Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Structural, electronic and magnetic properties of Cu(II) complexes of 2-substituted tropones bearing ferrocenyl group at 5-position

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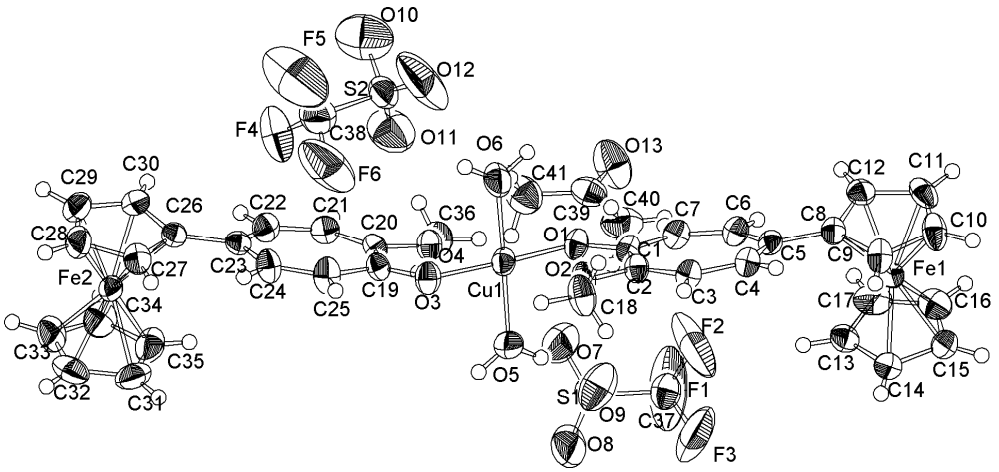
(a)



(b)

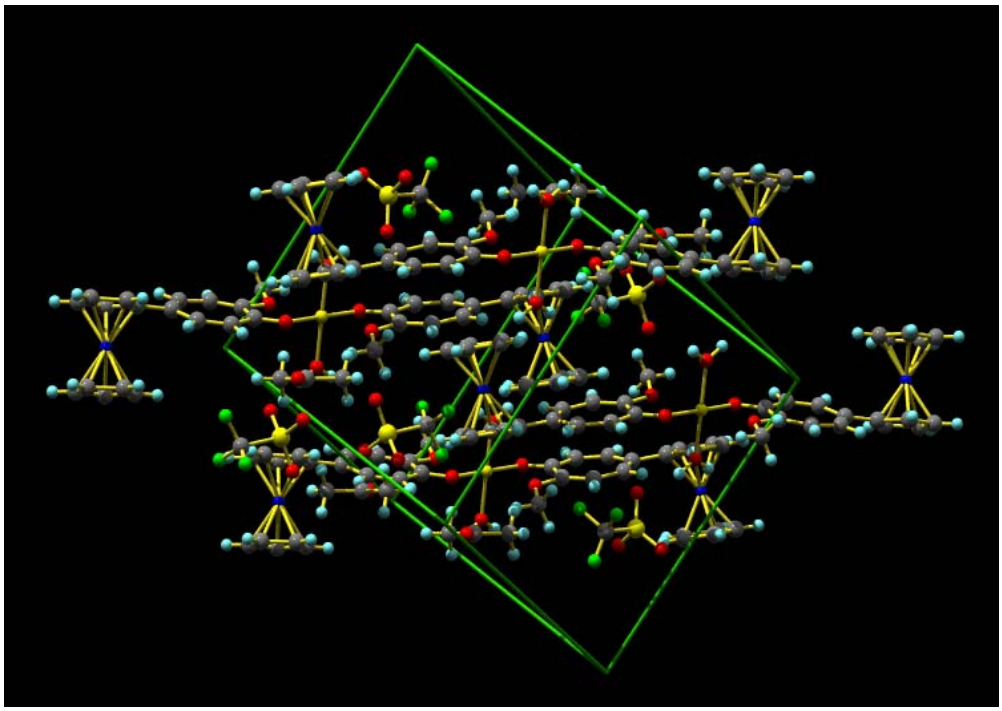


Figure S1. X-ray structure of **1** CH_3COCH_3. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S1. Crystal data and structure refinement for **1** CH_3COCH_3.

Identification code	**1** CH_3COCH_3	
Empirical formula	C41 H42 Cu F6 Fe2 O13 S2	
Formula weight	1096.11	
Temperature	173(2) K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.924(3) Å	α= 105.98(2)°.
	b = 15.246(3) Å	β= 92.31(2)°.
	c = 11.486(5) Å	γ = 105.50(2)°.
Volume	2241.9(12) $Å^3$	
Z	2	
Density (calculated)	1.624 Mg/m^3	
Absorption coefficient	1.289 mm^{-1}	
F(000)	1118	
Crystal size	0.60 x 0.50 x 0.30 mm^3	
Theta range for data collection	2.55 to 27.52°.	
Index ranges	-18<=h<=18, -19<=k<=19, -14<=l<=0	
Reflections collected	10780	
Independent reflections	10267 [R(int) = 0.0236]	
Completeness to theta = 27.52°	99.7 %	
Max. and min. transmission	0.6983 and 0.5117	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10267 / 0 / 586	
reflections with I > 2σ(I)	8420	
Goodness-of-fit on F^2	2.148	
Final R indices [I>2sigma(I)]	R1 = 0.0750, wR2 = 0.2468	
R indices (all data)	R1 = 0.0907, wR2 = 0.2574	
Largest diff. peak and hole	2.424 and -1.279 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1** CH_3COCH_3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1107(3)	-1396(3)	8531(3)	36(1)
C(2)	1172(3)	-680(3)	9692(4)	37(1)
C(3)	735(3)	-799(3)	10705(4)	40(1)
C(4)	159(3)	-1620(3)	10964(4)	38(1)
C(5)	-190(3)	-2558(3)	10219(4)	34(1)
C(6)	-8(3)	-2856(3)	8994(4)	40(1)
C(7)	523(3)	-2372(3)	8284(4)	40(1)
C(8)	-747(3)	-3288(3)	10734(3)	37(1)
C(9)	-1308(3)	-3149(3)	11769(4)	44(1)
C(10)	-1733(4)	-4075(4)	11921(4)	52(1)
C(11)	-1454(4)	-4761(3)	11033(5)	51(1)
C(12)	-844(3)	-4287(3)	10287(4)	43(1)
C(13)	-2729(3)	-3609(4)	8863(4)	47(1)
C(14)	-3282(3)	-3424(3)	9877(5)	47(1)
C(15)	-3747(3)	-4315(3)	10081(5)	51(1)
C(16)	-3474(4)	-5033(3)	9202(5)	54(1)
C(17)	-2833(4)	-4588(4)	8454(4)	53(1)
Fe(1)	-2218(1)	-4058(1)	10227(1)	32(1)
O(1)	1581(2)	-1164(2)	7698(3)	43(1)
O(2)	1756(3)	182(2)	9664(3)	47(1)
C(18)	1985(4)	976(3)	10765(5)	58(1)
Cu(1)	2400(1)	88(1)	7751(1)	39(1)
C(19)	3762(3)	1468(3)	6883(4)	36(1)
C(20)	3646(3)	696(3)	5772(3)	34(1)
C(21)	4183(3)	712(3)	4791(4)	41(1)
C(22)	4942(3)	1423(3)	4558(4)	43(1)
C(23)	5382(3)	2359(3)	5240(4)	35(1)
C(24)	5097(4)	2775(3)	6380(4)	46(1)
C(25)	4429(4)	2397(3)	7067(4)	49(1)
C(26)	6195(3)	2970(3)	4789(4)	40(1)
C(27)	6586(3)	3989(3)	5259(4)	46(1)

C(28)	7345(4)	4309(4)	4567(5)	58(1)
C(29)	7448(4)	3506(4)	3679(6)	60(1)
C(30)	6738(3)	2673(4)	3790(5)	48(1)
C(31)	4708(4)	3965(5)	3377(5)	65(2)
C(32)	5473(5)	4559(4)	2918(6)	65(1)
C(33)	5790(4)	3956(4)	1925(5)	61(1)
C(34)	5232(4)	3025(5)	1761(5)	60(1)
C(35)	4570(4)	3028(5)	2647(5)	64(2)
Fe(2)	6014(1)	3598(1)	3478(1)	38(1)
O(3)	3247(2)	1327(2)	7733(3)	45(1)
O(4)	2939(2)	-88(2)	5816(3)	42(1)
C(36)	2533(4)	-875(3)	4739(5)	54(1)
O(5)	1216(3)	392(3)	7172(3)	52(1)
O(6)	3587(3)	-209(3)	8308(4)	70(1)
S(1)	-1035(1)	-1362(1)	5470(1)	53(1)
O(7)	-280(4)	-1752(4)	4813(5)	91(2)
O(8)	-1557(4)	-1040(6)	4722(7)	130(3)
O(9)	-624(4)	-821(4)	6716(4)	90(2)
C(37)	-1970(4)	-2401(4)	5641(5)	60(1)
F(1)	-2308(6)	-3035(4)	4656(5)	175(4)
F(2)	-1599(6)	-2796(5)	6355(7)	173(3)
F(3)	-2636(4)	-2110(5)	6262(6)	142(2)
S(2)	6282(1)	1001(1)	8809(1)	62(1)
O(10)	6938(6)	443(5)	8180(7)	131(2)
O(11)	5444(5)	691(5)	7899(6)	115(2)
O(12)	6296(9)	1046(6)	10027(7)	173(4)
C(38)	6946(6)	2193(5)	8862(8)	80(2)
F(4)	6904(5)	2284(4)	7707(5)	127(2)
F(5)	7824(6)	2444(6)	9302(11)	237(6)
F(6)	6416(7)	2750(4)	9299(6)	161(3)
C(39)	550(4)	-4253(4)	3473(5)	55(1)
C(40)	125(6)	-3830(5)	4570(6)	76(2)
C(41)	1222(5)	-3584(5)	2932(7)	75(2)
O(13)	376(5)	-5099(3)	3016(4)	90(2)

Table S3. Bond lengths [Å] and angles [°] for **1** CH_3COCH_3.

C(1)-O(1)	1.261(5)
C(1)-C(7)	1.435(6)
C(1)-C(2)	1.453(5)
C(2)-O(2)	1.358(5)
C(2)-C(3)	1.368(6)
C(3)-C(4)	1.410(6)
C(4)-C(5)	1.390(5)
C(5)-C(6)	1.410(6)
C(5)-C(8)	1.459(5)
C(6)-C(7)	1.358(6)
C(8)-C(12)	1.433(6)
C(8)-C(9)	1.447(6)
C(8)-Fe(1)	2.037(4)
C(9)-C(10)	1.439(6)
C(9)-Fe(1)	2.047(4)
C(10)-C(11)	1.395(8)
C(10)-Fe(1)	2.043(4)
C(11)-C(12)	1.433(7)
C(11)-Fe(1)	2.053(4)
C(12)-Fe(1)	2.036(4)
C(13)-C(17)	1.401(7)
C(13)-C(14)	1.428(7)
C(13)-Fe(1)	2.047(4)
C(14)-C(15)	1.428(6)
C(14)-Fe(1)	2.056(4)
C(15)-C(16)	1.415(8)
C(15)-Fe(1)	2.050(4)
C(16)-C(17)	1.434(8)
C(16)-Fe(1)	2.034(4)
C(17)-Fe(1)	2.030(4)
O(1)-Cu(1)	1.926(3)
O(2)-C(18)	1.444(5)
O(2)-Cu(1)	2.390(3)
Cu(1)-O(3)	1.948(3)

Cu(1)-O(6)	1.955(4)
Cu(1)-O(5)	1.967(3)
Cu(1)-O(4)	2.342(3)
C(19)-O(3)	1.266(5)
C(19)-C(25)	1.425(6)
C(19)-C(20)	1.447(5)
C(20)-O(4)	1.345(5)
C(20)-C(21)	1.379(6)
C(21)-C(22)	1.391(6)
C(22)-C(23)	1.380(6)
C(23)-C(24)	1.412(6)
C(23)-C(26)	1.472(6)
C(24)-C(25)	1.357(6)
C(26)-C(27)	1.436(6)
C(26)-C(30)	1.435(6)
C(26)-Fe(2)	2.035(4)
C(27)-C(28)	1.412(7)
C(27)-Fe(2)	2.030(4)
C(28)-C(29)	1.406(9)
C(28)-Fe(2)	2.042(5)
C(29)-C(30)	1.427(7)
C(29)-Fe(2)	2.047(5)
C(30)-Fe(2)	2.037(4)
C(31)-C(35)	1.401(10)
C(31)-C(32)	1.422(9)
C(31)-Fe(2)	2.048(5)
C(32)-C(33)	1.421(9)
C(32)-Fe(2)	2.047(5)
C(33)-C(34)	1.380(9)
C(33)-Fe(2)	2.039(5)
C(34)-C(35)	1.400(8)
C(34)-Fe(2)	2.051(5)
C(35)-Fe(2)	2.040(5)
O(4)-C(36)	1.433(5)
S(1)-O(8)	1.372(5)
S(1)-O(9)	1.445(5)

S(1)-O(7)	1.476(5)
S(1)-C(37)	1.825(6)
C(37)-F(1)	1.244(7)
C(37)-F(3)	1.291(7)
C(37)-F(2)	1.307(8)
S(2)-O(12)	1.381(7)
S(2)-O(11)	1.418(6)
S(2)-O(10)	1.487(7)
S(2)-C(38)	1.788(7)
C(38)-F(5)	1.221(9)
C(38)-F(6)	1.283(9)
C(38)-F(4)	1.373(9)
C(39)-O(13)	1.203(7)
C(39)-C(40)	1.473(8)
C(39)-C(41)	1.478(9)

