

SUPPORTING INFORMATION

Title: Disproportionation of O-Benzylhydroxylamine Catalyzed by a Ferric Bis-Picket Fence Porphyrin Complex

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Disproportionation of O-Benzylhydroxylamine Catalyzed by a Ferric Bis-Picket Fence Porphyrin Complex

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Supporting Information

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}(\text{3,5-Me-BAFP})(\text{NH}_3)_2]$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2750(1)	563(1)	1951(1)	30(1)
O(1)	827(1)	1840(1)	856(1)	57(1)
O(2)	212(1)	369(1)	1889(1)	54(1)
O(3)	3930(1)	1710(1)	4756(1)	41(1)
O(4)	2145(1)	732(1)	5243(1)	40(1)
O(5)	4707(1)	-582(1)	3125(1)	47(1)
O(6)	5334(1)	820(1)	1831(1)	49(1)
O(7)	2056(1)	598(1)	-1708(1)	44(1)
O(8)	2810(1)	-916(1)	-358(1)	42(1)
N(1)	2012(1)	498(1)	967(1)	34(1)
N(2)	3319(1)	256(1)	1249(1)	34(1)
N(3)	3481(1)	612(1)	2958(1)	32(1)
N(4)	2197(1)	903(1)	2635(1)	35(1)
N(5)	2943(1)	1196(1)	1486(1)	42(1)
N(6)	2549(1)	-84(1)	2393(1)	38(1)
C(1)	2002(1)	265(1)	193(1)	35(1)
C(2)	2536(1)	79(1)	-76(1)	35(1)
C(3)	3154(1)	87(1)	411(1)	35(1)
C(4)	3972(1)	185(1)	1482(1)	35(1)
C(5)	4334(1)	268(1)	2302(1)	34(1)
C(6)	4097(1)	448(1)	2997(1)	33(1)

C(7)	3463(1)	771(1)	3783(1)	32(1)
C(8)	2950(1)	1007(1)	4022(1)	34(1)
C(9)	2367(1)	1087(1)	3462(1)	34(1)
C(10)	1576(1)	1059(1)	2340(1)	38(1)
C(11)	1195(1)	937(1)	1554(1)	39(1)
C(12)	1392(1)	659(1)	928(1)	38(1)
C(13)	989(1)	505(1)	136(1)	42(1)
C(14)	1361(1)	262(1)	-314(1)	40(1)
C(15)	515(1)	1112(1)	1397(1)	41(1)
C(16)	346(1)	1563(1)	1064(2)	44(1)
C(17)	645(1)	2184(1)	213(2)	55(1)
C(18)	752(1)	2658(1)	431(2)	62(1)
C(19)	590(1)	3011(1)	-216(2)	62(1)
C(20)	328(2)	2864(1)	-1038(2)	67(1)
C(21)	232(1)	2386(1)	-1272(2)	66(1)
C(22)	393(1)	2044(1)	-627(2)	59(1)
C(23)	-35(2)	2244(2)	-2191(2)	92(1)
C(24)	684(2)	3528(1)	17(3)	83(1)
C(25)	-278(1)	1738(1)	991(2)	47(1)
C(26)	-732(1)	1451(1)	1245(1)	45(1)
C(27)	-587(1)	996(1)	1560(1)	45(1)
C(28)	39(1)	831(1)	1626(1)	43(1)
C(29)	-102(1)	148(1)	2466(2)	47(1)
C(30)	-283(1)	-322(1)	2304(2)	52(1)
C(31)	-567(1)	-571(1)	2884(2)	54(1)

C(32)	-683(1)	-336(1)	3605(2)	52(1)
C(33)	-513(1)	140(1)	3772(2)	48(1)
C(34)	-204(1)	382(1)	3198(2)	47(1)
C(35)	-663(1)	398(1)	4541(2)	59(1)
C(36)	-748(2)	-1090(1)	2719(2)	73(1)
C(37)	1372(1)	1355(1)	2978(1)	42(1)
C(38)	1860(1)	1372(1)	3672(1)	39(1)
C(39)	3033(1)	1200(1)	4924(1)	35(1)
C(40)	3498(1)	1542(1)	5239(1)	36(1)
C(41)	3719(1)	1881(1)	3920(1)	39(1)
C(42)	3147(1)	2122(1)	3674(1)	40(1)
C(43)	2975(1)	2300(1)	2832(1)	41(1)
C(44)	3395(1)	2239(1)	2270(1)	42(1)
C(45)	3973(1)	1996(1)	2513(1)	42(1)
C(46)	4135(1)	1814(1)	3354(1)	41(1)
C(47)	4394(1)	1896(1)	1872(2)	51(1)
C(48)	2335(1)	2538(1)	2538(2)	49(1)
C(49)	3590(1)	1712(1)	6089(1)	40(1)
C(50)	3203(1)	1546(1)	6634(1)	41(1)
C(51)	2729(1)	1217(1)	6344(1)	39(1)
C(52)	2652(1)	1045(1)	5501(1)	36(1)
C(53)	2260(1)	287(1)	4909(1)	36(1)
C(54)	1744(1)	79(1)	4361(1)	40(1)
C(55)	1802(1)	-383(1)	4061(1)	42(1)
C(56)	2387(1)	-619(1)	4295(1)	41(1)

C(57)	2915(1)	-400(1)	4807(1)	41(1)
C(58)	2842(1)	56(1)	5131(1)	39(1)
C(59)	3564(1)	-631(1)	4989(2)	58(1)
C(60)	1244(1)	-612(1)	3469(2)	55(1)
C(61)	4068(1)	681(1)	4350(1)	35(1)
C(62)	4459(1)	490(1)	3864(1)	35(1)
C(63)	5018(1)	111(1)	2464(1)	34(1)
C(64)	5190(1)	-330(1)	2847(1)	37(1)
C(65)	4719(1)	-1077(1)	3079(2)	41(1)
C(66)	4704(1)	-1306(1)	2296(2)	45(1)
C(67)	4667(1)	-1799(1)	2257(2)	51(1)
C(68)	4632(1)	-2053(1)	3000(2)	51(1)
C(69)	4652(1)	-1827(1)	3785(2)	49(1)
C(70)	4695(1)	-1332(1)	3819(2)	45(1)
C(71)	4628(2)	-2118(1)	4583(2)	73(1)
C(72)	4666(2)	-2064(1)	1420(2)	85(1)
C(73)	5812(1)	-500(1)	2994(1)	38(1)
C(74)	6279(1)	-217(1)	2753(1)	36(1)
C(75)	6135(1)	225(1)	2379(1)	37(1)
C(76)	5508(1)	388(1)	2242(1)	37(1)
C(77)	5784(1)	1188(1)	1994(2)	45(1)
C(78)	5987(1)	1396(1)	1304(2)	47(1)
C(79)	6415(1)	1782(1)	1455(2)	54(1)
C(80)	6622(1)	1940(1)	2298(2)	59(1)
C(81)	6423(1)	1728(1)	2996(2)	58(1)

