1)-Fe(1)-N(4)	87.17(8)	C(13)-C(12)-C(11)	107.0(3)
O(1)-Fe(1)-N(2)	103.77(10)	C(13)-C(12)-H(12)	126.5
N(1)-Fe(1)-N(2)	87.27(9)	C(11)-C(12)-H(12)	126.5
N(4)-Fe(1)-N(2)	152.81(9)	C(3)-C(2)-C(1)	106.3(3)
O(1)-Fe(1)-N(3)	101.24(7)	C(3)-C(2)-H(2)	126.8
N(1)-Fe(1)-N(3)	155.92(9)	C(1)-C(2)-H(2)	126.8
N(4)-Fe(1)-N(3)	87.05(9)	C(2)-C(3)-C(4)	108.0(2)
N(2)-Fe(1)-N(3)	87.27(9)	C(2)-C(3)-H(3)	126.0
$Fe(1)^{i}$-O(1)-Fe(1)	179.79(15)	C(4)-C(3)-H(3)	126.0
C(19)-N(4)-C(16)	106.5(2)	C(29)-C(28)-C(33)	118.5(3)
C(19)-N(4)-Fe(1)	125.73(17)	C(29)-C(28)-C(10)	122.3(3)
C(16)-N(4)-Fe(1)	127.11(18)	C(33)-C(28)-C(10)	119.2(3)
C(9)-N(2)-C(6)	107.1(2)	C(7)-C(8)-C(9)	107.2(3)
C(9)-N(2)-Fe(1)	125.50(17)	C(7)-C(8)-H(8)	126.4
C(6)-N(2)-Fe(1)	126.99(19)	C(9)-C(8)-H(8)	126.4
C(1)-N(1)-C(4)	106.4(2)	C(40)-C(35)-C(36)	118.9(3)
C(1)-N(1)-Fe(1)	123.72(16)	C(40)-C(35)-C(15)	120.2(3)
C(4)-N(1)-Fe(1)	124.44(18)	C(36)-C(35)-C(15)	120.8(3)
C(11)-N(3)-C(14)	106.3(2)	C(32)-C(33)-C(28)	121.2(4)
C(11)-N(3)-Fe(1)	123.26(17)	C(32)-C(33)-H(33)	119.4
C(14)-N(3)-Fe(1)	124.06(18)	C(28)-C(33)-H(33)	119.4
N(4)-C(16)-C(15)	125.1(2)	C(25)-C(26)-C(21)	119.8(3)
N(4)-C(16)-C(17)	109.1(2)	C(25)-C(26)-H(26)	120.1