O(1)-C(1)-C(7)	117.7(4)
O(1)-C(1)-C(2)	119.7(4)
C(7)-C(1)-C(2)	122.7(3)
O(2)-C(2)-C(3)	121.8(4)
O(2)-C(2)-C(1)	110.1(3)
C(3)-C(2)-C(1)	128.1(4)
C(2)-C(3)-C(4)	131.5(4)
C(5)-C(4)-C(3)	129.9(4)
C(4)-C(5)-C(6)	123.7(4)
C(4)-C(5)-C(8)	118.8(4)
C(6)-C(5)-C(8)	117.5(3)
C(7)-C(6)-C(5)	131.7(4)
C(6)-C(7)-C(1)	132.1(4)
C(12)-C(8)-C(9)	107.4(4)
C(12)-C(8)-C(5)	125.6(4)
C(9)-C(8)-C(5)	127.0(4)
C(12)-C(8)-Fe(1)	69.4(2)
C(9)-C(8)-Fe(1)	69.6(2)
C(5)-C(8)-Fe(1)	125.8(3)
C(10)-C(9)-C(8)	106.6(4)

C(10)-C(9)-Fe(1)	69.3(2)
C(8)-C(9)-Fe(1)	68.9(2)
C(11)-C(10)-C(9)	109.7(4)
C(11)-C(10)-Fe(1)	70.5(2)
C(9)-C(10)-Fe(1)	69.6(2)
C(10)-C(11)-C(12)	107.9(4)
C(10)-C(11)-Fe(1)	69.7(3)
C(12)-C(11)-Fe(1)	68.9(2)
C(8)-C(12)-C(11)	108.4(4)
C(8)-C(12)-Fe(1)	69.4(2)
C(11)-C(12)-Fe(1)	70.1(3)
C(17)-C(13)-C(14)	108.9(4)
C(17)-C(13)-Fe(1)	69.2(3)
C(14)-C(13)-Fe(1)	70.0(3)
C(15)-C(14)-C(13)	107.4(4)
C(15)-C(14)-Fe(1)	69.4(3)
C(13)-C(14)-Fe(1)	69.3(2)
C(16)-C(15)-C(14)	107.8(4)
C(16)-C(15)-Fe(1)	69.1(3)
C(14)-C(15)-Fe(1)	69.9(3)
C(15)-C(16)-C(17)	108.3(4)
C(15)-C(16)-Fe(1)	70.3(3)
C(17)-C(16)-Fe(1)	69.2(3)
C(13)-C(17)-C(16)	107.6(4)
C(13)-C(17)-Fe(1)	70.6(3)
C(16)-C(17)-Fe(1)	69.5(3)
C(17)-Fe(1)-C(16)	41.3(2)
C(17)-Fe(1)-C(12)	106.6(2)
C(16)-Fe(1)-C(12)	123.8(2)
C(17)-Fe(1)-C(8)	122.2(2)
C(16)-Fe(1)-C(8)	159.9(2)
C(12)-Fe(1)-C(8)	41.20(17)
C(17)-Fe(1)-C(10)	157.8(2)
C(16)-Fe(1)-C(10)	122.3(2)
C(12)-Fe(1)-C(10)	68.2(2)
C(8)-Fe(1)-C(10)	69.07(17)

C(17)-Fe(1)-C(13)	40.2(2)
C(16)-Fe(1)-C(13)	68.2(2)
C(12)-Fe(1)-C(13)	121.27(19)
C(8)-Fe(1)-C(13)	106.36(18)
C(10)-Fe(1)-C(13)	161.0(2)
C(17)-Fe(1)-C(9)	159.3(2)
C(16)-Fe(1)-C(9)	157.6(2)
C(12)-Fe(1)-C(9)	69.29(19)
C(8)-Fe(1)-C(9)	41.49(16)
C(10)-Fe(1)-C(9)	41.19(18)
C(13)-Fe(1)-C(9)	123.33(19)
C(17)-Fe(1)-C(15)	68.9(2)
C(16)-Fe(1)-C(15)	40.6(2)
C(12)-Fe(1)-C(15)	160.50(19)
C(8)-Fe(1)-C(15)	157.32(19)
C(10)-Fe(1)-C(15)	108.4(2)
C(13)-Fe(1)-C(15)	68.4(2)
C(9)-Fe(1)-C(15)	121.6(2)
C(17)-Fe(1)-C(11)	122.2(2)
C(16)-Fe(1)-C(11)	107.97(19)
C(12)-Fe(1)-C(11)	41.01(19)
C(8)-Fe(1)-C(11)	69.24(17)
C(10)-Fe(1)-C(11)	39.8(2)
C(13)-Fe(1)-C(11)	157.5(2)
C(9)-Fe(1)-C(11)	68.8(2)
C(15)-Fe(1)-C(11)	124.11(19)
C(17)-Fe(1)-C(14)	68.5(2)
C(16)-Fe(1)-C(14)	68.3(2)
C(12)-Fe(1)-C(14)	157.07(19)
C(8)-Fe(1)-C(14)	120.98(18)
C(10)-Fe(1)-C(14)	124.7(2)
C(13)-Fe(1)-C(14)	40.72(19)
C(9)-Fe(1)-C(14)	106.9(2)
C(15)-Fe(1)-C(14)	40.70(18)
C(11)-Fe(1)-C(14)	160.5(2)
C(1)-O(1)-Cu(1)	127.0(3)

C(2)-O(2)-C(18)	118.9(3)
C(2)-O(2)-Cu(1)	111.6(2)
C(18)-O(2)-Cu(1)	129.2(3)
O(1)-Cu(1)-O(3)	177.38(12)
O(1)-Cu(1)-O(6)	89.92(15)
O(3)-Cu(1)-O(6)	89.63(15)
O(1)-Cu(1)-O(5)	90.62(15)
O(3)-Cu(1)-O(5)	89.80(15)
O(6)-Cu(1)-O(5)	179.17(15)
O(1)-Cu(1)-O(4)	105.16(11)
O(3)-Cu(1)-O(4)	72.26(11)
O(6)-Cu(1)-O(4)	89.42(16)
O(5)-Cu(1)-O(4)	89.83(13)
O(1)-Cu(1)-O(2)	71.55(11)
O(3)-Cu(1)-O(2)	111.04(11)
O(6)-Cu(1)-O(2)	92.31(16)
O(5)-Cu(1)-O(2)	88.47(14)
O(4)-Cu(1)-O(2)	176.27(10)
O(3)-C(19)-C(25)	117.7(4)
O(3)-C(19)-C(20)	119.5(4)
C(25)-C(19)-C(20)	122.8(4)
O(4)-C(20)-C(21)	122.5(3)
O(4)-C(20)-C(19)	110.6(3)
C(21)-C(20)-C(19)	126.9(4)
C(20)-C(21)-C(22)	132.3(4)
C(23)-C(22)-C(21)	130.6(4)
C(22)-C(23)-C(24)	123.1(4)
C(22)-C(23)-C(26)	119.9(4)
C(24)-C(23)-C(26)	117.0(4)
C(25)-C(24)-C(23)	131.3(4)
C(24)-C(25)-C(19)	132.8(4)
C(27)-C(26)-C(30)	106.8(4)
C(27)-C(26)-C(23)	126.2(4)
C(30)-C(26)-C(23)	127.1(4)
C(27)-C(26)-Fe(2)	69.2(2)
C(30)-C(26)-Fe(2)	69.4(2)

C(23)-C(26)-Fe(2)	125.6(3)
C(28)-C(27)-C(26)	108.9(5)
C(28)-C(27)-Fe(2)	70.1(3)
C(26)-C(27)-Fe(2)	69.5(2)
C(27)-C(28)-C(29)	107.8(5)
C(27)-C(28)-Fe(2)	69.3(3)
C(29)-C(28)-Fe(2)	70.1(3)
C(28)-C(29)-C(30)	109.0(4)
C(28)-C(29)-Fe(2)	69.7(3)
C(30)-C(29)-Fe(2)	69.1(3)
C(29)-C(30)-C(26)	107.5(4)
C(29)-C(30)-Fe(2)	70.0(3)
C(26)-C(30)-Fe(2)	69.3(2)
C(35)-C(31)-C(32)	106.6(5)
C(35)-C(31)-Fe(2)	69.7(3)
C(32)-C(31)-Fe(2)	69.7(3)
C(33)-C(32)-C(31)	107.4(5)
C(33)-C(32)-Fe(2)	69.3(3)
C(31)-C(32)-Fe(2)	69.7(3)
C(34)-C(33)-C(32)	108.6(5)
C(34)-C(33)-Fe(2)	70.7(3)
C(32)-C(33)-Fe(2)	70.0(3)
C(33)-C(34)-C(35)	107.9(6)
C(33)-C(34)-Fe(2)	69.8(3)
C(35)-C(34)-Fe(2)	69.6(3)
C(34)-C(35)-C(31)	109.5(5)
C(34)-C(35)-Fe(2)	70.4(3)
C(31)-C(35)-Fe(2)	70.3(3)
C(27)-Fe(2)-C(26)	41.36(18)
C(27)-Fe(2)-C(30)	69.0(2)
C(26)-Fe(2)-C(30)	41.27(18)
C(27)-Fe(2)-C(33)	149.6(2)
C(26)-Fe(2)-C(33)	168.3(2)
C(30)-Fe(2)-C(33)	129.8(2)
C(27)-Fe(2)-C(35)	131.2(2)
C(26)-Fe(2)-C(35)	108.6(2)

C(30)-Fe(2)-C(35)	116.9(2)
C(33)-Fe(2)-C(35)	66.9(2)
C(27)-Fe(2)-C(28)	40.6(2)
C(26)-Fe(2)-C(28)	69.27(19)
C(30)-Fe(2)-C(28)	68.9(2)
C(33)-Fe(2)-C(28)	117.2(2)
C(35)-Fe(2)-C(28)	169.3(3)
C(27)-Fe(2)-C(31)	108.6(2)
C(26)-Fe(2)-C(31)	116.0(2)
C(30)-Fe(2)-C(31)	148.9(2)
C(33)-Fe(2)-C(31)	68.2(2)
C(35)-Fe(2)-C(31)	40.1(3)
C(28)-Fe(2)-C(31)	130.5(3)
C(27)-Fe(2)-C(32)	116.8(2)
C(26)-Fe(2)-C(32)	149.1(2)
C(30)-Fe(2)-C(32)	168.9(2)
C(33)-Fe(2)-C(32)	40.7(2)
C(35)-Fe(2)-C(32)	67.3(3)
C(28)-Fe(2)-C(32)	108.8(2)
C(31)-Fe(2)-C(32)	40.6(2)
C(27)-Fe(2)-C(29)	67.9(2)
C(26)-Fe(2)-C(29)	68.84(19)
C(30)-Fe(2)-C(29)	40.9(2)
C(33)-Fe(2)-C(29)	109.2(2)
C(35)-Fe(2)-C(29)	149.8(3)
C(28)-Fe(2)-C(29)	40.2(2)
C(31)-Fe(2)-C(29)	169.1(3)
C(32)-Fe(2)-C(29)	130.6(2)
C(27)-Fe(2)-C(34)	169.6(2)
C(26)-Fe(2)-C(34)	130.3(2)
C(30)-Fe(2)-C(34)	108.6(2)
C(33)-Fe(2)-C(34)	39.4(2)
C(35)-Fe(2)-C(34)	40.0(2)
C(28)-Fe(2)-C(34)	149.1(2)
C(31)-Fe(2)-C(34)	67.9(2)
C(32)-Fe(2)-C(34)	67.5(3)

