Supporting Information for

Synthesis, Characterization, and Dioxygen Reactivity of Tetracarboxylate-Bridged Diiron(II) Complexes with Coordinated Substrates

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Experimental Section

General. All reagents were obtained from commercial suppliers and used as received unless otherwise noted. Dichloromethane, pentane, and toluene were saturated with argon and purified by passage through activated Al_2O_3 columns under argon.[1] Dioxygen (99.994%, BOC Gases) was dried by passing the gas stream through a column of Drierite. The compound $[Fe_2(\mu\text{-}O_2CAr^{Tol})_2(O_2CAr^{Tol})_2(THF)_2]$ was prepared as described in the literature.[2] Air-sensitive manipulations were carried out under nitrogen in an MBraun glovebox.

Syntheses.

$[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA)_2]$ (1). To a rapidly stirred CH_2Cl_2 (10 mL) solution of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_2(O_2CAr^{Tol})_2(THF)_2]$ (86.8 mg, 0.0615 mmol) was added benzylamine (BA) (14.1 mg, 2 equiv), to afford a greenish yellow precipitate (70.1 mg, 76%). This solid dissolved to THF (10 mL) upon gentle heating. Light green blocks of **1** suitable for X-ray crystallography were obtained by vapor diffusion of pentane into the THF solution. FT-

IR (KBr, cm^{-1}) 3324, 3271, 3024, 2919, 1607, 1585, 1550, 1514, 1452, 1404,1384, 1303, 1210, 1187, 1150, 1109, 1074, 1036, 1020, 996, 843, 814, 790, 763, 727, 706, 584, 526, 463. Anal. Calcd. for $C_{98}H_{86}N_2Fe_2O_8$: C, 76.86; H, 5.66; N, 1.83. Found: C, 76.81; H, 5.61; N, 1.87.

[$Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2$] (2). To a rapidly stirred yellow CH_2Cl_2 (10 mL) solution of [$Fe_2(\mu\text{-}O_2CAr^{Tol})_2(O_2CAr^{Tol})_2(THF)_2$] (94.8 mg, 0.064 mmol) was added dropwise neat 4-methoxybenzylamine ($BA^{p\text{-}OMe}$) (17.1 mg, 2 equiv). The resulting light greenish yellow solution was stirred for 10 min and filtered through Celite. Light green blocks of **2** (87.4 mg, 83%) suitable for X-ray crystallography were obtained by layering pentanes over the filtrate. FT-IR (KBr, cm^{-1}) 3332, 3274, 3021, 2918, 2863, 2833, 1607, 1586, 1550, 1514, 1453, 1404, 1303, 1248, 1178, 1110, 1073, 1035, 1020, 997, 842, 814, 791, 763, 726, 706, 643, 584, 558, 526, 462. Anal. Calcd. for $C_{100}H_{90}N_2Fe_2O_{10}$: C, 75.47; H, 5.70; N, 1.76. Found: C, 75.11; H, 5.39; N, 1.92.

α-*d_1*-4-Methoxybenzylamine (α-*d_1*-$BA^{p\text{-}OMe}$). To a stirred anhydrous THF (25 mL) suspension of lithium aluminum deuteride (2.6 g, 62 mmol), a solution of anisaldehyde oxime (3.0 g, 24 mmol) was slowly added at -78 °C. The mixture was warmed to room temperature and stirred for 2 days. The mixture was carefully hydrolyzed by addition of 2.6 g of water, 2.6 g of 15% NaOH (aq), and 3 $\times$ 2.6 g of water. Inorganic salts were removed by filtration and washed with ethylacetate (200 mL). The solution was dried ($MgSO_4$) and filtered through a Celite cake and concentrated to give 1.6 g (61 %) of the product. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.22 (d, *J* = 8.5 Hz, 2 H), 6.87 (d, *J* = 8.6 Hz, 2 H), 3. 79 (s, 3 H), 3. 77 (t, *J* = 0.05 Hz, 1 H).

[$Fe_2(\mu\text{-}O_2CAr^{Tol})_4(\alpha\text{-}d_1\text{-}BA^{p\text{-}OMe})_2$]. This compound was prepared as described above for **2**. FT-IR (KBr, cm^{-1}) 3332, 3275, 3051, 3022, 2918, 2862, 2299 ($\nu_{C\text{-}D}$), 1607, 1545, 1514, 1454, 1405, 1385, 1304, 1287, 1247, 1178, 1154, 1110, 1071, 1032, 942, 914, 858, 843, 816, 800, 787, 764, 736, 727, 713, 705, 638, 585, 546, 525, 461.

$[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2](PF_6)$. To a rapidly stirred yellow CH_2Cl_2 (7 mL) solution of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]$ (151.5 mg, 0.095 mmol) was added dropwise a CH_2Cl_2 (3 mL) solution of $AgPF_6$ (24.0 mg, 0.095 mmol). The resulting dark-forest green solution was stirred for 2 h and filtered through a Celite cake. Dichroic brown-green blocks of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2](PF_6)$ (43.2 mg, yield 26 %) suitable for X-ray crystallography were obtained by layering pentanes over the filtrate. FT-IR (KBr, cm^{-1}) 3300, 3243, 2919, 1613, 1583, 1514, 1441, 1405, 1386, 1304, 1252, 1182, 1155, 1110, 1074, 1034, 973, 847, 814, 793, 762, 727, 713, 705, 586, 557, 529, 491. Anal. Calcd. for $C_{100}H_{90}N_2Fe_2O_{10}F_6P$: C, 69.17; H, 5.22; N, 1.61. Found: C, 69.17; H, 5.16; N, 1.55.