C(82)	5995(1)	1348(1)	2833(2)	52(1)
C(83)	6677(2)	1895(1)	3908(2)	81(1)
C(84)	6676(2)	2005(1)	727(2)	69(1)
C(85)	4216(1)	-18(1)	775(1)	40(1)
C(86)	3713(1)	-78(1)	116(1)	40(1)
C(87)	2434(1)	-144(1)	-955(1)	37(1)
C(88)	2223(1)	119(1)	-1714(1)	40(1)
C(89)	2462(1)	935(1)	-1236(1)	42(1)
C(90)	2170(1)	1317(1)	-913(1)	42(1)
C(91)	2537(1)	1689(1)	-493(1)	42(1)
C(92)	3200(1)	1664(1)	-404(1)	45(1)
C(93)	3497(1)	1274(1)	-707(2)	48(1)
C(94)	3121(1)	907(1)	-1134(1)	45(1)
C(95)	4214(1)	1237(1)	-562(2)	70(1)
C(96)	2220(1)	2098(1)	-118(2)	49(1)
C(97)	2115(1)	-95(1)	-2528(1)	44(1)
C(98)	2212(1)	-579(1)	-2594(2)	46(1)
C(99)	2421(1)	-852(1)	-1864(1)	43(1)
C(100)	2534(1)	-633(1)	-1056(1)	40(1)
C(101)	2498(1)	-998(1)	326(1)	40(1)
C(102)	2869(1)	-1204(1)	1057(2)	43(1)
C(103)	2591(1)	-1330(1)	1755(2)	46(1)
C(104)	1940(1)	-1236(1)	1702(2)	44(1)
C(105)	1570(1)	-1022(1)	980(2)	42(1)
C(106)	1855(1)	-905(1)	281(2)	41(1)

C(107)	876(1)	-904(1)	944(2)	50(1)
C(108)	2983(1)	-1552(1)	2555(2)	60(1)
C(109)	1397(9)	7889(4)	4113(6)	236(9)
C(110)	1448(5)	7876(3)	5089(8)	165(4)
C(111)	1336(8)	8290(5)	5509(9)	172(5)
C(112)	1350(7)	8342(4)	6387(9)	162(4)
C(113)	1548(5)	7959(4)	6917(9)	144(4)
C(114)	1634(6)	7533(4)	6543(7)	131(3)
C(115)	1597(10)	7504(5)	5627(7)	179(5)
C(116)	1342(8)	8164(6)	6768(7)	225(9)
C(117)	1452(4)	7970(3)	5910(7)	122(3)
C(118)	1649(5)	7507(3)	5881(8)	126(3)
C(119)	1768(5)	7333(4)	5109(8)	136(3)
C(120)	1698(5)	7593(4)	4352(9)	136(3)
C(121)	1482(8)	8063(4)	4347(9)	164(4)
C(122)	1347(8)	8235(4)	5149(7)	137(4)

Table S2. Bond lengths (Å) and angles (degrees) for [Fe(3,5-Me-BAFP)(NH₃)₂].

Fe(1)-N(2)	1.9881(17)
Fe(1)-N(4)	1.9893(17)
Fe(1)-N(5)	1.9903(19)
Fe(1)-N(1)	1.9915(17)
Fe(1)-N(3)	2.0002(17)
Fe(1)-N(6)	2.0156(18)
O(1)-C(16)	1.376(3)
O(1)-C(17)	1.397(3)
O(2)-C(29)	1.378(3)
O(2)-C(28)	1.385(3)
O(3)-C(40)	1.387(3)
O(3)-C(41)	1.391(3)
O(4)-C(52)	1.389(3)
O(4)-C(53)	1.394(3)
O(5)-C(64)	1.386(3)
O(5)-C(65)	1.390(3)
O(6)-C(76)	1.387(3)
O(6)-C(77)	1.396(3)
O(7)-C(88)	1.386(3)
O(7)-C(89)	1.393(3)
O(8)-C(101)	1.390(3)
O(8)-C(100)	1.391(3)
N(1)-C(1)	1.380(3)
N(1)-C(12)	1.385(3)
N(2)-C(3)	1.382(2)
N(2)-C(4)	1.384(2)
N(3)-C(7)	1.379(2)
N(3)-C(6)	1.382(3)
N(4)-C(9)	1.381(3)
N(4)-C(10)	1.386(3)
C(1)-C(2)	1.392(3)
C(1)-C(14)	1.441(3)
C(2)-C(3)	1.390(3)
C(2)-C(87)	1.495(3)
C(3)-C(86)	1.438(3)
C(4)-C(5)	1.389(3)
C(4)-C(85)	1.436(3)
C(5)-C(6)	1.388(3)
C(5)-C(63)	1.498(3)
C(6)-C(62)	1.437(3)
C(7)-C(8)	1.392(3)
C(7)-C(61)	1.441(3)
C(8)-C(9)	1.396(3)

C(8)-C(39)	1.498(3)
C(9)-C(38)	1.432(3)
C(10)-C(11)	1.385(3)
C(10)-C(37)	1.434(3)
C(11)-C(12)	1.385(3)
C(11)-C(15)	1.505(3)
C(12)-C(13)	1.436(3)
C(13)-C(14)	1.350(3)
C(15)-C(16)	1.386(3)
C(15)-C(28)	1.387(3)
C(16)-C(25)	1.402(3)
C(17)-C(18)	1.378(4)
C(17)-C(22)	1.383(4)
C(18)-C(19)	1.413(4)
C(19)-C(20)	1.369(5)
C(19)-C(24)	1.497(4)
C(20)-C(21)	1.393(4)
C(21)-C(22)	1.390(4)
C(21)-C(23)	1.502(5)
C(25)-C(26)	1.377(4)
C(26)-C(27)	1.380(4)
C(27)-C(28)	1.396(3)
C(29)-C(34)	1.378(3)
C(29)-C(30)	1.381(4)
C(30)-C(31)	1.381(4)
C(31)-C(32)	1.377(4)
C(31)-C(36)	1.511(4)
C(32)-C(33)	1.393(4)
C(33)-C(34)	1.395(3)
C(33)-C(35)	1.498(4)
C(37)-C(38)	1.356(3)
C(39)-C(40)	1.398(3)
C(39)-C(52)	1.401(3)
C(40)-C(49)	1.397(3)
C(41)-C(42)	1.381(3)
C(41)-C(46)	1.387(3)
C(42)-C(43)	1.398(3)
C(43)-C(44)	1.387(3)
C(43)-C(48)	1.508(3)
C(44)-C(45)	1.395(3)
C(45)-C(46)	1.397(3)
C(45)-C(47)	1.504(3)
C(49)-C(50)	1.382(3)
C(50)-C(51)	1.380(3)
C(51)-C(52)	1.391(3)