C(29)-Fe(2)-C(34)	117.4(2)
C(19)-O(3)-Cu(1)	124.5(3)
C(20)-O(4)-C(36)	121.0(3)
C(20)-O(4)-Cu(1)	112.0(2)
C(36)-O(4)-Cu(1)	126.8(3)
O(8)-S(1)-O(9)	123.4(5)
O(8)-S(1)-O(7)	109.8(4)
O(9)-S(1)-O(7)	110.5(3)
O(8)-S(1)-C(37)	103.4(3)
O(9)-S(1)-C(37)	103.0(3)
O(7)-S(1)-C(37)	104.7(3)
F(1)-C(37)-F(3)	115.2(7)
F(1)-C(37)-F(2)	106.5(7)
F(3)-C(37)-F(2)	101.6(7)
F(1)-C(37)-S(1)	113.1(4)
F(3)-C(37)-S(1)	108.3(4)
F(2)-C(37)-S(1)	111.7(5)
O(12)-S(2)-O(11)	128.7(6)
O(12)-S(2)-O(10)	112.1(5)
O(11)-S(2)-O(10)	100.7(4)
O(12)-S(2)-C(38)	102.9(5)
O(11)-S(2)-C(38)	107.1(4)
O(10)-S(2)-C(38)	102.6(4)
F(5)-C(38)-F(6)	116.8(9)
F(5)-C(38)-F(4)	108.8(9)
F(6)-C(38)-F(4)	96.9(6)
F(5)-C(38)-S(2)	114.0(6)
F(6)-C(38)-S(2)	109.3(6)
F(4)-C(38)-S(2)	109.6(5)
O(13)-C(39)-C(40)	123.2(6)
O(13)-C(39)-C(41)	119.9(6)
C(40)-C(39)-C(41)	116.9(5)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **1** CH_3COCH_3. 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}
C(1)	29(2)	43(2)	31(2)	11(2)	4(1)	4(2)
C(2)	35(2)	33(2)	35(2)	8(2)	1(2)	1(1)
C(3)	40(2)	39(2)	37(2)	7(2)	7(2)	6(2)
C(4)	37(2)	40(2)	32(2)	8(2)	4(2)	4(2)
C(5)	26(2)	36(2)	36(2)	11(2)	0(1)	4(1)
C(6)	36(2)	36(2)	38(2)	4(2)	4(2)	2(2)
C(7)	41(2)	41(2)	30(2)	3(2)	6(2)	9(2)
C(8)	33(2)	42(2)	32(2)	14(2)	-1(1)	4(2)
C(9)	46(2)	45(2)	28(2)	8(2)	0(2)	-4(2)
C(10)	53(3)	61(3)	34(2)	25(2)	-5(2)	-6(2)
C(11)	49(2)	49(2)	56(3)	31(2)	-15(2)	2(2)
C(12)	36(2)	46(2)	46(2)	18(2)	-3(2)	11(2)
C(13)	45(2)	57(3)	44(2)	25(2)	-1(2)	16(2)
C(14)	42(2)	46(2)	59(3)	23(2)	8(2)	16(2)
C(15)	33(2)	52(3)	69(3)	28(2)	5(2)	7(2)
C(16)	42(2)	42(2)	65(3)	12(2)	-19(2)	1(2)
C(17)	56(3)	62(3)	34(2)	2(2)	-17(2)	21(2)
Fe(1)	30(1)	33(1)	30(1)	10(1)	-2(1)	4(1)
O(1)	41(2)	50(2)	34(1)	14(1)	10(1)	6(1)
O(2)	57(2)	33(1)	40(2)	8(1)	6(1)	-5(1)
C(18)	77(3)	33(2)	47(3)	6(2)	5(2)	-7(2)
Cu(1)	34(1)	48(1)	36(1)	19(1)	4(1)	6(1)
C(19)	44(2)	36(2)	31(2)	14(2)	7(2)	10(2)
C(20)	41(2)	32(2)	31(2)	13(1)	1(2)	9(2)
C(21)	46(2)	37(2)	37(2)	6(2)	5(2)	12(2)
C(22)	50(2)	45(2)	33(2)	10(2)	12(2)	15(2)
C(23)	34(2)	40(2)	35(2)	16(2)	0(2)	11(2)
C(24)	56(3)	36(2)	39(2)	10(2)	9(2)	3(2)
C(25)	60(3)	39(2)	35(2)	3(2)	12(2)	2(2)
C(26)	34(2)	49(2)	45(2)	25(2)	4(2)	12(2)
C(27)	40(2)	51(2)	41(2)	18(2)	-6(2)	2(2)

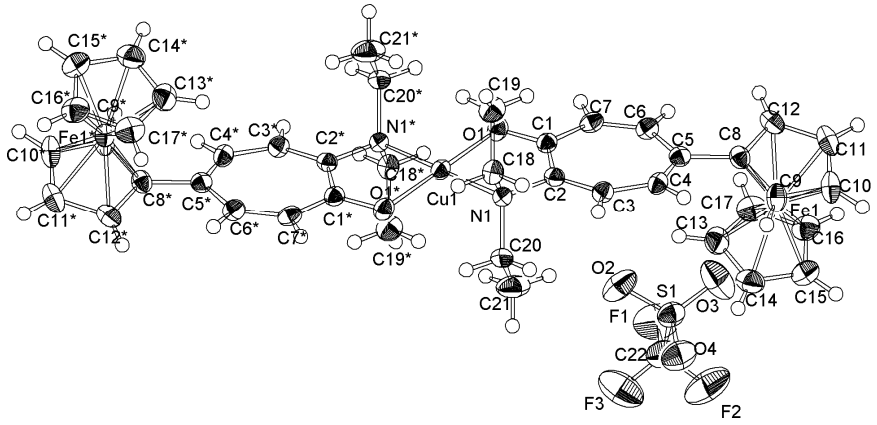
C(28)	35(2)	68(3)	73(3)	40(3)	1(2)	1(2)
C(29)	35(2)	86(4)	72(3)	43(3)	13(2)	18(2)
C(30)	41(2)	59(3)	58(3)	27(2)	15(2)	24(2)
C(31)	49(3)	110(5)	60(3)	41(3)	16(2)	46(3)
C(32)	72(3)	67(3)	70(3)	35(3)	-3(3)	33(3)
C(33)	68(3)	83(4)	42(3)	38(3)	10(2)	20(3)
C(34)	57(3)	84(4)	37(2)	20(2)	0(2)	16(3)
C(35)	39(2)	100(4)	59(3)	44(3)	2(2)	11(3)
Fe(2)	32(1)	50(1)	38(1)	21(1)	6(1)	12(1)
O(3)	53(2)	46(2)	33(1)	11(1)	12(1)	9(1)
O(4)	43(2)	37(1)	38(2)	9(1)	3(1)	2(1)
C(36)	54(3)	39(2)	53(3)	2(2)	-2(2)	-2(2)
O(5)	44(2)	66(2)	58(2)	30(2)	9(1)	22(2)
O(6)	40(2)	89(3)	92(3)	64(3)	-7(2)	2(2)
S(1)	66(1)	48(1)	44(1)	17(1)	-1(1)	11(1)
O(7)	82(3)	101(4)	100(4)	33(3)	40(3)	35(3)
O(8)	73(3)	202(7)	171(6)	149(6)	15(4)	34(4)
O(9)	65(3)	108(4)	68(3)	6(2)	11(2)	0(3)
C(37)	61(3)	67(3)	51(3)	21(2)	15(2)	15(3)
F(1)	219(7)	103(4)	93(3)	-21(3)	39(4)	-88(4)
F(2)	205(7)	124(5)	185(6)	119(5)	-45(5)	-26(5)
F(3)	95(3)	137(5)	186(6)	40(4)	90(4)	18(3)
S(2)	50(1)	67(1)	76(1)	43(1)	-3(1)	9(1)
O(10)	148(6)	93(4)	133(5)	-2(4)	-8(5)	48(4)
O(11)	99(4)	108(4)	132(5)	47(4)	-29(4)	15(3)
O(12)	342(14)	145(6)	111(5)	94(5)	91(7)	133(8)
C(38)	72(4)	65(4)	104(5)	31(4)	4(4)	13(3)
F(4)	156(5)	122(4)	119(4)	81(4)	40(4)	17(4)
F(5)	144(6)	140(6)	384(14)	130(8)	-152(8)	-58(5)
F(6)	313(10)	105(4)	119(4)	46(3)	76(5)	128(6)
C(39)	61(3)	53(3)	51(3)	13(2)	-9(2)	20(2)
C(40)	83(4)	83(4)	73(4)	18(3)	14(3)	47(4)
C(41)	76(4)	63(3)	79(4)	23(3)	-5(3)	10(3)
O(13)	144(5)	51(2)	66(3)	10(2)	20(3)	16(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1** CH_3COCH_3.

	x	y	z	U(eq)
H(1)	839	-225	11351	48
H(2)	-18	-1518	11770	46
H(3)	-311	-3514	8593	48
H(4)	505	-2752	7470	47
H(5)	-1382	-2562	12254	52
H(6)	-2141	-4200	12533	63
H(7)	-1637	-5426	10940	61
H(8)	-552	-4584	9610	51
H(9)	-2351	-3144	8521	56
H(10)	-3333	-2818	10332	56
H(11)	-4164	-4410	10696	61
H(12)	-3681	-5695	9122	64
H(13)	-2533	-4901	7798	64
H(14)	2410	1545	10604	87
H(15)	2340	827	11406	87
H(16)	1359	1094	11033	87
H(17)	4000	126	4154	50
H(18)	5200	1233	3805	51
H(19)	5432	3435	6728	55
H(20)	4400	2840	7820	59
H(21)	6370	4383	5928	55
H(22)	7720	4953	4680	69
H(23)	7915	3516	3099	72
H(24)	6642	2037	3294	58
H(25)	4359	4166	4047	78
H(26)	5726	5233	3220	77
H(27)	6301	4160	1453	73
H(28)	5288	2480	1155	72
H(29)	4100	2479	2739	77
H(30)	2029	-1376	4945	81

H(31)	3074	-1126	4401	81
H(32)	2219	-659	4133	81
H(39)	575	-67	7007	78
H(40)	1285	999	7057	78
H(41)	3526	-815	8420	105
H(42)	4226	253	8467	105
H(33)	-301	-4339	4847	114
H(34)	-277	-3439	4376	114
H(35)	672	-3430	5218	114
H(36)	1453	-3946	2210	112
H(37)	1802	-3183	3532	112
H(38)	856	-3181	2696	112

(a)



(b)

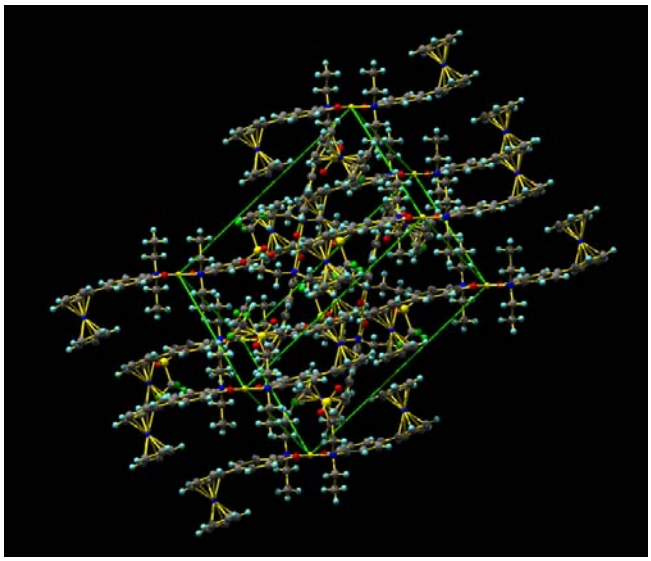


Figure S2. X-ray structure of **2**. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S6. Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C44 H46 Cu F6 Fe2 N2 O8 S2	
Formula weight	1084.19	
Temperature	298(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P21/a	
Unit cell dimensions	a = 16.055(3) Å	α= 90°.
	b = 18.374(5) Å	β= 100.75(2)°.
	c = 7.719(3) Å	γ = 90°.
Volume	2237.1(10) $Å^3$	
Z	2	
Density (calculated)	1.609 Mg/m^3	
Absorption coefficient	1.284 mm^{-1}	
F(000)	1110	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.57 to 27.48°.	
Index ranges	-11<=h<=20, 0<=k<=23, -10<=l<=9	
Reflections collected	6113	
Independent reflections	5118 [R(int) = 0.0226]	
Completeness to theta = 27.48°	99.9 %	
Max. and min. transmission	0.7832 and 0.7832	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5118 / 0 / 295	
reflections with I > 2σ(I)	3562	
Goodness-of-fit on F^2	0.916	
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.1092	
R indices (all data)	R1 = 0.0713, wR2 = 0.1330	
Largest diff. peak and hole	0.430 and -0.311 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	536(2)	-936(1)	2682(3)	26(1)
C(2)	-293(2)	-1211(1)	2051(3)	25(1)
C(3)	-680(2)	-1800(2)	2644(3)	27(1)
C(4)	-380(2)	-2328(1)	3907(3)	27(1)
C(5)	423(2)	-2416(1)	4928(3)	26(1)
C(6)	1103(2)	-1918(2)	4933(4)	30(1)
C(7)	1153(2)	-1294(2)	3998(4)	28(1)
C(8)	576(2)	-3059(2)	6050(3)	29(1)
C(9)	96(2)	-3723(2)	5785(4)	34(1)
C(10)	492(2)	-4238(2)	7057(4)	40(1)
C(11)	1208(2)	-3898(2)	8110(4)	42(1)
C(12)	1270(2)	-3179(2)	7495(4)	35(1)
C(13)	1801(2)	-3635(2)	3300(4)	42(1)
C(14)	1283(2)	-4264(2)	2965(4)	44(1)
C(15)	1627(2)	-4801(2)	4203(4)	43(1)
C(16)	2346(2)	-4507(2)	5291(4)	42(1)
C(17)	2464(2)	-3793(2)	4731(4)	42(1)
Fe(1)	1315(1)	-3895(1)	5493(1)	28(1)
O(1)	762(1)	-337(1)	2042(2)	30(1)
N(1)	-779(1)	-785(1)	593(3)	24(1)
C(18)	-1527(2)	-413(2)	1123(4)	30(1)
C(19)	-1280(2)	85(2)	2683(4)	39(1)
C(20)	-1085(2)	-1262(2)	-981(4)	35(1)
C(21)	-388(3)	-1683(2)	-1576(5)	54(1)
S(1)	-2333(1)	-3358(1)	996(1)	41(1)
O(2)	-2316(2)	-2590(1)	742(4)	61(1)
O(3)	-1971(2)	-3590(2)	2751(4)	79(1)
O(4)	-3115(2)	-3698(2)	187(4)	63(1)
C(22)	-1561(3)	-3680(2)	-266(6)	60(1)
F(1)	-791(2)	-3415(2)	346(4)	82(1)
F(2)	-1502(2)	-4403(2)	-233(5)	109(1)

F(3)	-1780(2)	-3504(2)	-1947(4)	104(1)
Cu(1)	0	0	0	25(1)

Table S8. Bond lengths [Å] and angles [°] for **2**.