C(15)-C(16)-C(17)	125.7(2)	C(21)-C(26)-H(26)	120.1
N(2)-C(6)-C(5)	125.6(2)	C(22)-C(21)-C(26)	119.1(3)
N(2)-C(6)-C(7)	108.9(3)	C(22)-C(21)-C(5)	120.6(3)
C(5)-C(6)-C(7)	125.5(2)	C(26)-C(21)-C(5)	120.2(3)
C(1)-C(20)-C(19)	123.7(3)	C(37)-C(36)-C(35)	120.1(3)
C(1)-C(20)-C(42)	119.0(2)	C(37)-C(36)-H(36)	120.0
C(19)-C(20)-C(42)	117.3(2)	C(35)-C(36)-H(36)	120.0
N(4)-C(19)-C(20)	125.7(2)	C(23)-C(24)-C(25)	119.2(3)
N(4)-C(19)-C(18)	109.9(2)	C(23)-C(24)-C(27)	120.6(4)
C(20)-C(19)-C(18)	124.4(3)	C(25)-C(24)-C(27)	120.1(4)
N(1)-C(1)-C(20)	125.7(3)	C(21)-C(22)-C(23)	120.3(3)
N(1)-C(1)-C(2)	110.0(2)	C(21)-C(22)-H(22)	119.8
C(20)-C(1)-C(2)	124.3(3)	C(23)-C(22)-H(22)	119.8
N(2)-C(9)-C(10)	126.1(2)	C(24)-C(23)-C(22)	120.6(3)
N(2)-C(9)-C(8)	109.1(2)	C(24)-C(23)-H(23)	119.7
C(10)-C(9)-C(8)	124.7(3)	C(22)-C(23)-H(23)	119.7
N(3)-C(11)-C(10)	125.1(2)	C(45)-C(44)-C(43)	121.6(3)
N(3)-C(11)-C(12)	110.0(2)	C(45)-C(44)-H(44)	119.2
C(10)-C(11)-C(12)	124.9(3)	C(43)-C(44)-H(44)	119.2
C(18)-C(17)-C(16)	107.2(2)	C(47)-C(46)-C(45)	120.8(3)
C(18)-C(17)-H(17)	126.4	C(47)-C(46)-H(46)	119.6
C(16)-C(17)-H(17)	126.4	C(45)-C(46)-H(46)	119.6
C(14)-C(15)-C(16)	124.7(2)	C(44)-C(45)-C(46)	118.1(3)
C(14)-C(15)-C(35)	117.6(3)	C(44)-C(45)-C(48)	120.9(3)
C(16)-C(15)-C(35)	117.6(2)	C(46)-C(45)-C(48)	121.0(3)
N(1)-C(4)-C(5)	125.3(3)	C(38)-C(39)-C(40)	120.1(3)
N(1)-C(4)-C(3)	109.2(2)	C(38)-C(39)-H(39)	119.9
C(5)-C(4)-C(3)	125.5(2)	C(40)-C(39)-H(39)	119.9
C(44)-C(43)-C(42)	120.3(3)	C(37)-C(38)-C(39)	119.4(3)
C(44)-C(43)-H(43)	119.8	C(37)-C(38)-C(41)	120.2(4)
C(42)-C(43)-H(43)	119.8	C(39)-C(38)-C(41)	120.4(4)
C(9)-C(10)-C(11)	124.4(3)	C(28)-C(29)-C(30)	120.5(4)
C(9)-C(10)-C(28)	117.5(2)	C(28)-C(29)-H(29)	119.7
C(11)-C(10)-C(28)	117.9(3)	C(30)-C(29)-H(29)	119.7
C(43)-C(42)-C(47)	118.4(3)	C(26)-C(25)-C(24)	120.9(3)
C(43)-C(42)-C(20)	122.2(2)	C(26)-C(25)-H(25)	119.5
C(47)-C(42)-C(20)	119.3(3)	C(24)-C(25)-H(25)	119.5
N(3)-C(14)-C(15)	125.1(3)	O(9)-C(48)-O(8)	124.1(4)
N(3)-C(14)-C(13)	109.6(2)	O(9)-C(48)-C(45)	121.0(4)

C(15)-C(14)-C(13)	125.3(2)	O(8)-C(48)-C(45)	114.8(4)
C(6)-C(5)-C(4)	124.8(2)	C(31)-C(32)-C(33)	120.2(4)
C(6)-C(5)-C(21)	118.8(2)	C(31)-C(32)-H(32)	119.9
C(4)-C(5)-C(21)	116.5(3)	C(33)-C(32)-H(32)	119.9
C(17)-C(18)-C(19)	107.2(2)	C(32)-C(31)-C(30)	120.1(3)
C(17)-C(18)-H(18)	126.4	C(32)-C(31)-C(34)	121.4(4)
C(19)-C(18)-H(18)	126.4	C(30)-C(31)-C(34)	118.5(5)
C(46)-C(47)-C(42)	120.7(3)	O(6)-C(41)-O(7)	125.1(4)
C(46)-C(47)-H(47)	119.6	O(6)-C(41)-C(38)	119.5(5)
C(42)-C(47)-H(47)	119.6	O(7)-C(41)-C(38)	115.3(5)
C(35)-C(40)-C(39)	120.6(3)	C(29)-C(30)-C(31)	119.4(4)
C(35)-C(40)-H(40)	119.7	C(29)-C(30)-H(30)	120.3
C(39)-C(40)-H(40)	119.7	C(31)-C(30)-H(30)	120.3
C(38)-C(37)-C(36)	120.8(4)	O(3)-C(27)-O(2)	125.1(4)
C(38)-C(37)-H(37)	119.6	O(3)-C(27)-C(24)	121.7(4)
C(36)-C(37)-H(37)	119.6	O(2)-C(27)-C(24)	113.1(4)
C(8)-C(7)-C(6)	107.5(2)	O(5)-C(34)-O(4)	122.3(4)
C(8)-C(7)-H(7)	126.3	O(5)-C(34)-C(31)	122.3(5)
C(6)-C(7)-H(7)	126.3	O(4)-C(34)-C(31)	115.4(5)
C(12)-C(13)-C(14)	107.2(2)		

Symmetry code: i) -x+1,y,-z+1/2

Table S2 Fractional atomic coordinates ($x10^4$) and equivalent thermal factors ($x10^3$) for μ-O-$[FeTCPP]_2 \cdot nDMF$.