C(53)-C(58)	1.382(3)
C(53)-C(54)	1.389(3)
C(54)-C(55)	1.390(3)
C(55)-C(56)	1.397(3)
C(55)-C(60)	1.504(3)
C(56)-C(57)	1.394(3)
C(57)-C(58)	1.394(3)
C(57)-C(59)	1.504(3)
C(61)-C(62)	1.347(3)
C(63)-C(64)	1.392(3)
C(63)-C(76)	1.401(3)
C(64)-C(73)	1.387(3)
C(65)-C(70)	1.377(3)
C(65)-C(66)	1.384(3)
C(66)-C(67)	1.383(4)
C(67)-C(68)	1.385(4)
C(67)-C(72)	1.512(4)
C(68)-C(69)	1.380(4)
C(69)-C(70)	1.389(4)
C(69)-C(71)	1.507(4)
C(73)-C(74)	1.382(3)
C(74)-C(75)	1.379(3)
C(75)-C(76)	1.388(3)
C(77)-C(78)	1.376(3)
C(77)-C(82)	1.385(4)
C(78)-C(79)	1.405(4)
C(79)-C(80)	1.388(4)
C(79)-C(84)	1.502(4)
C(80)-C(81)	1.388(4)
C(81)-C(82)	1.391(4)
C(81)-C(83)	1.507(4)
C(85)-C(86)	1.349(3)
C(87)-C(100)	1.398(3)
C(87)-C(88)	1.401(3)
C(88)-C(97)	1.393(3)
C(89)-C(90)	1.382(3)
C(89)-C(94)	1.386(3)
C(90)-C(91)	1.392(3)
C(91)-C(92)	1.395(3)
C(91)-C(96)	1.506(3)
C(92)-C(93)	1.392(4)
C(93)-C(94)	1.392(3)
C(93)-C(95)	1.504(3)
C(97)-C(98)	1.379(3)
C(98)-C(99)	1.381(3)

C(99)-C(100)	1.391(3)
C(101)-C(106)	1.384(3)
C(101)-C(102)	1.390(3)
C(102)-C(103)	1.391(3)
C(103)-C(104)	1.399(3)
C(103)-C(108)	1.504(3)
C(104)-C(105)	1.387(3)
C(105)-C(106)	1.396(3)
C(105)-C(107)	1.508(3)
C(109)-C(110)	1.521(10)
C(110)-C(115)	1.342(8)
C(110)-C(111)	1.377(8)
C(111)-C(112)	1.386(8)
C(112)-C(113)	1.375(9)
C(113)-C(114)	1.357(8)
C(114)-C(115)	1.431(8)
C(116)-C(117)	1.517(10)
C(117)-C(118)	1.367(8)
C(117)-C(122)	1.392(8)
C(118)-C(119)	1.379(8)
C(119)-C(120)	1.380(8)
C(120)-C(121)	1.393(8)
C(121)-C(122)	1.433(8)
N(2)-Fe(1)-N(4)	177.01(7)
N(2)-Fe(1)-N(5)	89.32(7)
N(4)-Fe(1)-N(5)	87.72(8)
N(2)-Fe(1)-N(1)	90.18(7)
N(4)-Fe(1)-N(1)	90.15(7)
N(5)-Fe(1)-N(1)	89.05(7)
N(2)-Fe(1)-N(3)	90.33(7)
N(4)-Fe(1)-N(3)	89.42(7)
N(5)-Fe(1)-N(3)	92.62(7)
N(1)-Fe(1)-N(3)	178.26(7)
N(2)-Fe(1)-N(6)	89.88(7)
N(4)-Fe(1)-N(6)	93.10(7)
N(5)-Fe(1)-N(6)	178.63(7)
N(1)-Fe(1)-N(6)	89.85(7)
N(3)-Fe(1)-N(6)	88.49(7)
C(16)-O(1)-C(17)	116.61(18)
C(29)-O(2)-C(28)	118.69(17)
C(40)-O(3)-C(41)	120.56(16)
C(52)-O(4)-C(53)	119.37(15)
C(64)-O(5)-C(65)	117.91(16)
C(76)-O(6)-C(77)	116.51(16)

C(88)-O(7)-C(89)	121.66(16)
C(101)-O(8)-C(100)	120.97(16)
C(1)-N(1)-C(12)	105.30(16)
C(1)-N(1)-Fe(1)	127.22(13)
C(12)-N(1)-Fe(1)	127.43(14)
C(3)-N(2)-C(4)	105.01(16)
C(3)-N(2)-Fe(1)	127.65(13)
C(4)-N(2)-Fe(1)	127.29(13)
C(7)-N(3)-C(6)	105.38(16)
C(7)-N(3)-Fe(1)	127.53(13)
C(6)-N(3)-Fe(1)	126.78(13)
C(9)-N(4)-C(10)	104.94(16)
C(9)-N(4)-Fe(1)	127.92(14)
C(10)-N(4)-Fe(1)	126.70(13)
N(1)-C(1)-C(2)	124.98(18)
N(1)-C(1)-C(14)	110.05(17)
C(2)-C(1)-C(14)	124.91(18)
C(3)-C(2)-C(1)	124.78(18)
C(3)-C(2)-C(87)	117.96(17)
C(1)-C(2)-C(87)	117.26(17)
N(2)-C(3)-C(2)	124.71(18)
N(2)-C(3)-C(86)	110.30(17)
C(2)-C(3)-C(86)	124.98(18)
N(2)-C(4)-C(5)	124.88(18)
N(2)-C(4)-C(85)	110.43(17)
C(5)-C(4)-C(85)	124.57(18)
C(6)-C(5)-C(4)	124.86(18)
C(6)-C(5)-C(63)	117.72(17)
C(4)-C(5)-C(63)	117.17(17)
N(3)-C(6)-C(5)	125.17(17)
N(3)-C(6)-C(62)	110.19(17)
C(5)-C(6)-C(62)	124.65(18)
N(3)-C(7)-C(8)	125.04(17)
N(3)-C(7)-C(61)	110.02(17)
C(8)-C(7)-C(61)	124.86(18)
C(7)-C(8)-C(9)	123.79(18)
C(7)-C(8)-C(39)	118.26(17)
C(9)-C(8)-C(39)	117.92(17)
N(4)-C(9)-C(8)	125.03(18)
N(4)-C(9)-C(38)	110.72(17)
C(8)-C(9)-C(38)	124.25(18)
C(11)-C(10)-N(4)	125.37(19)
C(11)-C(10)-C(37)	124.30(19)
N(4)-C(10)-C(37)	110.30(18)
C(10)-C(11)-C(12)	124.62(19)