C(1)-O(1)	1.286(3)
C(1)-C(2)	1.423(4)
C(1)-C(7)	1.439(4)
C(2)-C(3)	1.368(4)
C(2)-N(1)	1.470(3)
C(3)-C(4)	1.396(4)
C(4)-C(5)	1.390(4)
C(5)-C(6)	1.424(4)
C(5)-C(8)	1.458(4)
C(6)-C(7)	1.365(4)
C(8)-C(9)	1.438(4)
C(8)-C(12)	1.439(4)
C(8)-Fe(1)	2.035(3)
C(9)-C(10)	1.425(4)
C(9)-Fe(1)	2.036(3)
C(10)-C(11)	1.423(5)
C(10)-Fe(1)	2.049(3)
C(11)-C(12)	1.414(5)
C(11)-Fe(1)	2.059(3)
C(12)-Fe(1)	2.041(3)
C(13)-C(17)	1.413(5)
C(13)-C(14)	1.419(5)
C(13)-Fe(1)	2.048(3)
C(14)-C(15)	1.412(5)
C(14)-Fe(1)	2.058(3)
C(15)-C(16)	1.403(5)
C(15)-Fe(1)	2.049(3)
C(16)-C(17)	1.406(5)
C(16)-Fe(1)	2.032(3)
C(17)-Fe(1)	2.047(3)
O(1)-Cu(1)	1.910(2)
N(1)-C(18)	1.504(3)
N(1)-C(20)	1.505(3)
N(1)-Cu(1)	2.016(2)

C(18)-C(19)	1.505(4)
C(20)-C(21)	1.501(5)
S(1)-O(2)	1.425(3)
S(1)-O(3)	1.436(3)
S(1)-O(4)	1.438(3)
S(1)-C(22)	1.812(4)
C(22)-F(3)	1.320(5)
C(22)-F(1)	1.330(5)
C(22)-F(2)	1.331(5)
Cu(1)-O(1)#1	1.910(2)
Cu(1)-N(1)#1	2.016(2)

O(1)-C(1)-C(2)	119.1(2)
O(1)-C(1)-C(7)	117.2(2)
C(2)-C(1)-C(7)	123.8(2)
C(3)-C(2)-C(1)	128.4(2)
C(3)-C(2)-N(1)	118.0(2)
C(1)-C(2)-N(1)	113.7(2)
C(2)-C(3)-C(4)	131.7(3)
C(5)-C(4)-C(3)	129.8(2)
C(4)-C(5)-C(6)	123.7(2)
C(4)-C(5)-C(8)	117.9(2)
C(6)-C(5)-C(8)	118.4(2)
C(7)-C(6)-C(5)	131.2(3)
C(6)-C(7)-C(1)	131.1(2)
C(9)-C(8)-C(12)	107.3(3)
C(9)-C(8)-C(5)	125.2(2)
C(12)-C(8)-C(5)	127.2(3)
C(9)-C(8)-Fe(1)	69.38(16)
C(12)-C(8)-Fe(1)	69.57(16)
C(5)-C(8)-Fe(1)	121.73(18)
C(10)-C(9)-C(8)	107.9(3)
C(10)-C(9)-Fe(1)	70.04(17)
C(8)-C(9)-Fe(1)	69.26(16)
C(11)-C(10)-C(9)	108.1(3)
C(11)-C(10)-Fe(1)	70.14(17)

C(9)-C(10)-Fe(1)	69.12(16)
C(12)-C(11)-C(10)	108.6(3)
C(12)-C(11)-Fe(1)	69.15(17)
C(10)-C(11)-Fe(1)	69.34(17)
C(11)-C(12)-C(8)	108.1(3)
C(11)-C(12)-Fe(1)	70.51(19)
C(8)-C(12)-Fe(1)	69.09(16)
C(17)-C(13)-C(14)	107.8(3)
C(17)-C(13)-Fe(1)	69.76(18)
C(14)-C(13)-Fe(1)	70.16(18)
C(15)-C(14)-C(13)	107.7(3)
C(15)-C(14)-Fe(1)	69.57(19)
C(13)-C(14)-Fe(1)	69.41(18)
C(16)-C(15)-C(14)	108.1(3)
C(16)-C(15)-Fe(1)	69.21(19)
C(14)-C(15)-Fe(1)	70.22(19)
C(15)-C(16)-C(17)	108.5(3)
C(15)-C(16)-Fe(1)	70.57(19)
C(17)-C(16)-Fe(1)	70.41(18)
C(16)-C(17)-C(13)	107.9(3)
C(16)-C(17)-Fe(1)	69.26(19)
C(13)-C(17)-Fe(1)	69.86(18)
C(16)-Fe(1)-C(8)	161.74(13)
C(16)-Fe(1)-C(9)	155.26(13)
C(8)-Fe(1)-C(9)	41.37(12)
C(16)-Fe(1)-C(12)	124.00(13)
C(8)-Fe(1)-C(12)	41.34(11)
C(9)-Fe(1)-C(12)	69.27(13)
C(16)-Fe(1)-C(17)	40.33(14)
C(8)-Fe(1)-C(17)	125.71(13)
C(9)-Fe(1)-C(17)	162.59(13)
C(12)-Fe(1)-C(17)	108.63(13)
C(16)-Fe(1)-C(13)	67.92(14)
C(8)-Fe(1)-C(13)	109.02(12)
C(9)-Fe(1)-C(13)	125.29(13)
C(12)-Fe(1)-C(13)	123.26(13)

C(17)-Fe(1)-C(13)	40.39(13)
C(16)-Fe(1)-C(10)	119.93(13)
C(8)-Fe(1)-C(10)	69.05(12)
C(9)-Fe(1)-C(10)	40.84(11)
C(12)-Fe(1)-C(10)	68.56(14)
C(17)-Fe(1)-C(10)	155.87(13)
C(13)-Fe(1)-C(10)	161.07(14)
C(16)-Fe(1)-C(15)	40.22(13)
C(8)-Fe(1)-C(15)	157.04(13)
C(9)-Fe(1)-C(15)	120.45(13)
C(12)-Fe(1)-C(15)	159.68(13)
C(17)-Fe(1)-C(15)	67.65(14)
C(13)-Fe(1)-C(15)	67.81(14)
C(10)-Fe(1)-C(15)	106.21(14)
C(16)-Fe(1)-C(14)	67.74(14)
C(8)-Fe(1)-C(14)	122.49(13)
C(9)-Fe(1)-C(14)	107.56(14)
C(12)-Fe(1)-C(14)	158.84(13)
C(17)-Fe(1)-C(14)	67.78(14)
C(13)-Fe(1)-C(14)	40.43(14)
C(10)-Fe(1)-C(14)	123.55(14)
C(15)-Fe(1)-C(14)	40.22(14)
C(16)-Fe(1)-C(11)	106.97(13)
C(8)-Fe(1)-C(11)	68.67(12)
C(9)-Fe(1)-C(11)	68.53(13)
C(12)-Fe(1)-C(11)	40.34(13)
C(17)-Fe(1)-C(11)	121.80(14)
C(13)-Fe(1)-C(11)	157.81(14)
C(10)-Fe(1)-C(11)	40.52(13)
C(15)-Fe(1)-C(11)	123.16(14)
C(14)-Fe(1)-C(11)	159.65(14)
C(1)-O(1)-Cu(1)	114.29(17)
C(2)-N(1)-C(18)	111.7(2)
C(2)-N(1)-C(20)	110.8(2)
C(18)-N(1)-C(20)	109.1(2)
C(2)-N(1)-Cu(1)	106.98(15)

C(18)-N(1)-Cu(1)	107.30(16)
C(20)-N(1)-Cu(1)	110.91(16)
N(1)-C(18)-C(19)	112.9(2)
C(21)-C(20)-N(1)	113.4(2)
O(2)-S(1)-O(3)	114.2(2)
O(2)-S(1)-O(4)	114.13(16)
O(3)-S(1)-O(4)	116.5(2)
O(2)-S(1)-C(22)	102.6(2)
O(3)-S(1)-C(22)	102.3(2)
O(4)-S(1)-C(22)	104.69(19)
F(3)-C(22)-F(1)	108.6(4)
F(3)-C(22)-F(2)	105.6(4)
F(1)-C(22)-F(2)	107.4(4)
F(3)-C(22)-S(1)	111.4(3)
F(1)-C(22)-S(1)	111.8(3)
F(2)-C(22)-S(1)	111.7(3)
O(1)#1-Cu(1)-O(1)	180.0
O(1)#1-Cu(1)-N(1)#1	84.83(8)
O(1)-Cu(1)-N(1)#1	95.17(8)
O(1)#1-Cu(1)-N(1)	95.17(8)
O(1)-Cu(1)-N(1)	84.83(8)
N(1)#1-Cu(1)-N(1)	180.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

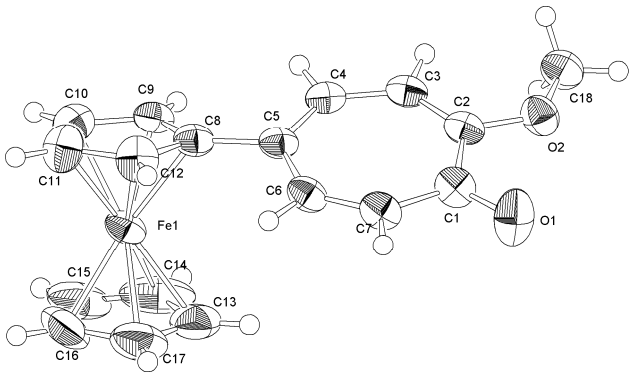
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(1)	24(1)	26(1)	-2(1)	8(1)	0(1)
C(2)	25(1)	26(1)	22(1)	-3(1)	4(1)	2(1)
C(3)	23(1)	27(1)	30(1)	-1(1)	4(1)	-2(1)
C(4)	29(1)	23(1)	32(1)	1(1)	9(1)	-2(1)
C(5)	28(1)	27(1)	26(1)	-3(1)	8(1)	4(1)
C(6)	26(1)	29(1)	34(1)	-1(1)	1(1)	1(1)
C(7)	22(1)	27(1)	35(1)	-6(1)	3(1)	-2(1)
C(8)	29(1)	31(1)	26(1)	3(1)	8(1)	5(1)
C(9)	29(1)	35(2)	41(2)	12(1)	11(1)	2(1)
C(10)	39(2)	39(2)	46(2)	20(1)	15(1)	6(1)
C(11)	46(2)	51(2)	31(2)	15(1)	9(1)	10(1)
C(12)	37(2)	45(2)	25(1)	1(1)	5(1)	7(1)
C(13)	51(2)	40(2)	40(2)	3(1)	24(2)	3(1)
C(14)	50(2)	49(2)	34(2)	-8(1)	9(1)	2(2)
C(15)	46(2)	34(2)	51(2)	-7(1)	10(2)	1(1)
C(16)	40(2)	38(2)	48(2)	-6(1)	6(1)	10(1)
C(17)	34(2)	48(2)	48(2)	-8(1)	17(1)	-2(1)
Fe(1)	28(1)	27(1)	29(1)	4(1)	6(1)	2(1)
O(1)	28(1)	26(1)	35(1)	2(1)	5(1)	-4(1)
N(1)	26(1)	22(1)	24(1)	-1(1)	5(1)	0(1)
C(18)	24(1)	30(1)	36(1)	4(1)	6(1)	3(1)
C(19)	38(2)	38(2)	44(2)	-4(1)	18(1)	3(1)
C(20)	46(2)	30(1)	26(1)	-4(1)	0(1)	-10(1)
C(21)	66(2)	55(2)	47(2)	-23(2)	28(2)	-16(2)
S(1)	38(1)	40(1)	47(1)	-5(1)	9(1)	-9(1)
O(2)	43(1)	38(1)	97(2)	-11(1)	-1(1)	-4(1)
O(3)	66(2)	119(3)	50(2)	22(2)	10(1)	-8(2)
O(4)	50(2)	59(2)	77(2)	-12(1)	5(1)	-24(1)
C(22)	62(2)	58(2)	62(3)	-16(2)	13(2)	-1(2)
F(1)	44(1)	103(2)	102(2)	-28(2)	24(1)	0(1)
F(2)	125(3)	53(2)	152(3)	-37(2)	32(2)	22(2)

F(3)	110(2)	152(3)	55(2)	-12(2)	31(2)	8(2)
Cu(1)	26(1)	22(1)	27(1)	-1(1)	7(1)	-2(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(1)	-1245	-1859	2109	32
H(2)	-778	-2673	4093	33
H(3)	1599	-2038	5708	36
H(4)	1675	-1061	4255	34
H(5)	-388	-3802	4935	41
H(6)	313	-4714	7178	48
H(7)	1574	-4113	9046	51
H(8)	1687	-2842	7946	42
H(9)	1719	-3197	2688	50
H(10)	804	-4314	2087	53
H(11)	1414	-5268	4283	52
H(12)	2687	-4745	6226	51
H(13)	2900	-3479	5215	51
H(14)	-1916	-779	1407	36
H(15)	-1823	-132	132	36
H(16)	-1779	308	2964	58
H(17)	-905	456	2403	58
H(18)	-998	-191	3678	58
H(19)	-1501	-1602	-690	42
H(20)	-1365	-961	-1948	42
H(21)	-622	-1976	-2579	81
H(22)	-116	-1992	-635	81
H(23)	20	-1351	-1894	81

(a)



(b)

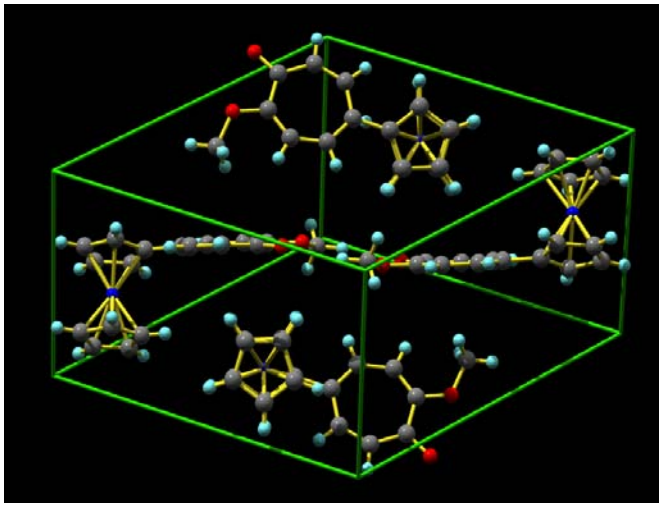


Figure S3. X-ray structure of **4**. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S11. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C18 H16 Fe O2	
Formula weight	320.16	
Temperature	213(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P21/a	
Unit cell dimensions	a = 12.891(7) Å	α= 90°.
	b = 8.762(5) Å	β= 111.26(5)°.
	c = 13.727(9) Å	γ = 90°.
Volume	1445.0(15) $Å^3$	
Z	4	