Atoms	X	Y	Z	U_{eq}, Å^2
Fe(1)	5001(1)	865(1)	3598(1)	29(1)
O(1)	5000	864(1)	2500	34(1)
N(4)	5154(1)	-111(1)	3956(1)	33(1)
N(2)	4853(1)	1844(1)	3853(1)	35(1)
N(1)	4504(1)	569(1)	3712(1)	32(1)
N(3)	5506(1)	1162(1)	4029(1)	33(1)
O(8)	4007(1)	-3549(1)	2286(2)	106(1)
O(3)	2844(1)	3526(2)	2943(3)	113(2)
O(7)	7117(1)	-1761(2)	3786(3)	107(1)
O(9)	3764(1)	-3516(2)	3447(3)	95(1)
C(16)	5485(1)	-347(1)	4145(2)	36(1)
C(6)	4523(1)	2076(1)	3853(2)	37(1)
O(6)	7357(1)	-1062(2)	4790(3)	114(1)

C(20)	4582(1)	-660(1)	3675(2)	33(1)
C(19)	4944(1)	-663(1)	3923(2)	35(1)
C(1)	4384(1)	-73(1)	3566(2)	35(1)
C(9)	5066(1)	2392(1)	3959(2)	37(1)
C(11)	5622(1)	1804(1)	3953(2)	36(1)
C(17)	5476(1)	-1063(1)	4286(2)	38(1)
C(15)	5783(1)	44(1)	4142(2)	36(1)
C(4)	4221(1)	986(1)	3578(2)	37(1)
C(43)	4148(1)	-1541(1)	3928(2)	38(1)
C(10)	5420(1)	2390(1)	3943(2)	39(1)
C(42)	4412(1)	-1319(1)	3498(2)	36(1)
C(14)	5787(1)	747(1)	4045(2)	34(1)
C(5)	4228(1)	1691(1)	3687(2)	37(1)
C(18)	5143(1)	-1254(1)	4150(2)	37(1)
C(47)	4508(1)	-1728(2)	2860(2)	46(1)
C(40)	6166(1)	-830(2)	3648(2)	44(1)
C(37)	6712(1)	-450(2)	4841(2)	56(1)
C(7)	4535(1)	2789(1)	4025(2)	43(1)
C(13)	6083(1)	1143(1)	3957(2)	39(1)
C(12)	5982(1)	1796(2)	3901(2)	41(1)
C(2)	4015(1)	-63(1)	3304(2)	40(1)
C(3)	3919(1)	587(2)	3313(2)	44(1)
C(28)	5590(1)	3052(1)	3857(2)	43(1)
C(8)	4865(1)	2986(1)	4077(2)	43(1)
C(35)	6120(1)	-319(1)	4209(2)	39(1)
C(33)	5510(1)	3418(2)	3101(2)	54(1)
C(26)	3806(1)	2562(2)	3025(2)	49(1)
C(21)	3886(1)	2038(1)	3611(2)	43(1)
C(36)	6396(1)	-134(2)	4818(2)	46(1)
C(24)	3245(1)	2667(2)	3447(3)	67(1)
C(22)	3645(1)	1843(2)	4108(3)	57(1)
C(23)	3324(1)	2157(2)	4020(3)	71(1)
C(44)	3991(1)	-2158(2)	3733(2)	45(1)
C(46)	4350(1)	-2340(2)	2670(2)	56(1)
C(45)	4088(1)	-2569(2)	3114(2)	53(1)
C(39)	6483(1)	-1144(2)	3675(2)	56(1)
C(38)	6758(1)	-951(2)	4274(3)	61(1)
C(29)	5825(1)	3320(2)	4488(2)	59(1)
C(25)	3489(1)	2866(2)	2946(3)	63(1)

C(48)	3931(1)	-3255(2)	2949(3)	74(1)
C(32)	5665(1)	4019(2)	2987(3)	62(1)
C(31)	5892(1)	4290(2)	3617(3)	67(1)
C(41)	7106(1)	-1281(3)	4297(4)	82(2)
C(30)	5979(1)	3938(2)	4381(3)	72(1)
C(27)	2903(1)	3018(3)	3368(4)	91(2)
C(34)	6051(2)	4965(2)	3527(4)	90(2)
O(5)	6226(2)	5235(2)	4096(3)	137(2)
O(2)	2692(1)	2736(2)	3798(4)	142(2)
O(4)	5980(2)	5238(2)	2795(3)	127(2)

$$U_{eq} = \frac{1}{3}\left[U_{11}\left(aa^*\right)^2 + U_{22}\left(bb^*\right)^2 + U_{33}\left(cc^*\right)^2 + 2U_{13}aca^*c^*\cos\beta\right]$$

Table S3 Anisotropic displacement parameters (A^2 x 10^3) for μ-O-[FeTCPP]$_2$·nDMF.