C(10)-C(11)-C(15)	116.48(18)
C(12)-C(11)-C(15)	118.88(18)
C(11)-C(12)-N(1)	124.79(19)
C(11)-C(12)-C(13)	124.91(19)
N(1)-C(12)-C(13)	110.28(18)
C(14)-C(13)-C(12)	107.05(19)
C(13)-C(14)-C(1)	107.24(18)
C(16)-C(15)-C(28)	117.72(19)
C(16)-C(15)-C(11)	122.0(2)
C(28)-C(15)-C(11)	120.2(2)
O(1)-C(16)-C(15)	116.94(19)
O(1)-C(16)-C(25)	121.4(2)
C(15)-C(16)-C(25)	121.6(2)
C(18)-C(17)-C(22)	121.8(3)
C(18)-C(17)-O(1)	118.2(3)
C(22)-C(17)-O(1)	119.9(2)
C(17)-C(18)-C(19)	119.1(3)
C(20)-C(19)-C(18)	118.1(3)
C(20)-C(19)-C(24)	122.1(3)
C(18)-C(19)-C(24)	119.8(3)
C(19)-C(20)-C(21)	123.3(3)
C(22)-C(21)-C(20)	117.7(3)
C(22)-C(21)-C(23)	121.1(3)
C(20)-C(21)-C(23)	121.2(3)
C(17)-C(22)-C(21)	119.9(3)
C(26)-C(25)-C(16)	118.7(2)
C(25)-C(26)-C(27)	121.5(2)
C(26)-C(27)-C(28)	118.5(2)
O(2)-C(28)-C(15)	116.13(19)
O(2)-C(28)-C(27)	121.8(2)
C(15)-C(28)-C(27)	122.0(2)
O(2)-C(29)-C(34)	120.9(2)
O(2)-C(29)-C(30)	117.4(2)
C(34)-C(29)-C(30)	121.6(2)
C(29)-C(30)-C(31)	120.2(2)
C(32)-C(31)-C(30)	118.4(2)
C(32)-C(31)-C(36)	121.4(3)
C(30)-C(31)-C(36)	120.2(3)
C(31)-C(32)-C(33)	122.0(2)
C(32)-C(33)-C(34)	118.9(2)
C(32)-C(33)-C(35)	121.7(2)
C(34)-C(33)-C(35)	119.4(2)
C(29)-C(34)-C(33)	118.8(2)
C(38)-C(37)-C(10)	107.13(18)
C(37)-C(38)-C(9)	106.88(18)

C(40)-C(39)-C(52)	116.19(18)
C(40)-C(39)-C(8)	121.99(18)
C(52)-C(39)-C(8)	121.82(18)
O(3)-C(40)-C(49)	115.19(18)
O(3)-C(40)-C(39)	122.54(17)
C(49)-C(40)-C(39)	122.1(2)
C(42)-C(41)-C(46)	121.7(2)
C(42)-C(41)-O(3)	122.59(19)
C(46)-C(41)-O(3)	115.60(19)
C(41)-C(42)-C(43)	119.7(2)
C(44)-C(43)-C(42)	118.6(2)
C(44)-C(43)-C(48)	121.1(2)
C(42)-C(43)-C(48)	120.3(2)
C(43)-C(44)-C(45)	122.0(2)
C(44)-C(45)-C(46)	118.7(2)
C(44)-C(45)-C(47)	121.2(2)
C(46)-C(45)-C(47)	120.0(2)
C(41)-C(46)-C(45)	119.2(2)
C(50)-C(49)-C(40)	119.4(2)
C(51)-C(50)-C(49)	120.47(19)
C(50)-C(51)-C(52)	119.2(2)
O(4)-C(52)-C(51)	115.91(18)
O(4)-C(52)-C(39)	121.42(17)
C(51)-C(52)-C(39)	122.5(2)
C(58)-C(53)-C(54)	121.7(2)
C(58)-C(53)-O(4)	122.54(18)
C(54)-C(53)-O(4)	115.68(18)
C(53)-C(54)-C(55)	119.3(2)
C(54)-C(55)-C(56)	119.0(2)
C(54)-C(55)-C(60)	119.7(2)
C(56)-C(55)-C(60)	121.3(2)
C(57)-C(56)-C(55)	121.6(2)
C(56)-C(57)-C(58)	118.7(2)
C(56)-C(57)-C(59)	122.0(2)
C(58)-C(57)-C(59)	119.2(2)
C(53)-C(58)-C(57)	119.6(2)
C(62)-C(61)-C(7)	107.21(17)
C(61)-C(62)-C(6)	107.11(18)
C(64)-C(63)-C(76)	117.01(18)
C(64)-C(63)-C(5)	120.09(18)
C(76)-C(63)-C(5)	122.90(19)
O(5)-C(64)-C(73)	121.3(2)
O(5)-C(64)-C(63)	115.99(18)
C(73)-C(64)-C(63)	122.58(19)
C(70)-C(65)-C(66)	121.1(2)

C(70)-C(65)-O(5)	118.0(2)
C(66)-C(65)-O(5)	120.7(2)
C(67)-C(66)-C(65)	119.5(2)
C(66)-C(67)-C(68)	119.1(2)
C(66)-C(67)-C(72)	121.3(3)
C(68)-C(67)-C(72)	119.6(3)
C(69)-C(68)-C(67)	121.7(2)
C(68)-C(69)-C(70)	118.8(2)
C(68)-C(69)-C(71)	119.9(3)
C(70)-C(69)-C(71)	121.3(3)
C(65)-C(70)-C(69)	119.8(2)
C(74)-C(73)-C(64)	118.4(2)
C(75)-C(74)-C(73)	121.27(19)
C(74)-C(75)-C(76)	119.3(2)
O(6)-C(76)-C(75)	121.38(19)
O(6)-C(76)-C(63)	117.06(17)
C(75)-C(76)-C(63)	121.4(2)
C(78)-C(77)-C(82)	121.5(2)
C(78)-C(77)-O(6)	118.6(2)
C(82)-C(77)-O(6)	119.9(2)
C(77)-C(78)-C(79)	119.1(2)
C(80)-C(79)-C(78)	118.8(2)
C(80)-C(79)-C(84)	120.2(3)
C(78)-C(79)-C(84)	120.9(3)
C(81)-C(80)-C(79)	122.2(3)
C(80)-C(81)-C(82)	118.2(3)
C(80)-C(81)-C(83)	120.8(3)
C(82)-C(81)-C(83)	121.0(3)
C(77)-C(82)-C(81)	120.2(2)
C(86)-C(85)-C(4)	107.04(18)
C(85)-C(86)-C(3)	107.19(18)
C(100)-C(87)-C(88)	116.63(19)
C(100)-C(87)-C(2)	121.06(19)
C(88)-C(87)-C(2)	122.3(2)
O(7)-C(88)-C(97)	115.1(2)
O(7)-C(88)-C(87)	122.88(18)
C(97)-C(88)-C(87)	121.8(2)
C(90)-C(89)-C(94)	121.2(2)
C(90)-C(89)-O(7)	116.35(19)
C(94)-C(89)-O(7)	122.3(2)
C(89)-C(90)-C(91)	120.2(2)
C(90)-C(91)-C(92)	118.3(2)
C(90)-C(91)-C(96)	120.1(2)
C(92)-C(91)-C(96)	121.6(2)
C(93)-C(92)-C(91)	121.8(2)