Density (calculated)	1.472 Mg/m^3
Absorption coefficient	1.044 mm^{-1}
F(000)	664
Crystal size	0.50 x 0.40 x 0.20 mm^3
Theta range for data collection	2.82 to 27.51°.
Index ranges	-16<=h<=0, 0<=k<=11, -16<=l<=17
Reflections collected	3482
Independent reflections	3331 [R(int) = 0.0304]
Completeness to theta = 27.51°	100.0 %
Max. and min. transmission	0.8184 and 0.6233
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3331 / 0 / 191
reflections with I > 2σ(I)	2428
Goodness-of-fit on F^2	1.514
Final R indices [I>2sigma(I)]	R1 = 0.0713, wR2 = 0.1973
R indices (all data)	R1 = 0.0977, wR2 = 0.2088
Largest diff. peak and hole	1.930 and -1.295 $e.Å^{-3}$

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6317(4)	5943(4)	3337(3)	45(1)
C(2)	6875(3)	5096(4)	4324(3)	40(1)
C(3)	7897(3)	4416(4)	4642(3)	42(1)
C(4)	8688(3)	4265(4)	4166(3)	40(1)
C(5)	8685(3)	4796(4)	3222(3)	38(1)
C(6)	7807(3)	5709(4)	2521(3)	42(1)
C(7)	6842(4)	6188(4)	2593(3)	44(1)
C(8)	9624(3)	4432(4)	2890(3)	41(1)
C(9)	10361(3)	3153(5)	3228(3)	43(1)
C(10)	11132(4)	3230(5)	2722(4)	50(1)
C(11)	10891(4)	4526(5)	2083(4)	58(1)
C(12)	9961(4)	5277(4)	2183(4)	51(1)
C(13)	7936(4)	2379(7)	929(4)	66(1)
C(14)	8688(7)	1112(6)	1319(5)	93(2)
C(15)	9448(6)	1149(8)	834(5)	90(2)
C(16)	9231(6)	2431(10)	159(4)	88(2)
C(17)	8276(5)	3142(7)	228(4)	78(2)
Fe(1)	9552(1)	3111(1)	1646(1)	40(1)
O(1)	5367(3)	6440(5)	3152(3)	68(1)
O(2)	6215(2)	5063(3)	4886(2)	48(1)
C(18)	6510(4)	4100(6)	5789(3)	58(1)

Table S13. Bond lengths [Å] and angles [°] for **4**.

C(1)-O(1)	1.236(5)
C(1)-C(7)	1.432(6)
C(1)-C(2)	1.483(5)
C(2)-O(2)	1.339(5)
C(2)-C(3)	1.365(6)
C(3)-C(4)	1.402(6)
C(4)-C(5)	1.375(6)
C(5)-C(6)	1.434(5)
C(5)-C(8)	1.475(6)
C(6)-C(7)	1.349(6)
C(8)-C(12)	1.409(6)
C(8)-C(9)	1.433(5)
C(8)-Fe(1)	2.037(4)
C(9)-C(10)	1.405(6)
C(9)-Fe(1)	2.040(4)
C(10)-C(11)	1.399(6)
C(10)-Fe(1)	2.039(5)
C(11)-C(12)	1.417(6)
C(11)-Fe(1)	2.032(5)
C(12)-Fe(1)	2.035(4)
C(13)-C(17)	1.367(9)
C(13)-C(14)	1.443(9)
C(13)-Fe(1)	2.057(5)
C(14)-C(15)	1.369(10)
C(14)-Fe(1)	2.036(6)
C(15)-C(16)	1.419(11)
C(15)-Fe(1)	2.026(5)
C(16)-C(17)	1.414(9)
C(16)-Fe(1)	2.020(5)
C(17)-Fe(1)	2.043(5)
O(2)-C(18)	1.433(5)
O(1)-C(1)-C(7)	119.4(4)
O(1)-C(1)-C(2)	118.7(4)

C(7)-C(1)-C(2)	121.9(4)
O(2)-C(2)-C(3)	123.2(3)
O(2)-C(2)-C(1)	109.7(3)
C(3)-C(2)-C(1)	127.1(4)
C(2)-C(3)-C(4)	132.3(4)
C(5)-C(4)-C(3)	130.7(4)
C(4)-C(5)-C(6)	123.6(4)
C(4)-C(5)-C(8)	119.7(3)
C(6)-C(5)-C(8)	116.7(4)
C(7)-C(6)-C(5)	130.4(4)
C(6)-C(7)-C(1)	133.8(4)
C(12)-C(8)-C(9)	107.4(4)
C(12)-C(8)-C(5)	126.3(4)
C(9)-C(8)-C(5)	126.2(4)
C(12)-C(8)-Fe(1)	69.7(2)
C(9)-C(8)-Fe(1)	69.5(2)
C(5)-C(8)-Fe(1)	126.1(3)
C(10)-C(9)-C(8)	107.9(4)
C(10)-C(9)-Fe(1)	69.8(3)
C(8)-C(9)-Fe(1)	69.3(2)
C(11)-C(10)-C(9)	108.3(4)
C(11)-C(10)-Fe(1)	69.6(3)
C(9)-C(10)-Fe(1)	69.9(2)
C(10)-C(11)-C(12)	108.6(4)
C(10)-C(11)-Fe(1)	70.2(3)
C(12)-C(11)-Fe(1)	69.7(3)
C(8)-C(12)-C(11)	107.8(4)
C(8)-C(12)-Fe(1)	69.8(2)
C(11)-C(12)-Fe(1)	69.5(3)
C(17)-C(13)-C(14)	107.1(6)
C(17)-C(13)-Fe(1)	70.0(3)
C(14)-C(13)-Fe(1)	68.6(3)
C(15)-C(14)-C(13)	107.7(6)
C(15)-C(14)-Fe(1)	69.9(4)
C(13)-C(14)-Fe(1)	70.2(3)
C(14)-C(15)-C(16)	109.3(5)

C(14)-C(15)-Fe(1)	70.7(3)
C(16)-C(15)-Fe(1)	69.2(3)
C(17)-C(16)-C(15)	106.0(6)
C(17)-C(16)-Fe(1)	70.5(3)
C(15)-C(16)-Fe(1)	69.7(3)
C(13)-C(17)-C(16)	109.9(6)
C(13)-C(17)-Fe(1)	71.1(3)
C(16)-C(17)-Fe(1)	68.8(3)
C(16)-Fe(1)-C(15)	41.0(3)
C(16)-Fe(1)-C(11)	108.6(3)
C(15)-Fe(1)-C(11)	124.0(3)
C(16)-Fe(1)-C(12)	124.9(3)
C(15)-Fe(1)-C(12)	161.2(3)
C(11)-Fe(1)-C(12)	40.79(18)
C(16)-Fe(1)-C(14)	68.2(3)
C(15)-Fe(1)-C(14)	39.4(3)
C(11)-Fe(1)-C(14)	158.2(3)
C(12)-Fe(1)-C(14)	158.7(3)
C(16)-Fe(1)-C(8)	160.9(3)
C(15)-Fe(1)-C(8)	156.5(3)
C(11)-Fe(1)-C(8)	68.30(18)
C(12)-Fe(1)-C(8)	40.49(17)
C(14)-Fe(1)-C(8)	122.0(3)
C(16)-Fe(1)-C(10)	122.1(2)
C(15)-Fe(1)-C(10)	106.9(2)
C(11)-Fe(1)-C(10)	40.21(19)
C(12)-Fe(1)-C(10)	68.30(18)
C(14)-Fe(1)-C(10)	121.8(2)
C(8)-Fe(1)-C(10)	68.52(17)
C(16)-Fe(1)-C(9)	156.8(2)
C(15)-Fe(1)-C(9)	120.5(2)
C(11)-Fe(1)-C(9)	67.85(19)
C(12)-Fe(1)-C(9)	68.44(18)
C(14)-Fe(1)-C(9)	106.2(2)
C(8)-Fe(1)-C(9)	41.17(15)
C(10)-Fe(1)-C(9)	40.29(18)

C(16)-Fe(1)-C(17)	40.7(3)
C(15)-Fe(1)-C(17)	67.5(2)
C(11)-Fe(1)-C(17)	125.3(3)
C(12)-Fe(1)-C(17)	110.2(2)
C(14)-Fe(1)-C(17)	67.3(3)
C(8)-Fe(1)-C(17)	124.6(2)
C(10)-Fe(1)-C(17)	159.5(3)
C(9)-Fe(1)-C(17)	159.8(2)
C(16)-Fe(1)-C(13)	67.9(3)
C(15)-Fe(1)-C(13)	67.6(3)
C(11)-Fe(1)-C(13)	159.4(2)
C(12)-Fe(1)-C(13)	123.3(2)
C(14)-Fe(1)-C(13)	41.3(3)
C(8)-Fe(1)-C(13)	108.0(2)
C(10)-Fe(1)-C(13)	159.2(2)
C(9)-Fe(1)-C(13)	123.6(2)
C(17)-Fe(1)-C(13)	39.0(3)
C(2)-O(2)-C(18)	119.1(3)

Symmetry transformations used to generate equivalent atoms:

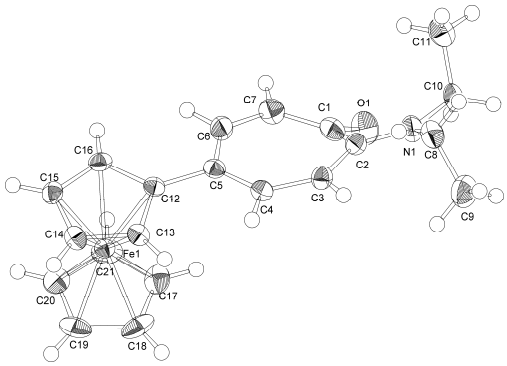
Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	56(2)	31(2)	46(2)	8(2)	19(2)	6(2)
C(2)	52(2)	30(2)	35(2)	-1(1)	13(2)	-3(2)
C(3)	49(2)	41(2)	30(2)	1(2)	7(2)	-2(2)
C(4)	41(2)	37(2)	36(2)	-2(2)	4(1)	1(2)
C(5)	44(2)	27(2)	38(2)	-8(1)	9(2)	1(1)
C(6)	56(2)	36(2)	34(2)	2(2)	15(2)	5(2)
C(7)	56(2)	35(2)	38(2)	8(2)	14(2)	11(2)
C(8)	47(2)	31(2)	41(2)	-9(2)	11(2)	-4(2)
C(9)	47(2)	43(2)	33(2)	-5(2)	7(2)	1(2)
C(10)	48(2)	43(2)	57(3)	-6(2)	14(2)	1(2)
C(11)	59(3)	44(2)	77(3)	6(2)	33(2)	-3(2)
C(12)	64(3)	26(2)	68(3)	3(2)	29(2)	-1(2)
C(13)	63(3)	65(3)	56(3)	-23(3)	4(2)	-8(3)
C(14)	127(6)	42(3)	66(4)	-16(3)	-15(4)	-17(3)
C(15)	100(5)	77(4)	59(3)	-37(3)	-9(3)	40(4)
C(16)	91(4)	136(6)	35(2)	-12(3)	19(3)	31(4)
C(17)	83(4)	84(4)	44(3)	-3(3)	-4(3)	24(3)
Fe(1)	56(1)	31(1)	31(1)	-1(1)	12(1)	7(1)
O(1)	64(2)	71(2)	80(2)	42(2)	39(2)	31(2)
O(2)	57(2)	48(2)	42(2)	9(1)	22(1)	7(1)
C(18)	58(3)	77(3)	37(2)	12(2)	15(2)	3(2)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1)	8111	3964	5307	50
H(2)	9326	3707	4557	48
H(3)	7922	6025	1914	51
H(4)	6425	6818	2034	53
H(5)	10333	2396	3704	52
H(6)	11709	2531	2800	60
H(7)	11282	4845	1659	69
H(8)	9629	6178	1839	61
H(9)	7327	2631	1120	79
H(10)	8662	391	1816	111
H(11)	10023	437	934	108
H(12)	9640	2745	-251	106
H(13)	7926	4011	-151	93
H(14)	6630	3067	5598	87
H(15)	5913	4102	6062	87
H(16)	7187	4478	6320	87

(a)



(b)

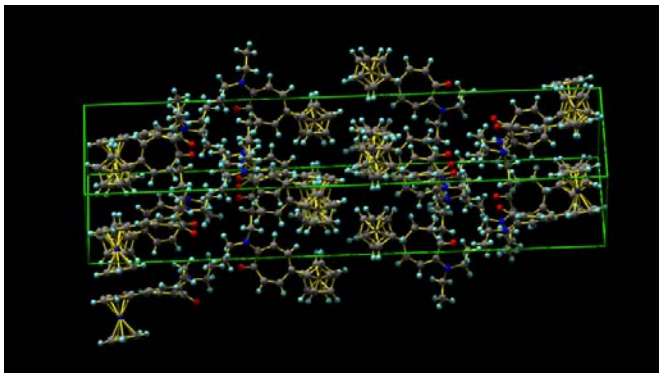


Figure S4. X-ray structure of **5**. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S16. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	C21 H23 Fe N O	
Formula weight	361.25	
Temperature	197(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 9.7399(13) Å	α= 90°.
	b = 8.0421(11) Å	β= 90°.
	c = 43.669(6) Å	γ = 90°.
Volume	3420.6(8) $Å^3$	
Z	8	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.888 mm^{-1}	