Atoms	U11	U22	U33	U23	U13	U12
Fe(1)	28(1)	26(1)	37(1)	3(1)	13(1)	10(1)
O(1)	35(1)	24(1)	44(1)	0	15(1)	0
N(4)	30(1)	30(1)	41(1)	6(1)	17(1)	11(1)
N(2)	36(1)	30(1)	41(1)	0(1)	14(1)	13(1)
N(1)	29(1)	30(1)	41(1)	4(1)	15(1)	11(1)
N(3)	31(1)	30(1)	39(1)	1(1)	10(1)	11(1)
O(8)	188(4)	34(1)	98(2)	-19(1)	34(3)	-4(2)
O(3)	75(2)	119(3)	153(3)	59(3)	42(2)	71(2)
O(7)	59(2)	106(3)	164(4)	6(3)	43(2)	51(2)
O(9)	120(3)	45(2)	125(3)	-10(2)	34(2)	-28(2)
C(16)	36(1)	34(1)	40(1)	5(1)	15(1)	14(1)
C(6)	35(1)	34(1)	44(1)	3(1)	16(1)	16(1)
O(6)	43(2)	143(3)	155(4)	23(3)	8(2)	41(2)
C(20)	36(1)	32(1)	34(1)	4(1)	14(1)	7(1)
C(19)	38(1)	29(1)	43(1)	5(1)	21(1)	9(1)
C(1)	34(1)	35(1)	39(1)	4(1)	18(1)	9(1)
C(9)	39(1)	33(1)	40(1)	0(1)	12(1)	11(1)
C(11)	33(1)	36(1)	42(1)	3(1)	10(1)	7(1)
C(17)	40(2)	35(1)	39(1)	5(1)	12(1)	16(1)
C(15)	35(1)	37(1)	40(1)	4(1)	14(1)	16(1)
C(4)	33(1)	35(1)	44(2)	4(1)	14(1)	14(1)
C(43)	39(1)	32(1)	44(2)	2(1)	12(1)	6(1)
C(10)	44(2)	33(1)	41(1)	1(1)	9(1)	11(1)