C(94)-C(93)-C(92)	119.0(2)
C(94)-C(93)-C(95)	119.7(2)
C(92)-C(93)-C(95)	121.2(2)
C(89)-C(94)-C(93)	119.4(2)
C(98)-C(97)-C(88)	119.5(2)
C(97)-C(98)-C(99)	120.7(2)
C(98)-C(99)-C(100)	119.2(2)
C(99)-C(100)-O(8)	116.2(2)
C(99)-C(100)-C(87)	122.2(2)
O(8)-C(100)-C(87)	121.26(18)
C(106)-C(101)-C(102)	121.3(2)
C(106)-C(101)-O(8)	123.3(2)
C(102)-C(101)-O(8)	115.42(18)
C(101)-C(102)-C(103)	119.9(2)
C(102)-C(103)-C(104)	118.5(2)
C(102)-C(103)-C(108)	120.9(2)
C(104)-C(103)-C(108)	120.7(2)
C(105)-C(104)-C(103)	121.9(2)
C(104)-C(105)-C(106)	118.9(2)
C(104)-C(105)-C(107)	121.6(2)
C(106)-C(105)-C(107)	119.5(2)
C(101)-C(106)-C(105)	119.6(2)
C(115)-C(110)-C(111)	113.1(12)
C(115)-C(110)-C(109)	128.2(9)
C(111)-C(110)-C(109)	118.7(9)
C(110)-C(111)-C(112)	126.5(13)
C(113)-C(112)-C(111)	117.9(13)
C(114)-C(113)-C(112)	118.2(12)
C(113)-C(114)-C(115)	120.2(12)
C(110)-C(115)-C(114)	123.5(13)
C(118)-C(117)-C(122)	118.5(9)
C(118)-C(117)-C(116)	118.2(8)
C(122)-C(117)-C(116)	123.3(8)
C(117)-C(118)-C(119)	118.3(10)
C(118)-C(119)-C(120)	124.7(11)
C(119)-C(120)-C(121)	118.9(12)
C(120)-C(121)-C(122)	115.8(12)
C(117)-C(122)-C(121)	123.6(10)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for abm1104.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^2 U_{11} + \dots + 2hkabU_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	28(1)	34(1)	28(1)	-1(1)	6(1)	0(1)
O(1)	38(1)	56(1)	75(1)	7(1)	4(1)	1(1)
O(2)	50(1)	60(1)	54(1)	12(1)	21(1)	18(1)
O(3)	41(1)	44(1)	36(1)	0(1)	4(1)	-2(1)
O(4)	39(1)	40(1)	41(1)	-7(1)	12(1)	0(1)
O(5)	42(1)	38(1)	67(1)	-3(1)	26(1)	0(1)
O(6)	32(1)	56(1)	55(1)	19(1)	0(1)	-1(1)
O(7)	43(1)	49(1)	37(1)	-7(1)	-2(1)	4(1)
O(8)	34(1)	50(1)	43(1)	-3(1)	8(1)	6(1)
N(1)	31(1)	39(1)	33(1)	-4(1)	7(1)	4(1)
N(2)	28(1)	41(1)	30(1)	-2(1)	4(1)	-1(1)
N(3)	31(1)	33(1)	32(1)	-2(1)	9(1)	-1(1)
N(4)	33(1)	39(1)	31(1)	-2(1)	3(1)	3(1)
N(5)	48(1)	44(1)	35(1)	-1(1)	7(1)	-1(1)
N(6)	37(1)	42(1)	36(1)	-2(1)	7(1)	-2(1)
C(1)	32(1)	40(1)	32(1)	-3(1)	4(1)	3(1)
C(2)	34(1)	40(1)	32(1)	-5(1)	4(1)	2(1)
C(3)	31(1)	42(1)	32(1)	-4(1)	6(1)	1(1)
C(4)	26(1)	44(1)	34(1)	-3(1)	6(1)	0(1)
C(5)	28(1)	39(1)	34(1)	-2(1)	6(1)	-1(1)

C(6)	29(1)	36(1)	32(1)	-1(1)	5(1)	0(1)
C(7)	33(1)	34(1)	29(1)	-1(1)	5(1)	-1(1)
C(8)	36(1)	33(1)	31(1)	-3(1)	6(1)	0(1)
C(9)	35(1)	37(1)	31(1)	-4(1)	6(1)	0(1)
C(10)	34(1)	42(1)	37(1)	-3(1)	6(1)	6(1)
C(11)	33(1)	45(1)	36(1)	-3(1)	4(1)	7(1)
C(12)	31(1)	46(1)	36(1)	-2(1)	6(1)	6(1)
C(13)	32(1)	53(1)	37(1)	-7(1)	0(1)	6(1)
C(14)	34(1)	50(1)	34(1)	-8(1)	2(1)	3(1)
C(15)	34(1)	52(1)	36(1)	-8(1)	4(1)	9(1)
C(16)	36(1)	49(1)	46(1)	-6(1)	3(1)	4(1)
C(17)	42(1)	50(2)	75(2)	6(1)	16(1)	4(1)
C(18)	52(1)	57(2)	83(2)	-9(1)	25(1)	0(1)
C(19)	58(2)	53(2)	86(2)	1(1)	37(1)	2(1)
C(20)	68(2)	56(2)	88(2)	8(2)	40(2)	4(1)
C(21)	63(2)	69(2)	69(2)	6(2)	23(1)	5(1)
C(22)	54(1)	52(2)	72(2)	0(1)	16(1)	1(1)
C(23)	121(3)	86(3)	70(2)	8(2)	20(2)	14(2)
C(24)	91(2)	57(2)	115(3)	-6(2)	53(2)	4(2)
C(25)	39(1)	48(1)	51(1)	-4(1)	2(1)	8(1)
C(26)	36(1)	55(2)	45(1)	-7(1)	5(1)	10(1)
C(27)	36(1)	58(2)	42(1)	-2(1)	9(1)	7(1)
C(28)	41(1)	53(1)	36(1)	0(1)	7(1)	13(1)
C(29)	38(1)	58(2)	45(1)	5(1)	6(1)	9(1)
C(30)	45(1)	55(2)	53(1)	-2(1)	0(1)	12(1)