F(000)	1520
Crystal size	0.40 x 0.40 x 0.03 mm^3
Theta range for data collection	2.29 to 23.25°.
Index ranges	-10<=h<=10, -8<=k<=8, -37<=l<=48
Reflections collected	13509
Independent reflections	2447 [R(int) = 0.0244]
Completeness to theta = 23.25°	99.8 %
Max. and min. transmission	0.9191 and 0.6736
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2447 / 0 / 220
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0744
R indices (all data)	R1 = 0.0330, wR2 = 0.0783
Extinction coefficient	0.00020(11)
Largest diff. peak and hole	0.218 and -0.209 e.$Å^{-3}$

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9544(2)	4459(3)	3183(1)	31(1)
C(2)	9898(2)	6187(3)	3277(1)	27(1)
C(3)	10196(2)	6522(3)	3585(1)	27(1)
C(4)	9914(2)	5668(3)	3855(1)	23(1)
C(5)	9099(2)	4301(2)	3915(1)	23(1)
C(6)	8442(2)	3394(3)	3680(1)	31(1)
C(7)	8632(2)	3485(3)	3371(1)	33(1)
C(8)	10172(2)	9157(3)	3155(1)	38(1)
C(9)	11644(3)	9739(3)	3180(1)	52(1)
C(10)	9885(2)	7153(3)	2730(1)	38(1)
C(11)	8393(3)	7107(3)	2633(1)	45(1)
C(12)	8888(2)	3768(2)	4235(1)	22(1)
C(13)	9642(2)	4327(3)	4499(1)	23(1)
C(14)	9127(2)	3466(3)	4760(1)	27(1)
C(15)	8071(2)	2387(3)	4663(1)	27(1)
C(16)	7921(2)	2559(3)	4342(1)	26(1)
C(17)	11211(2)	912(3)	4130(1)	39(1)
C(18)	11913(2)	1365(3)	4399(1)	42(1)
C(19)	11365(2)	423(3)	4643(1)	39(1)
C(20)	10323(2)	-608(3)	4525(1)	35(1)
C(21)	10225(2)	-308(3)	4208(1)	36(1)
Fe(1)	9869(1)	1825(1)	4445(1)	21(1)
N(1)	10044(2)	7400(2)	3064(1)	33(1)
O(1)	9952(2)	3877(2)	2937(1)	44(1)

Table S18. Bond lengths [Å] and angles [°] for **5**.

C(1)-O(1)	1.238(3)
C(1)-C(7)	1.441(3)
C(1)-C(2)	1.489(3)
C(2)-N(1)	1.357(3)
C(2)-C(3)	1.400(3)
C(3)-C(4)	1.393(3)
C(4)-C(5)	1.381(3)
C(5)-C(6)	1.414(3)
C(5)-C(12)	1.475(3)
C(6)-C(7)	1.364(3)
C(8)-N(1)	1.474(3)
C(8)-C(9)	1.512(3)
C(10)-N(1)	1.477(3)
C(10)-C(11)	1.515(3)
C(12)-C(16)	1.432(3)
C(12)-C(13)	1.436(3)
C(12)-Fe(1)	2.0487(19)
C(13)-C(14)	1.428(3)
C(13)-Fe(1)	2.037(2)
C(14)-C(15)	1.411(3)
C(14)-Fe(1)	2.038(2)
C(15)-C(16)	1.415(3)
C(15)-Fe(1)	2.043(2)
C(16)-Fe(1)	2.0371(19)
C(17)-C(18)	1.409(3)
C(17)-C(21)	1.415(3)
C(17)-Fe(1)	2.038(2)
C(18)-C(19)	1.413(3)
C(18)-Fe(1)	2.035(2)
C(19)-C(20)	1.408(3)
C(19)-Fe(1)	2.035(2)
C(20)-C(21)	1.408(4)
C(20)-Fe(1)	2.036(2)
C(21)-Fe(1)	2.034(2)

O(1)-C(1)-C(7)	119.1(2)
O(1)-C(1)-C(2)	121.2(2)
C(7)-C(1)-C(2)	119.49(19)
N(1)-C(2)-C(3)	119.9(2)
N(1)-C(2)-C(1)	120.3(2)
C(3)-C(2)-C(1)	119.5(2)
C(4)-C(3)-C(2)	132.6(2)
C(5)-C(4)-C(3)	131.9(2)
C(4)-C(5)-C(6)	122.10(19)
C(4)-C(5)-C(12)	119.50(18)
C(6)-C(5)-C(12)	118.40(18)
C(7)-C(6)-C(5)	129.1(2)
C(6)-C(7)-C(1)	132.6(2)
N(1)-C(8)-C(9)	113.4(2)
N(1)-C(10)-C(11)	112.30(19)
C(16)-C(12)-C(13)	106.71(17)
C(16)-C(12)-C(5)	126.69(18)
C(13)-C(12)-C(5)	126.57(19)
C(16)-C(12)-Fe(1)	69.05(11)
C(13)-C(12)-Fe(1)	69.00(11)
C(5)-C(12)-Fe(1)	125.50(14)
C(14)-C(13)-C(12)	108.06(19)
C(14)-C(13)-Fe(1)	69.53(12)
C(12)-C(13)-Fe(1)	69.85(11)
C(15)-C(14)-C(13)	108.23(18)
C(15)-C(14)-Fe(1)	69.95(11)
C(13)-C(14)-Fe(1)	69.46(12)
C(14)-C(15)-C(16)	108.27(18)
C(14)-C(15)-Fe(1)	69.59(11)
C(16)-C(15)-Fe(1)	69.49(11)
C(15)-C(16)-C(12)	108.74(18)
C(15)-C(16)-Fe(1)	69.93(11)
C(12)-C(16)-Fe(1)	69.91(11)
C(18)-C(17)-C(21)	107.9(2)
C(18)-C(17)-Fe(1)	69.67(13)

C(21)-C(17)-Fe(1)	69.52(13)
C(17)-C(18)-C(19)	107.9(2)
C(17)-C(18)-Fe(1)	69.86(13)
C(19)-C(18)-Fe(1)	69.66(13)
C(20)-C(19)-C(18)	108.1(2)
C(20)-C(19)-Fe(1)	69.80(13)
C(18)-C(19)-Fe(1)	69.70(13)
C(21)-C(20)-C(19)	108.0(2)
C(21)-C(20)-Fe(1)	69.69(13)
C(19)-C(20)-Fe(1)	69.72(13)
C(20)-C(21)-C(17)	108.1(2)
C(20)-C(21)-Fe(1)	69.83(13)
C(17)-C(21)-Fe(1)	69.80(13)
C(21)-Fe(1)-C(19)	68.10(10)
C(21)-Fe(1)-C(18)	68.24(10)
C(19)-Fe(1)-C(18)	40.64(10)
C(21)-Fe(1)-C(20)	40.48(10)
C(19)-Fe(1)-C(20)	40.48(10)
C(18)-Fe(1)-C(20)	68.27(10)
C(21)-Fe(1)-C(16)	106.89(9)
C(19)-Fe(1)-C(16)	157.11(10)
C(18)-Fe(1)-C(16)	160.33(10)
C(20)-Fe(1)-C(16)	121.25(9)
C(21)-Fe(1)-C(13)	155.41(9)
C(19)-Fe(1)-C(13)	125.21(9)
C(18)-Fe(1)-C(13)	107.26(10)
C(20)-Fe(1)-C(13)	162.41(10)
C(16)-Fe(1)-C(13)	68.78(9)
C(21)-Fe(1)-C(17)	40.68(10)
C(19)-Fe(1)-C(17)	68.17(10)
C(18)-Fe(1)-C(17)	40.48(10)
C(20)-Fe(1)-C(17)	68.26(10)
C(16)-Fe(1)-C(17)	123.53(9)
C(13)-Fe(1)-C(17)	120.17(9)
C(21)-Fe(1)-C(14)	161.85(10)
C(19)-Fe(1)-C(14)	109.02(9)

C(18)-Fe(1)-C(14)	122.10(10)
C(20)-Fe(1)-C(14)	125.74(9)
C(16)-Fe(1)-C(14)	68.38(9)
C(13)-Fe(1)-C(14)	41.01(8)
C(17)-Fe(1)-C(14)	156.57(10)
C(21)-Fe(1)-C(15)	124.74(9)
C(19)-Fe(1)-C(15)	122.61(9)
C(18)-Fe(1)-C(15)	157.68(10)
C(20)-Fe(1)-C(15)	108.65(9)
C(16)-Fe(1)-C(15)	40.58(8)
C(13)-Fe(1)-C(15)	68.62(9)
C(17)-Fe(1)-C(15)	160.86(10)
C(14)-Fe(1)-C(15)	40.46(8)
C(21)-Fe(1)-C(12)	119.65(9)
C(19)-Fe(1)-C(12)	161.21(9)
C(18)-Fe(1)-C(12)	123.37(9)
C(20)-Fe(1)-C(12)	155.65(9)
C(16)-Fe(1)-C(12)	41.04(8)
C(13)-Fe(1)-C(12)	41.14(8)
C(17)-Fe(1)-C(12)	105.73(9)
C(14)-Fe(1)-C(12)	69.09(8)
C(15)-Fe(1)-C(12)	68.89(8)
C(2)-N(1)-C(8)	120.81(19)
C(2)-N(1)-C(10)	124.7(2)
C(8)-N(1)-C(10)	113.86(19)

Symmetry transformations used to generate equivalent atoms:

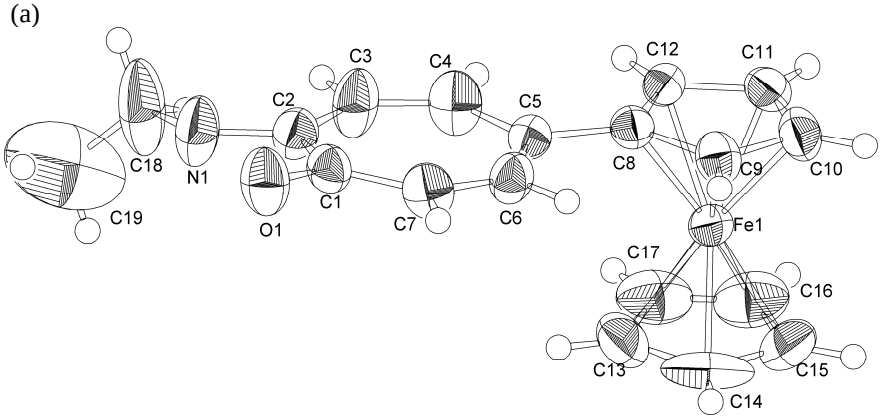
Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(1)	33(1)	24(1)	-3(1)	-5(1)	5(1)
C(2)	25(1)	30(1)	26(1)	1(1)	3(1)	2(1)
C(3)	29(1)	24(1)	28(1)	0(1)	1(1)	-3(1)
C(4)	26(1)	22(1)	22(1)	-4(1)	-2(1)	1(1)
C(5)	22(1)	23(1)	24(1)	-1(1)	-1(1)	5(1)
C(6)	32(1)	30(1)	30(1)	1(1)	-3(1)	-7(1)
C(7)	39(1)	31(1)	30(1)	-5(1)	-7(1)	-8(1)
C(8)	44(1)	35(1)	35(1)	8(1)	0(1)	0(1)
C(9)	55(2)	48(2)	52(2)	9(1)	2(1)	-15(1)
C(10)	44(1)	47(2)	22(1)	9(1)	4(1)	0(1)
C(11)	50(2)	56(2)	31(1)	4(1)	-2(1)	0(1)
C(12)	22(1)	19(1)	25(1)	0(1)	-1(1)	4(1)
C(13)	28(1)	16(1)	25(1)	-2(1)	-2(1)	1(1)
C(14)	33(1)	25(1)	22(1)	-2(1)	1(1)	4(1)
C(15)	24(1)	26(1)	30(1)	4(1)	6(1)	4(1)
C(16)	19(1)	24(1)	33(1)	0(1)	-3(1)	3(1)
C(17)	39(1)	39(1)	40(1)	1(1)	15(1)	12(1)
C(18)	18(1)	32(1)	77(2)	-7(1)	6(1)	3(1)
C(19)	33(1)	41(1)	42(1)	-4(1)	-11(1)	18(1)
C(20)	33(1)	19(1)	54(2)	5(1)	3(1)	8(1)
C(21)	34(1)	28(1)	45(2)	-13(1)	-4(1)	8(1)
Fe(1)	20(1)	19(1)	24(1)	-1(1)	-1(1)	1(1)
N(1)	38(1)	34(1)	27(1)	4(1)	2(1)	-4(1)
O(1)	59(1)	44(1)	29(1)	-9(1)	7(1)	2(1)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5**.

	x	y	z	U(eq)
H(1)	10676	7509	3614	32
H(2)	10357	6096	4026	28
H(3)	7789	2627	3745	37
H(4)	8062	2781	3260	40
H(5)	9723	9312	3351	46
H(6)	9698	9844	3006	46
H(7)	12093	9151	3343	78
H(8)	11660	10911	3222	78
H(9)	12113	9526	2991	78
H(10)	10324	6117	2672	45
H(11)	10348	8048	2623	45
H(12)	7955	6150	2721	68
H(13)	8339	7044	2414	68
H(14)	7939	8097	2703	68
H(15)	10343	5112	4498	28
H(16)	9435	3593	4961	32
H(17)	7561	1684	4788	32
H(18)	7298	1982	4221	31
H(19)	11368	1338	3935	47
H(20)	12613	2147	4414	51
H(21)	11643	475	4847	47
H(22)	9794	-1355	4636	42
H(23)	9617	-822	4074	43

(a)



(b)

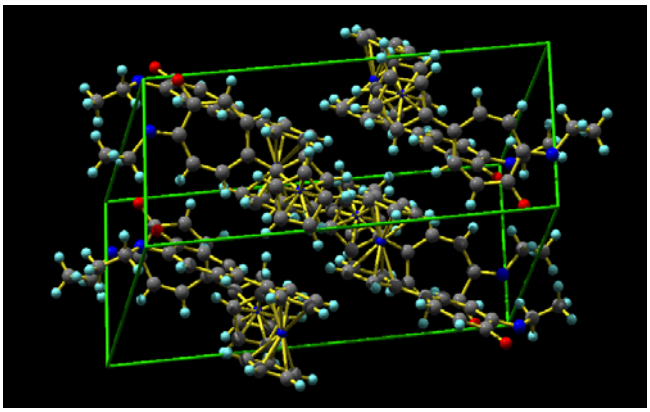


Figure S5. X-ray structure of **6**. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S21. Crystal data and structure refinement for **6**.