C(42)	36(1)	32(1)	42(1)	4(1)	10(1)	9(1)
C(14)	28(1)	39(1)	37(1)	3(1)	10(1)	10(1)
C(5)	35(1)	36(1)	44(2)	2(1)	14(1)	15(1)
C(18)	42(2)	31(1)	42(1)	5(1)	17(1)	10(1)
C(47)	58(2)	37(2)	46(2)	3(1)	19(1)	13(1)
C(40)	42(2)	42(2)	53(2)	6(1)	18(1)	18(1)
C(37)	36(2)	63(2)	70(2)	20(2)	9(2)	14(1)
C(7)	45(2)	34(1)	52(2)	-1(1)	15(1)	18(1)
C(13)	34(1)	40(1)	47(2)	6(1)	17(1)	10(1)
C(12)	36(1)	39(1)	51(2)	5(1)	14(1)	7(1)
C(2)	32(1)	38(1)	51(2)	1(1)	8(1)	6(1)
C(3)	29(1)	42(2)	62(2)	0(1)	12(1)	13(1)
C(28)	47(2)	32(1)	51(2)	3(1)	16(1)	11(1)
C(8)	47(2)	32(1)	52(2)	-3(1)	13(1)	12(1)
C(35)	31(1)	39(1)	51(2)	7(1)	16(1)	14(1)
C(33)	65(2)	43(2)	58(2)	8(1)	17(2)	18(2)
C(26)	43(2)	46(2)	60(2)	9(1)	16(1)	20(1)
C(21)	37(2)	37(1)	56(2)	1(1)	15(1)	16(1)
C(36)	36(2)	47(2)	58(2)	10(1)	15(1)	11(1)
C(24)	45(2)	60(2)	101(3)	17(2)	24(2)	33(2)
C(22)	45(2)	52(2)	78(2)	16(2)	26(2)	25(2)
C(23)	47(2)	70(2)	104(3)	23(2)	37(2)	33(2)
C(44)	48(2)	34(1)	55(2)	4(1)	12(1)	1(1)
C(46)	84(3)	31(1)	54(2)	-1(1)	19(2)	11(2)
C(45)	69(2)	29(1)	60(2)	2(1)	5(2)	8(1)
C(39)	52(2)	54(2)	68(2)	9(2)	28(2)	25(2)
C(38)	37(2)	65(2)	86(3)	26(2)	24(2)	23(2)
C(29)	76(2)	37(2)	64(2)	9(1)	6(2)	-7(2)
C(25)	58(2)	59(2)	76(2)	16(2)	19(2)	33(2)
C(48)	100(3)	33(2)	89(3)	-2(2)	13(3)	1(2)
C(32)	87(3)	40(2)	65(2)	13(2)	29(2)	21(2)
C(31)	91(3)	29(2)	89(3)	11(2)	42(2)	8(2)
C(41)	48(2)	91(3)	113(4)	37(3)	29(2)	38(2)
C(30)	99(3)	44(2)	73(3)	6(2)	9(2)	-20(2)
C(27)	59(3)	87(3)	136(4)	29(3)	40(3)	49(2)
C(34)	150(5)	30(2)	104(4)	8(2)	59(4)	-1(2)
O(5)	205(5)	59(2)	144(4)	18(2)	17(3)	-64(3)
O(2)	72(2)	104(3)	269(6)	75(3)	90(3)	63(2)
O(4)	246(5)	34(2)	116(3)	15(2)	79(3)	-4(2)

Table S4 Fractional atomic coordinates (x10^4) and isotropic thermal factors (x10^3) of hydrogen atoms for μ-O-[FeTCPP]$_2$·nDMF.

Atoms	X	Y	Z	U_{iso} Å^2
H(17)	5669	-1349	4445	45
H(43)	4075	-1267	4355	45
H(18)	5058	-1698	4195	45
H(47)	4684	-1582	2554	55
H(40)	5978	-968	3241	53
H(37)	6899	-319	5253	67
H(7)	4344	3069	4089	52
H(13)	6309	978	3940	47
H(12)	6123	2176	3840	49
H(2)	3870	-440	3155	48
H(3)	3691	754	3170	53
H(8)	4950	3432	4174	52
H(33)	5345	3242	2663	65
H(26)	3971	2706	2684	58
H(36)	6368	208	5216	56
H(22)	3697	1494	4512	68
H(23)	3158	2017	4361	85
H(44)	3813	-2302	4032	54
H(46)	4418	-2611	2235	67
H(39)	6512	-1491	3283	67
H(29)	5883	3079	5002	71
H(25)	3435	3218	2546	76
H(32)	5614	4250	2464	75
H(30)	6140	4122	4820	87

$$U_{iso} = \exp\left[-8\pi^2 U\left(sen\theta/\lambda\right)^2\right]$$

Table S5. Catalytic oxidation conditions.

Reaction	Catalyst	Substrate	Oxidant	Solvent
1	5.5 mg ($1.9 \cdot 10^{-3}$ mmol)	Benzyl alcohol 12.5 µL (0.12 mmol)	TBHP 32.8 µL (0.18 mmol)	Aetonitrile 2mL
2	5.6 mg ($2.0 \cdot 10^{-3}$ mmol)	Benzyl alcohol 12.5 µL (0.12 mmol)	$PhI(OAc)_2$ 77.2 mg (0.24 mmol)	Aetonitrile 2mL
3	5.2 mg ($1.8 \cdot 10^{-3}$ mmol)	1-Phenylethanol 14.5 µL (0.12 mmol)	TBHP 32.8 µL (0.18 mmol)	Aetonitrile 2mL
4	5.0 mg ($1.7 \cdot 10^{-3}$ mmol)	1-hexanol 15.2 µL (0.12 mmol)	TBHP 32.8 µL (0.18 mmol)	Aetonitrile 2mL
5	5.4 mg ($1.9 \cdot 10^{-3}$ mmol)	1-octanol 18.9 µL (0.12 mmol)	TBHP 32.8 µL (0.18 mmol)	Aetonitrile 2mL