C(31)	41(1)	52(2)	62(2)	-1(1)	-7(1)	6(1)
C(32)	37(1)	57(2)	60(2)	11(1)	3(1)	-2(1)
C(33)	39(1)	59(2)	46(1)	6(1)	8(1)	2(1)
C(34)	38(1)	53(2)	49(1)	3(1)	7(1)	-1(1)
C(35)	58(2)	71(2)	52(1)	4(1)	19(1)	-2(1)
C(36)	67(2)	53(2)	88(2)	-1(2)	-10(2)	3(1)
C(37)	38(1)	49(1)	39(1)	-6(1)	8(1)	10(1)
C(38)	40(1)	43(1)	34(1)	-8(1)	8(1)	5(1)
C(39)	37(1)	34(1)	31(1)	-3(1)	4(1)	5(1)
C(40)	38(1)	35(1)	34(1)	-4(1)	4(1)	4(1)
C(41)	45(1)	33(1)	38(1)	-2(1)	4(1)	-4(1)
C(42)	48(1)	34(1)	40(1)	-2(1)	10(1)	-1(1)
C(43)	48(1)	31(1)	44(1)	0(1)	7(1)	-1(1)
C(44)	52(1)	34(1)	39(1)	0(1)	9(1)	-5(1)
C(45)	48(1)	35(1)	44(1)	-1(1)	10(1)	-6(1)
C(46)	44(1)	36(1)	42(1)	-4(1)	6(1)	-4(1)
C(47)	56(1)	50(2)	49(1)	2(1)	17(1)	-3(1)
C(48)	52(1)	47(1)	47(1)	6(1)	8(1)	4(1)
C(49)	44(1)	35(1)	38(1)	-7(1)	2(1)	5(1)
C(50)	49(1)	40(1)	32(1)	-7(1)	4(1)	9(1)
C(51)	45(1)	40(1)	33(1)	-1(1)	9(1)	10(1)
C(52)	38(1)	35(1)	35(1)	-5(1)	7(1)	4(1)
C(53)	41(1)	36(1)	33(1)	-2(1)	11(1)	1(1)
C(54)	36(1)	45(1)	41(1)	-1(1)	10(1)	1(1)
C(55)	41(1)	46(1)	41(1)	-3(1)	12(1)	-5(1)

C(56)	48(1)	38(1)	39(1)	-1(1)	10(1)	0(1)
C(57)	48(1)	40(1)	35(1)	3(1)	7(1)	5(1)
C(58)	44(1)	42(1)	31(1)	-1(1)	4(1)	1(1)
C(59)	55(2)	53(2)	59(2)	-6(1)	-4(1)	15(1)
C(60)	44(1)	60(2)	61(2)	-16(1)	11(1)	-7(1)
C(61)	37(1)	38(1)	30(1)	-2(1)	3(1)	0(1)
C(62)	31(1)	38(1)	33(1)	-3(1)	2(1)	1(1)
C(63)	28(1)	44(1)	29(1)	-5(1)	4(1)	0(1)
C(64)	34(1)	39(1)	39(1)	-6(1)	13(1)	-2(1)
C(65)	34(1)	38(1)	51(1)	-2(1)	12(1)	0(1)
C(66)	44(1)	48(1)	43(1)	0(1)	10(1)	-1(1)
C(67)	49(1)	49(2)	55(1)	-11(1)	10(1)	-3(1)
C(68)	41(1)	39(1)	71(2)	0(1)	9(1)	-2(1)
C(69)	35(1)	54(2)	57(1)	11(1)	6(1)	-6(1)
C(70)	37(1)	57(2)	42(1)	-3(1)	10(1)	-6(1)
C(71)	66(2)	80(2)	71(2)	24(2)	9(1)	-21(2)
C(72)	109(3)	71(2)	78(2)	-32(2)	28(2)	-23(2)
C(73)	38(1)	39(1)	37(1)	-4(1)	11(1)	3(1)
C(74)	32(1)	46(1)	31(1)	-6(1)	7(1)	3(1)
C(75)	30(1)	50(1)	32(1)	1(1)	5(1)	-2(1)
C(76)	32(1)	45(1)	32(1)	4(1)	3(1)	1(1)
C(77)	30(1)	47(1)	59(1)	11(1)	10(1)	4(1)
C(78)	39(1)	45(1)	59(1)	12(1)	13(1)	10(1)
C(79)	49(1)	40(1)	77(2)	12(1)	25(1)	11(1)
C(80)	53(1)	39(1)	88(2)	-3(1)	24(1)	2(1)

C(81)	52(1)	50(2)	75(2)	-10(1)	18(1)	5(1)
C(82)	42(1)	58(2)	58(1)	4(1)	14(1)	6(1)
C(83)	84(2)	75(2)	85(2)	-25(2)	23(2)	-8(2)
C(84)	68(2)	51(2)	95(2)	18(2)	34(2)	1(1)
C(85)	31(1)	56(1)	35(1)	-6(1)	9(1)	3(1)
C(86)	34(1)	53(1)	33(1)	-8(1)	8(1)	3(1)
C(87)	28(1)	48(1)	35(1)	-9(1)	4(1)	3(1)
C(88)	32(1)	48(1)	37(1)	-9(1)	4(1)	4(1)
C(89)	45(1)	48(1)	31(1)	-1(1)	6(1)	-1(1)
C(90)	42(1)	48(1)	36(1)	1(1)	5(1)	3(1)
C(91)	49(1)	44(1)	35(1)	4(1)	9(1)	-2(1)
C(92)	49(1)	50(1)	37(1)	1(1)	11(1)	-9(1)
C(93)	44(1)	60(2)	42(1)	-2(1)	16(1)	-5(1)
C(94)	47(1)	57(2)	35(1)	-4(1)	15(1)	2(1)
C(95)	48(1)	85(2)	83(2)	-24(2)	29(1)	-12(1)
C(96)	54(1)	47(1)	45(1)	0(1)	10(1)	1(1)
C(97)	33(1)	62(2)	34(1)	-8(1)	1(1)	5(1)
C(98)	32(1)	62(2)	41(1)	-18(1)	2(1)	5(1)
C(99)	30(1)	51(1)	46(1)	-15(1)	5(1)	2(1)
C(100)	27(1)	52(1)	39(1)	-7(1)	4(1)	2(1)
C(101)	36(1)	40(1)	45(1)	-6(1)	9(1)	-1(1)
C(102)	34(1)	45(1)	49(1)	-2(1)	8(1)	4(1)
C(103)	41(1)	42(1)	53(1)	-3(1)	8(1)	2(1)
C(104)	42(1)	42(1)	50(1)	-3(1)	12(1)	-2(1)
C(105)	34(1)	40(1)	51(1)	-9(1)	7(1)	-3(1)