Identification code	**6**	
Empirical formula	C19 H19 Fe N O	
Formula weight	333.20	
Temperature	296(2) K	
Wavelength	0.71069 Å	
Crystal system	monoclinic	
Space group	$P2_1/a$	
Unit cell dimensions	a = 8.4296(15) Å	α= 90°.
	b = 9.8744(17) Å	β= 101.570(11)°.
	c = 19.5262(17) Å	γ = 90°.

Volume	1592.3(4) $Å^3$
Z	4
Density (calculated)	1.390 Mg/m^3
Absorption coefficient	0.948 mm^{-1}
F(000)	696
Crystal size	0.35 x 0.28 x 0.10 mm^3
Theta range for data collection	2.96 to 27.49°.
Index ranges	-10<=h<=0, 0<=k<=12, -24<=l<=25
Reflections collected	3903
Independent reflections	3651 [R(int) = 0.0949]
Completeness to theta = 27.49°	99.9 %
Max. and min. transmission	0.9112 and 0.7327
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3651 / 0 / 200
Goodness-of-fit on F^2	1.483
Final R indices [I>2sigma(I)]	R1 = 0.0685, wR2 = 0.1960
R indices (all data)	R1 = 0.1435, wR2 = 0.2411
Largest diff. peak and hole	2.124 and -1.169 $e.Å^{-3}$

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8323(7)	161(6)	8777(3)	45(1)
C(2)	7235(7)	1073(6)	9057(3)	49(1)
C(3)	5918(8)	1760(7)	8661(3)	64(2)
C(4)	5208(7)	1728(7)	7961(3)	61(2)
C(5)	5540(6)	954(5)	7414(3)	38(1)
C(6)	6821(7)	23(5)	7511(3)	48(1)
C(7)	7985(7)	-305(6)	8075(3)	53(1)
C(8)	4555(6)	1136(5)	6703(3)	39(1)
C(9)	4729(7)	431(6)	6077(3)	46(1)
C(10)	3564(7)	924(6)	5517(3)	52(1)
C(11)	2656(7)	1921(6)	5776(3)	48(1)
C(12)	3258(6)	2061(5)	6508(3)	41(1)
C(13)	1969(11)	-1178(9)	6994(4)	87(3)
C(14)	2119(10)	-1868(6)	6378(6)	89(3)
C(15)	896(10)	-1330(8)	5832(4)	76(2)
C(16)	79(9)	-343(9)	6117(6)	82(2)
C(17)	705(11)	-258(8)	6798(6)	81(2)
Fe(1)	2476(1)	133(1)	6268(1)	38(1)
O(1)	9569(6)	-234(5)	9196(2)	65(1)
N(1)	7698(7)	1209(6)	9756(3)	70(2)
C(18)	6760(14)	1964(11)	10194(4)	116(4)
C(19)	6610(20)	1344(15)	10796(9)	211(9)

Table S23. Bond lengths [Å] and angles [°] for **6**.

C(1)-O(1)	1.257(7)
C(1)-C(7)	1.420(8)
C(1)-C(2)	1.466(8)
C(2)-N(1)	1.350(7)
C(2)-C(3)	1.395(8)
C(3)-C(4)	1.377(8)
C(4)-C(5)	1.387(7)
C(5)-C(6)	1.402(7)
C(5)-C(8)	1.479(7)
C(6)-C(7)	1.359(8)
C(8)-C(12)	1.417(7)
C(8)-C(9)	1.439(7)
C(8)-Fe(1)	2.044(5)
C(9)-C(10)	1.402(8)
C(9)-Fe(1)	2.029(5)
C(10)-C(11)	1.402(8)
C(10)-Fe(1)	2.034(5)
C(11)-C(12)	1.425(7)
C(11)-Fe(1)	2.030(5)
C(12)-Fe(1)	2.039(5)
C(13)-C(17)	1.394(12)
C(13)-C(14)	1.410(12)
C(13)-Fe(1)	2.029(7)
C(14)-C(15)	1.429(11)
C(14)-Fe(1)	2.017(6)
C(15)-C(16)	1.374(12)
C(15)-Fe(1)	2.032(7)
C(16)-C(17)	1.332(13)
C(16)-Fe(1)	2.037(7)
C(17)-Fe(1)	2.018(7)
N(1)-C(18)	1.478(9)
C(18)-C(19)	1.352(15)
O(1)-C(1)-C(7)	120.5(5)

O(1)-C(1)-C(2)	116.9(5)
C(7)-C(1)-C(2)	122.6(5)
N(1)-C(2)-C(3)	123.3(5)
N(1)-C(2)-C(1)	111.2(5)
C(3)-C(2)-C(1)	125.5(5)
C(4)-C(3)-C(2)	132.7(6)
C(3)-C(4)-C(5)	131.4(5)
C(4)-C(5)-C(6)	121.8(5)
C(4)-C(5)-C(8)	119.6(5)
C(6)-C(5)-C(8)	118.6(4)
C(7)-C(6)-C(5)	132.6(5)
C(6)-C(7)-C(1)	132.7(5)
C(12)-C(8)-C(9)	106.8(4)
C(12)-C(8)-C(5)	126.0(5)
C(9)-C(8)-C(5)	127.2(5)
C(12)-C(8)-Fe(1)	69.5(3)
C(9)-C(8)-Fe(1)	68.7(3)
C(5)-C(8)-Fe(1)	127.2(3)
C(10)-C(9)-C(8)	108.6(5)
C(10)-C(9)-Fe(1)	70.0(3)
C(8)-C(9)-Fe(1)	69.9(3)
C(11)-C(10)-C(9)	108.1(5)
C(11)-C(10)-Fe(1)	69.7(3)
C(9)-C(10)-Fe(1)	69.6(3)
C(10)-C(11)-C(12)	108.6(5)
C(10)-C(11)-Fe(1)	70.0(3)
C(12)-C(11)-Fe(1)	69.8(3)
C(8)-C(12)-C(11)	107.9(5)
C(8)-C(12)-Fe(1)	69.9(3)
C(11)-C(12)-Fe(1)	69.2(3)
C(17)-C(13)-C(14)	106.0(7)
C(17)-C(13)-Fe(1)	69.4(4)
C(14)-C(13)-Fe(1)	69.2(4)
C(13)-C(14)-C(15)	106.4(7)
C(13)-C(14)-Fe(1)	70.1(4)
C(15)-C(14)-Fe(1)	69.9(4)

C(16)-C(15)-C(14)	107.9(8)
C(16)-C(15)-Fe(1)	70.5(4)
C(14)-C(15)-Fe(1)	68.8(4)
C(17)-C(16)-C(15)	108.5(8)
C(17)-C(16)-Fe(1)	70.0(5)
C(15)-C(16)-Fe(1)	70.0(4)
C(16)-C(17)-C(13)	111.2(8)
C(16)-C(17)-Fe(1)	71.6(5)
C(13)-C(17)-Fe(1)	70.3(4)
C(14)-Fe(1)-C(17)	67.4(3)
C(14)-Fe(1)-C(13)	40.8(3)
C(17)-Fe(1)-C(13)	40.3(3)
C(14)-Fe(1)-C(9)	109.1(3)
C(17)-Fe(1)-C(9)	159.8(4)
C(13)-Fe(1)-C(9)	123.9(3)
C(14)-Fe(1)-C(11)	158.4(3)
C(17)-Fe(1)-C(11)	122.9(3)
C(13)-Fe(1)-C(11)	158.8(4)
C(9)-Fe(1)-C(11)	68.0(2)
C(14)-Fe(1)-C(15)	41.3(3)
C(17)-Fe(1)-C(15)	65.7(4)
C(13)-Fe(1)-C(15)	68.1(3)
C(9)-Fe(1)-C(15)	125.8(3)
C(11)-Fe(1)-C(15)	121.7(3)
C(14)-Fe(1)-C(10)	123.5(3)
C(17)-Fe(1)-C(10)	158.5(4)
C(13)-Fe(1)-C(10)	159.6(4)
C(9)-Fe(1)-C(10)	40.4(2)
C(11)-Fe(1)-C(10)	40.3(2)
C(15)-Fe(1)-C(10)	108.9(3)
C(14)-Fe(1)-C(16)	68.0(3)
C(17)-Fe(1)-C(16)	38.3(4)
C(13)-Fe(1)-C(16)	67.2(4)
C(9)-Fe(1)-C(16)	160.9(4)
C(11)-Fe(1)-C(16)	107.4(3)
C(15)-Fe(1)-C(16)	39.5(3)

C(10)-Fe(1)-C(16)	124.2(4)
C(14)-Fe(1)-C(12)	159.8(3)
C(17)-Fe(1)-C(12)	107.4(3)
C(13)-Fe(1)-C(12)	122.6(3)
C(9)-Fe(1)-C(12)	68.6(2)
C(11)-Fe(1)-C(12)	41.0(2)
C(15)-Fe(1)-C(12)	156.2(3)
C(10)-Fe(1)-C(12)	68.6(2)
C(16)-Fe(1)-C(12)	120.9(3)
C(14)-Fe(1)-C(8)	124.3(3)
C(17)-Fe(1)-C(8)	122.7(3)
C(13)-Fe(1)-C(8)	107.6(3)
C(9)-Fe(1)-C(8)	41.4(2)
C(11)-Fe(1)-C(8)	68.7(2)
C(15)-Fe(1)-C(8)	162.5(3)
C(10)-Fe(1)-C(8)	68.9(2)
C(16)-Fe(1)-C(8)	156.2(3)
C(12)-Fe(1)-C(8)	40.6(2)
C(2)-N(1)-C(18)	123.8(6)
C(19)-C(18)-N(1)	115.4(8)

Symmetry transformations used to generate equivalent atoms:

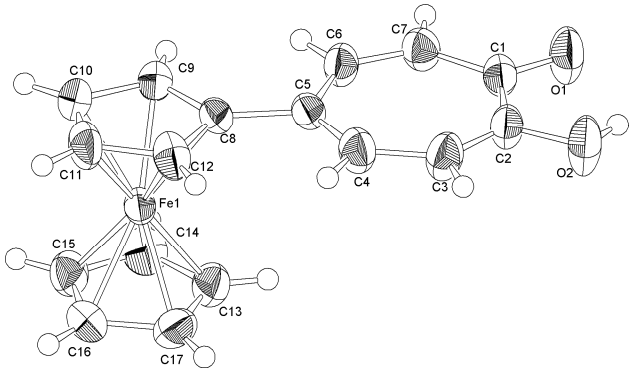
Table S24. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(3)	49(3)	41(3)	5(2)	1(2)	1(2)
C(2)	54(3)	50(3)	43(3)	-4(2)	6(3)	5(3)
C(3)	71(4)	74(4)	44(3)	-16(3)	6(3)	29(3)
C(4)	56(4)	68(4)	57(4)	-2(3)	7(3)	29(3)
C(5)	37(3)	41(3)	38(3)	-2(2)	8(2)	-2(2)
C(6)	56(3)	45(3)	40(3)	-7(2)	5(2)	10(3)
C(7)	54(3)	52(3)	52(4)	1(3)	12(3)	20(3)
C(8)	38(3)	41(3)	39(3)	1(2)	7(2)	-4(2)
C(9)	42(3)	59(3)	40(3)	2(2)	15(2)	2(2)
C(10)	54(3)	67(4)	35(3)	6(3)	8(2)	-7(3)
C(11)	51(3)	44(3)	45(3)	11(2)	2(2)	-5(2)
C(12)	48(3)	35(2)	38(3)	-1(2)	0(2)	-1(2)
C(13)	103(6)	96(6)	55(4)	26(4)	-3(4)	-49(5)
C(14)	80(5)	30(3)	170(9)	13(4)	58(6)	-4(3)
C(15)	94(6)	66(4)	66(5)	-15(4)	11(4)	-35(4)
C(16)	54(4)	73(5)	117(8)	0(5)	16(5)	-13(4)
C(17)	79(5)	67(5)	111(7)	-1(4)	56(5)	-11(4)
Fe(1)	40(1)	34(1)	40(1)	-1(1)	10(1)	-2(1)
O(1)	55(3)	84(3)	50(3)	3(2)	-2(2)	21(2)
N(1)	86(4)	79(4)	41(3)	-15(3)	1(3)	27(3)
C(18)	171(9)	129(8)	41(4)	-13(4)	7(5)	90(7)
C(19)	320(20)	140(12)	247(18)	-4(12)	239(18)	28(13)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(1)	5422	2358	8920	76
H(2)	4355	2333	7833	73
H(3)	6889	-465	7110	57
H(4)	8702	-964	7983	63
H(5)	5488	-240	6049	56
H(6)	3419	638	5055	62
H(7)	1803	2409	5513	57
H(8)	2869	2655	6805	50
H(9)	2587	-1310	7440	105
H(10)	2866	-2541	6336	107
H(11)	690	-1600	5366	91
H(12)	-769	179	5874	98
H(13)	346	337	7103	97
H(14)	7273	2836	10309	139
H(15)	5684	2132	9920	139
H(16)	5979	533	10689	316
H(17)	6078	1942	11066	316
H(18)	7663	1116	11059	316

(a)



(b)

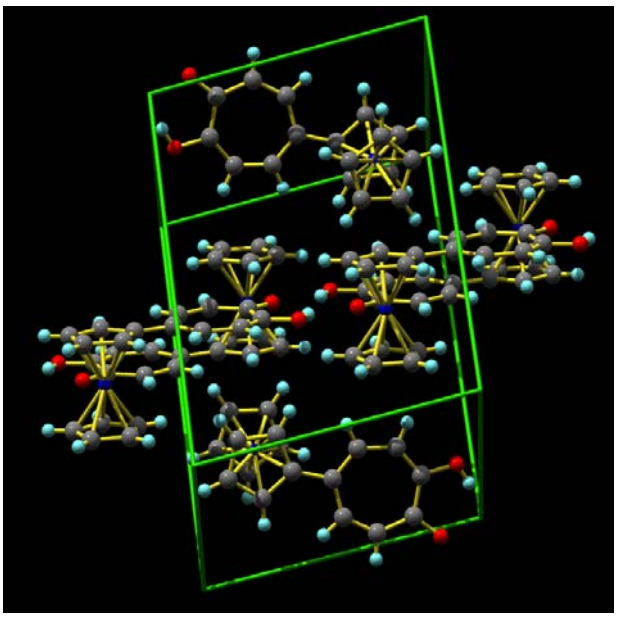


Figure S6. X-ray structure of **7**. (a) ORTEP drawing (50% probability) and (b) packing structure.

Table S26. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	C17 H14 Fe O2	
Formula weight	306.13	
Temperature	296(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 8.720(4) Å	α= 90°.
	b = 14.728(3) Å	β= 104.76(2)°.
	c = 10.4776(18) Å	γ = 90°.

Volume	1301.3(6) $Å^3$
Z	4
Density (calculated)	1.563 Mg/m^3
Absorption coefficient	1.156 mm^{-1}
F(000)	632
Crystal size	0.35 x 0.22 x 0.20 mm^3
Theta range for data collection	2.72 to 27.50°.
Index ranges	-11<=h<=0, 0<=k<=19, -13<=l<=13
Reflections collected	3176
Independent reflections	2989 [R(int) = 0.0221]
Completeness to theta = 27.50°	99.9 %
Max. and min. transmission	0.8018 and 0.6879
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2989 / 0 / 181
Goodness-of-fit on F^2	0.839
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.1098
R indices (all data)	R1 = 0.0971, wR2 = 0.1406
Largest diff. peak and hole	0.345 and -0.322 $e.Å^{-3}$

Table S27. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3733(4)	4914(3)	12614(3)	44(1)
C(2)	2769(5)	4217(3)	13015(3)	46(1)
C(3)	1584(5)	3721(3)	12246(4)	54(1)
C(4)	964(5)	3691(3)	10867(4)	51(1)
C(5)	1375(4)	4172(2)	9884(3)	38(1)
C(6)	2549(5)	4846(3)	10123(3)	45(1)
C(7)	3529(5)	5158(3)	11261(4)	47(1)
C(8)	495(4)	3991(2)	8493(3)	41(1)
C(9)	768(6)	4401(3)	7336(4)	53(1)
C(10)	-335(6)	4039(3)	6220(4)	58(1)
C(11)	-1283(5)	3406(3)	6667(4)	54(1)
C(12)	-790(4)	3368(3)	8064(4)	50(1)
C(13)	3121(5)	2429(3)	8240(4)	52(1)
C(14)	3249(5)	2803(3)	7023(4)	54(1)
C(15)	2083(5)	2391(3)	6007(4)	51(1)
C(16)	1246(5)	1761(3)	6565(4)	51(1)
C(17)	1890(6)	1784(3)	7952(4)	53(1)
Fe(1)	1041(1)	3033(1)	7271(1)	35(1)
O(1)	4777(4)	5280(2)	13505(3)	65(1)
O(2)	3099(4)	4068(2)	14313(3)	70(1)

Table S28. Bond lengths [Å] and angles [°] for **7**.

C(1)-O(1)	1.249(4)
C(1)-C(7)	1.430(5)
C(1)-C(2)	1.455(6)
C(2)-O(2)	1.335(4)
C(2)-C(3)	1.352(5)
C(3)-C(4)	1.408(5)
C(4)-C(5)	1.372(5)
C(5)-C(6)	1.401(5)
C(5)-C(8)	1.488(5)
C(6)-C(7)	1.358(5)
C(8)-C(9)	1.427(5)
C(8)-C(12)	1.430(6)
C(8)-Fe(1)	2.042(3)
C(9)-C(10)	1.416(6)
C(9)-Fe(1)	2.032(4)
C(10)-C(11)	1.403(7)
C(10)-Fe(1)	2.043(4)
C(11)-C(12)	1.418(5)
C(11)-Fe(1)	2.039(4)
C(12)-Fe(1)	2.040(4)
C(13)-C(17)	1.407(6)
C(13)-C(14)	1.419(6)
C(13)-Fe(1)	2.043(4)
C(14)-C(15)	1.408(6)
C(14)-Fe(1)	2.035(4)
C(15)-C(16)	1.398(6)
C(15)-Fe(1)	2.021(4)
C(16)-C(17)	1.419(6)
C(16)-Fe(1)	2.039(4)
C(17)-Fe(1)	2.042(4)
O(1)-C(1)-C(7)	121.1(4)
O(1)-C(1)-C(2)	117.0(3)
C(7)-C(1)-C(2)	121.9(3)

O(2)-C(2)-C(3)	116.9(4)
O(2)-C(2)-C(1)	114.9(3)
C(3)-C(2)-C(1)	128.3(3)
C(2)-C(3)-C(4)	131.6(4)
C(5)-C(4)-C(3)	130.4(4)
C(4)-C(5)-C(6)	123.4(3)
C(4)-C(5)-C(8)	118.3(3)
C(6)-C(5)-C(8)	118.2(3)
C(7)-C(6)-C(5)	131.6(4)
C(6)-C(7)-C(1)	132.6(4)
C(9)-C(8)-C(12)	107.0(3)
C(9)-C(8)-C(5)	126.9(4)
C(12)-C(8)-C(5)	126.2(4)
C(9)-C(8)-Fe(1)	69.1(2)
C(12)-C(8)-Fe(1)	69.4(2)
C(5)-C(8)-Fe(1)	126.4(2)
C(10)-C(9)-C(8)	108.5(4)
C(10)-C(9)-Fe(1)	70.1(2)
C(8)-C(9)-Fe(1)	69.9(2)
C(11)-C(10)-C(9)	107.9(4)
C(11)-C(10)-Fe(1)	69.7(2)
C(9)-C(10)-Fe(1)	69.2(2)
C(10)-C(11)-C(12)	108.8(4)
C(10)-C(11)-Fe(1)	70.1(2)
C(12)-C(11)-Fe(1)	69.7(2)
C(11)-C(12)-C(8)	107.8(4)
C(11)-C(12)-Fe(1)	69.6(2)
C(8)-C(12)-Fe(1)	69.6(2)
C(17)-C(13)-C(14)	107.5(4)
C(17)-C(13)-Fe(1)	69.8(2)
C(14)-C(13)-Fe(1)	69.4(2)
C(15)-C(14)-C(13)	107.7(4)
C(15)-C(14)-Fe(1)	69.2(2)
C(13)-C(14)-Fe(1)	69.9(2)
C(16)-C(15)-C(14)	108.9(4)
C(16)-C(15)-Fe(1)	70.5(2)

C(14)-C(15)-Fe(1)	70.2(2)
C(15)-C(16)-C(17)	107.4(4)
C(15)-C(16)-Fe(1)	69.2(2)
C(17)-C(16)-Fe(1)	69.8(2)
C(13)-C(17)-C(16)	108.5(4)
C(13)-C(17)-Fe(1)	69.9(2)
C(16)-C(17)-Fe(1)	69.5(2)
C(15)-Fe(1)-C(9)	124.17(18)
C(15)-Fe(1)-C(14)	40.61(17)
C(9)-Fe(1)-C(14)	106.97(19)
C(15)-Fe(1)-C(16)	40.28(18)
C(9)-Fe(1)-C(16)	160.94(16)
C(14)-Fe(1)-C(16)	68.14(18)
C(15)-Fe(1)-C(11)	119.98(17)
C(9)-Fe(1)-C(11)	68.11(19)
C(14)-Fe(1)-C(11)	154.52(18)
C(16)-Fe(1)-C(11)	107.89(18)
C(15)-Fe(1)-C(12)	155.40(17)
C(9)-Fe(1)-C(12)	68.66(19)
C(14)-Fe(1)-C(12)	163.03(17)
C(16)-Fe(1)-C(12)	121.33(19)
C(11)-Fe(1)-C(12)	40.70(16)
C(15)-Fe(1)-C(17)	67.95(17)
C(9)-Fe(1)-C(17)	156.41(17)
C(14)-Fe(1)-C(17)	67.95(18)
C(16)-Fe(1)-C(17)	40.69(17)
C(11)-Fe(1)-C(17)	126.5(2)
C(12)-Fe(1)-C(17)	109.08(19)
C(15)-Fe(1)-C(8)	161.75(17)
C(9)-Fe(1)-C(8)	41.03(16)
C(14)-Fe(1)-C(8)	125.07(17)
C(16)-Fe(1)-C(8)	156.74(17)
C(11)-Fe(1)-C(8)	68.65(15)
C(12)-Fe(1)-C(8)	41.01(16)
C(17)-Fe(1)-C(8)	121.67(16)
C(15)-Fe(1)-C(13)	68.37(17)

C(9)-Fe(1)-C(13)	120.82(18)
C(14)-Fe(1)-C(13)	40.73(17)
C(16)-Fe(1)-C(13)	68.35(18)
C(11)-Fe(1)-C(13)	163.38(19)
C(12)-Fe(1)-C(13)	126.24(17)
C(17)-Fe(1)-C(13)	40.29(18)
C(8)-Fe(1)-C(13)	108.02(16)
C(15)-Fe(1)-C(10)	106.61(17)
C(9)-Fe(1)-C(10)	40.66(16)
C(14)-Fe(1)-C(10)	119.8(2)
C(16)-Fe(1)-C(10)	124.35(17)
C(11)-Fe(1)-C(10)	40.20(19)
C(12)-Fe(1)-C(10)	68.36(19)
C(17)-Fe(1)-C(10)	162.20(19)
C(8)-Fe(1)-C(10)	68.79(15)
C(13)-Fe(1)-C(10)	155.4(2)

Symmetry transformations used to generate equivalent atoms:

Table S29. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	50(2)	46(2)	33(2)	-3(2)	4(2)	-5(2)
C(2)	51(2)	54(2)	29(2)	0(2)	5(2)	-4(2)
C(3)	63(3)	58(2)	37(2)	8(2)	6(2)	-16(2)
C(4)	55(2)	52(2)	41(2)	-4(2)	2(2)	-13(2)
C(5)	39(2)	39(2)	33(2)	-6(1)	6(1)	3(2)
C(6)	52(2)	49(2)	31(2)	1(2)	8(2)	-5(2)
C(7)	55(2)	46(2)	40(2)	-1(2)	11(2)	-10(2)
C(8)	49(2)	40(2)	33(2)	-7(1)	5(2)	10(2)
C(9)	75(3)	40(2)	35(2)	0(2)	-2(2)	-2(2)
C(10)	79(3)	52(2)	33(2)	0(2)	-4(2)	12(2)
C(11)	43(2)	71(3)	39(2)	-15(2)	-7(2)	9(2)
C(12)	41(2)	66(3)	41(2)	-12(2)	7(2)	0(2)
C(13)	50(2)	58(2)	42(2)	-2(2)	2(2)	10(2)
C(14)	42(2)	66(3)	56(2)	-4(2)	19(2)	0(2)
C(15)	57(2)	60(2)	38(2)	-4(2)	16(2)	9(2)
C(16)	61(2)	44(2)	47(2)	-10(2)	10(2)	-3(2)
C(17)	65(3)	46(2)	48(2)	11(2)	15(2)	9(2)
Fe(1)	39(1)	37(1)	27(1)	-2(1)	6(1)	-3(1)
O(1)	73(2)	78(2)	36(1)	0(2)	-4(1)	-30(2)
O(2)	81(2)	89(2)	32(1)	5(2)	-2(1)	-35(2)

Table S30. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(1)	1088	3329	12712	65
H(2)	143	3277	10577	61
H(3)	2680	5130	9365	53
H(4)	4199	5622	11135	56
H(5)	1540	4833	7319	63
H(6)	-416	4193	5344	70
H(7)	-2101	3068	6135	65
H(8)	-1225	3002	8605	60
H(9)	3738	2581	9074	62
H(10)	3972	3242	6916	65
H(11)	1900	2518	5112	61
H(12)	419	1393	6111	62
H(13)	1554	1433	8568	64
H(14)	3831	4398	14691	105