C(106)	34(1)	41(1)	47(1)	-7(1)	5(1)	0(1)
C(107)	36(1)	60(2)	54(1)	-4(1)	9(1)	-1(1)
C(108)	51(1)	69(2)	60(2)	14(1)	13(1)	11(1)
C(109)	440(30)	67(8)	165(7)	3(6)	-38(13)	-87(12)
C(110)	224(11)	75(6)	184(7)	-5(5)	5(9)	-28(7)
C(111)	154(11)	105(7)	238(9)	-43(7)	-5(11)	-30(7)
C(112)	133(9)	101(6)	240(10)	-45(7)	6(10)	-36(6)
C(113)	83(6)	110(6)	222(9)	-60(6)	-14(7)	-7(5)
C(114)	127(8)	108(6)	156(6)	-42(5)	26(7)	-12(6)
C(115)	247(13)	120(7)	150(6)	0(5)	-6(10)	-18(10)
C(116)	280(30)	215(18)	159(9)	-39(11)	1(14)	1(18)
C(117)	75(5)	112(6)	192(7)	23(5)	55(6)	15(5)
C(118)	61(5)	96(6)	210(9)	34(6)	4(7)	-14(5)
C(119)	74(5)	97(6)	227(10)	-21(5)	2(7)	-6(5)
C(120)	104(6)	95(6)	212(9)	-40(6)	40(7)	-33(5)
C(121)	237(11)	80(7)	175(8)	-14(6)	39(9)	-44(7)
C(122)	154(9)	66(6)	202(8)	15(5)	59(9)	35(6)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Fe}(3,5\text{-Me-BAFP})(\text{NH}_3)_2]$.

	x	y	z	U(eq)
H(5A)	3199	1366	1910	64
H(5B)	2572	1358	1301	64
H(5C)	3146	1153	1035	64
H(6A)	2290	-247	1962	58
H(6B)	2347	-46	2847	58
H(6C)	2918	-249	2569	58
H(13A)	544	564	-37	50
H(14A)	1227	115	-863	48
H(18A)	934	2746	1009	75
H(20A)	207	3101	-1471	81
H(22A)	330	1715	-762	71
H(23A)	316	2210	-2508	138
H(23B)	-332	2491	-2468	138
H(23C)	-261	1939	-2198	138
H(24A)	688	3715	-508	125
H(24B)	1092	3569	422	125
H(24C)	334	3638	289	125
H(25A)	-385	2050	770	57
H(26A)	-1154	1569	1203	55
H(27A)	-905	800	1727	54
H(30A)	-212	-473	1792	63

H(32A)	-886	-504	4002	63
H(34A)	-66	703	3309	56
H(35A)	-437	705	4609	89
H(35B)	-525	204	5062	89
H(35C)	-1124	454	4455	89
H(36A)	-434	-1293	3090	109
H(36B)	-753	-1167	2110	109
H(36C)	-1173	-1146	2849	109
H(37A)	970	1510	2924	50
H(38A)	1865	1540	4197	47
H(42A)	2873	2167	4075	49
H(44A)	3285	2367	1701	50
H(46A)	4526	1648	3536	49
H(47A)	4843	1915	2162	76
H(47B)	4309	2131	1404	76
H(47C)	4304	1574	1631	76
H(48A)	2276	2613	1919	73
H(48B)	2319	2833	2867	73
H(48C)	1994	2322	2635	73
H(49A)	3916	1939	6290	48
H(50A)	3265	1660	7213	49
H(51A)	2458	1108	6716	47
H(54A)	1355	250	4193	48
H(56A)	2426	-937	4100	50
H(58A)	3191	208	5501	47

H(59A)	3822	-504	4590	87
H(59B)	3517	-977	4910	87
H(59C)	3776	-562	5586	87
H(60A)	852	-552	3689	83
H(60B)	1316	-958	3447	83
H(60C)	1202	-477	2887	83
H(61A)	4171	744	4953	42
H(62A)	4892	399	4059	42
H(66A)	4718	-1126	1789	54
H(68A)	4592	-2390	2970	61
H(70A)	4708	-1170	4352	54
H(71A)	5047	-2264	4796	110
H(71B)	4306	-2370	4440	110
H(71C)	4516	-1911	5032	110
H(72A)	5087	-2207	1435	127
H(72B)	4568	-1841	933	127
H(72C)	4341	-2316	1350	127
H(73A)	5916	-803	3255	45
H(74A)	6708	-329	2846	44
H(75A)	6461	417	2218	45
H(78A)	5840	1281	733	56
H(80A)	6908	2203	2401	71
H(82A)	5847	1198	3299	63
H(83A)	6340	1868	4249	121
H(83B)	6813	2229	3897	121

H(83C)	7042	1697	4169	121
H(84A)	6775	2342	859	103
H(84B)	6356	1981	189	103
H(84C)	7065	1836	657	103
H(85A)	4649	-95	771	48
H(86A)	3727	-206	-439	48
H(90A)	1718	1325	-978	51
H(92A)	3456	1919	-131	54
H(94A)	3315	641	-1354	54
H(95A)	4404	1547	-373	105
H(95B)	4342	1143	-1103	105
H(95C)	4362	997	-115	105
H(96A)	1921	2258	-581	73
H(96B)	2546	2326	157	73
H(96C)	1987	1975	314	73
H(97A)	1976	92	-3033	52
H(98A)	2134	-727	-3148	55
H(99A)	2487	-1186	-1912	51
H(10A)	3311	-1260	1080	52
H(10C)	1746	-1323	2174	53
H(10B)	1609	-762	-222	49
H(10G)	731	-1056	1432	75
H(10H)	621	-1022	399	75
H(10I)	826	-557	977	75
H(10D)	3258	-1801	2387	90

H(10E)	2698	-1693	2904	90
H(10F)	3249	-1306	2893	90
H(10J)	1788	8027	3977	355
H(10K)	1029	8084	3850	355
H(10L)	1341	7563	3882	355
H(111)	1240	8568	5161	206
H(112)	1226	8634	6616	194
H(113)	1622	7990	7529	173
H(114)	1719	7254	6889	157
H(115)	1683	7205	5388	214
H(11A)	1651	8419	6967	338
H(11B)	1394	7907	7197	338
H(11C)	907	8294	6693	338
H(118)	1702	7309	6380	151
H(119)	1908	7012	5096	164
H(120)	1795	7454	3843	163
H(121)	1428	8257	3843	197
H(122)	1176	8548	5162	165

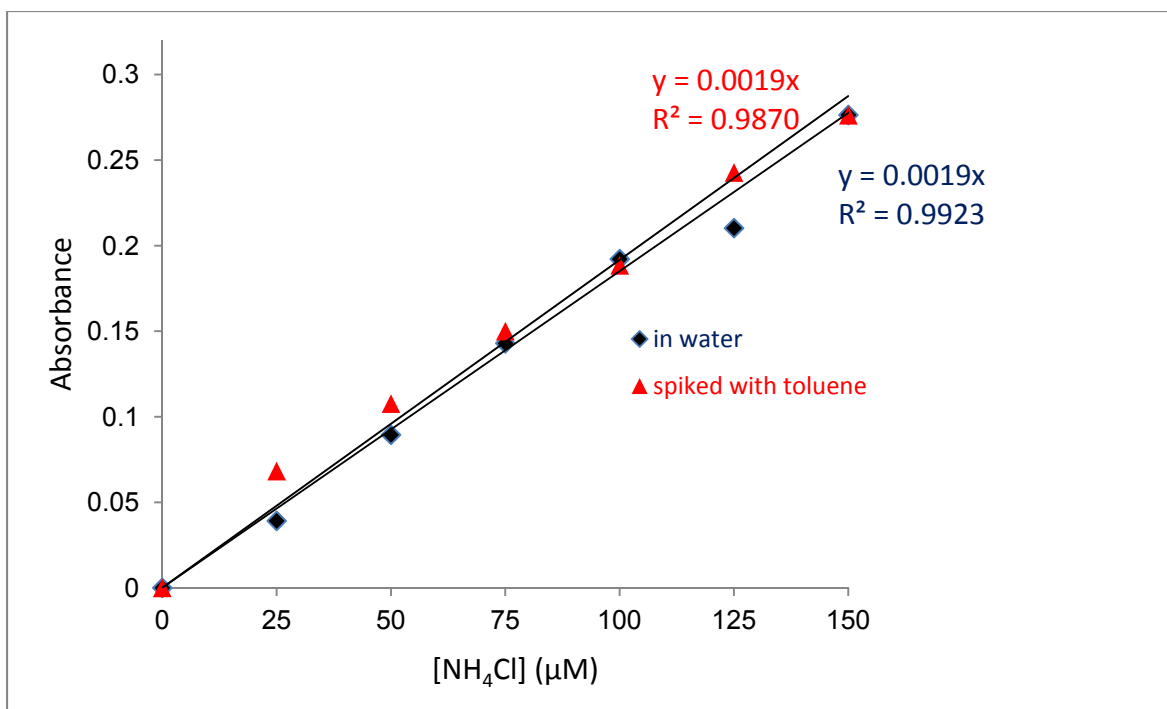


Figure S1. Calibration curve of absorbance versus NH₄Cl concentration (µM) in water (blue) and water-toluene mixtures (red).

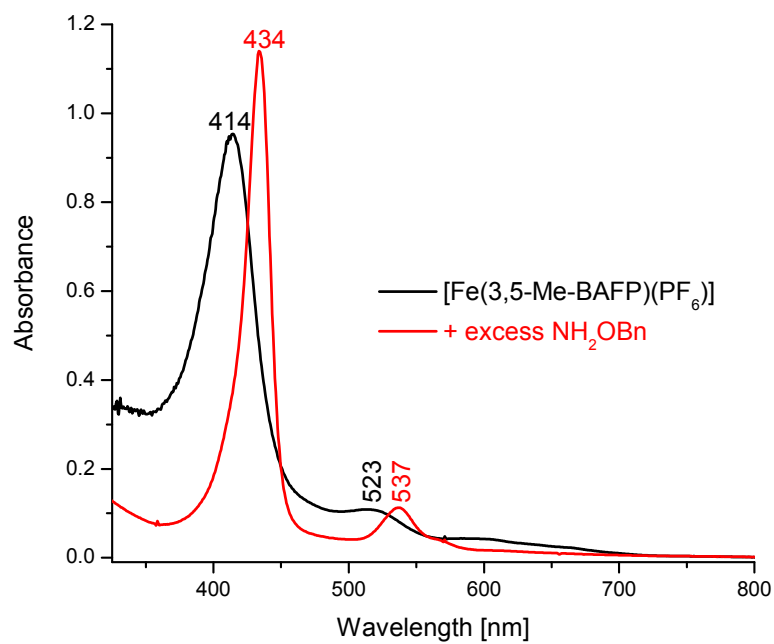


Figure S2. UV-visible spectra of $[\text{Fe}(3,5\text{-Me-BAFP})(\text{PF}_6)]$ (black) and of the product of the reaction of this complex with excess NH_2OBn (red) in toluene at room temperature.

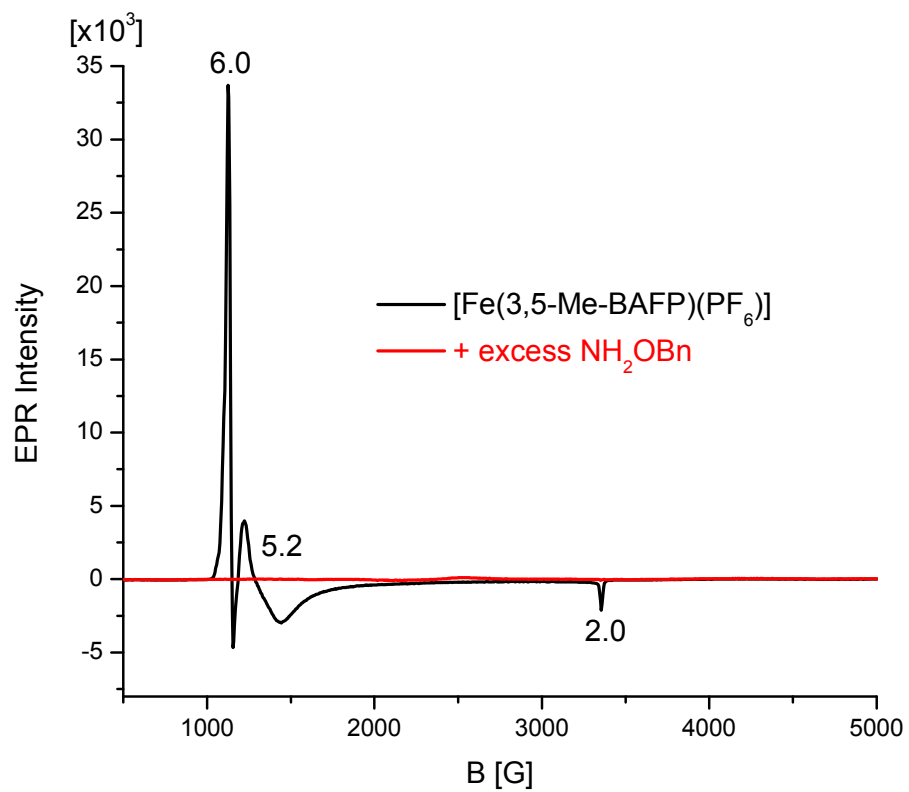


Figure S3. EPR spectra of $[\text{Fe}(3,5\text{-Me-BAFP})(\text{PF}_6)]$ (black) and of the product of the reaction of this complex with excess NH_2OBn (red) in 2-Me-THF. Spectra measured at 6 K.