Physical Measurements. ^{1}H-NMR spectra were recorded on a Bruker 400 MHz spectrometer housed in the Massachusetts Institute of Technology Department of Chemistry Instrument Facility (MIT DCIF); chemical shifts were referenced to residual solvent peaks. FT-IR spectra were recorded with both a Bio-Rad FTS 135 spectrometer and a Thermo Nicolet Avatar 360 spectrometer. UV-vis spectra were recorded on a Hewlett-Packard 8453 diode array spectrophotometer.

^{57}Fe Mössbauer Spectroscopy. Mössbauer spectra were obtained on an MS1 spectrometer (WEB Research Co.) with a ^{57}Co source in a Rh matrix maintained at room temperature in the DCIF. Solid samples were prepared by suspending ca 0.015 mmol of the powdered material in Apeizon N grease and packing the mixture into a nylon sample holder. All data were collected at 4.2 K and the isomer shift (δ) values are reported with respect to natural iron foil that was used for velocity calibration at room temperature. The spectra were fit to Lorentzian lines by using the WMOSS plot and fit program.[3]

X-ray Crystallographic Studies. Intensity data were collected on a Bruker (formerly Siemens) CCD diffractometer with graphite-monochromatized Mo $K\alpha$ radiation (λ = 0.71073 Å), controlled by a Pentium-based PC running the SMART software package. Single crystals were mounted at room temperature on the tips of quartz fibers, coated with Paratone-N oil, and cooled to 173 K under a stream of cold nitrogen maintained by a Bruker LT-2A nitrogen cryostat. Data collection and reduction protocols are described elsewhere.[4] The structures were solved by Patterson methods and refined on F^2 by using the SHELXTL software package.[5] Empirical absorption corrections were applied with SADABS,[6] part of the SHELXTL program package, and the structures were checked for higher symmetry by the program PLATON.[7] All non-hydrogen atoms were refined anisotropically unless otherwise noted. In general, hydrogen atoms were assigned idealized positions and given thermal parameters equivalent to either 1.5 (methyl hydrogen atoms and NH_2 hydrogen atoms) or 1.2 (all other hydrogen atoms) times the thermal parameter of the carbon atom to which they were attached.

Magnetic Susceptibility Measurement. Magnetic susceptibility data for powdered solid were measured between 5 and 300 K with applied magnetic fields of 0.1 or 1 *T* using a Quantum design MPMS SQUID susceptometer. The sample was loaded in a gel capsule and suspended in a plastic straw. The susceptibilities of the straw and gel capsule were independently determined over the same temperature range and field for correction of their contribution to the total measured susceptibility. Underlying diamagnetism of the sample was calculated from Pascal's constants.[8]

Electrochemistry. Cyclic voltammetric measurements were performed in an MBraun glovebox under nitrogen with an EG&G model 263 potentiostat. A three-electrode configuration consisting a platinum working electrode, a $AgNO_3/Ag$ (0.1 M in acetonitrile with 0.5 M $(Bu_4N)PF_6$) reference electrode, and a platinum mesh auxiliary electrode was used. The supporting electrode was 0.5 M $(Bu_4N)PF_6$ in CH_2Cl_2. All cyclic voltammograms were externally referenced to the Cp_2Fe/Cp_2Fe^+ couple. Conversion from Cp_2Fe/Cp_2Fe^+ scale to NHE scale was based on following values: Cp_2Fe/Cp_2Fe^+ = +460 mV vs SCE (in CH_2Cl_2 with the $(Bu_4N)PF_6$ supporting electrolyte),[9] SCE = +242 mV vs NHE.[10]

Resonance Raman Spectroscopy. Resonance Raman spectra of frozen solutions of $[Fe_2(\square\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]$ **(2)** oxygenated with either $^{16}O_2$ or $^{18}O_2$ at –78 °C were obtained by using a Kr^+ ion laser with excitation provided at 647.1 nm and 8 milliwatt of power at the sample. A monochromator (1200 grooves/nm grating) with an entrance slit of 18 microns and a TE-CCD-1100-PB-VISAR detector cooled to –30 °C with a circulating water bath was employed in a standard backscattering configuration. Data were collected at –196 °C in dichloromethane using a glass cryostat, similar in design to one described previously, that incorporates a copper cold finger.[11] The sample concentration was 5 mM for each measurement. Each measurement was made on more than one freshly prepared sample and the measurements were made in triplicate to ensure the authenticity of the results. The dichloromethane bands at 1156 cm^{-1}, 897 cm^{-1}, 704 cm^{-1}, and 286 cm^{-1} were used as an internal calibration standard. Data were processed using WinSpec 3.2.1 (Princeton Instruments, Inc.) and were further manipulated using Kaleidagraph.

Stopped-flow Oxidation Kinetics. Kinetic experiments were performed by using a Canterbury Stopped-Flow SF-40 and MG-6000 Rapid Diode array System (Hi-Tech

Scientific). A solution of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]$ in CH_2Cl_2 was prepared in a glove box under a nitrogen atmosphere and stored in a gas-tight syringe prior to loading into the stopped-flow apparatus. Dioxygen was introduced to the system as a saturated solution in solvent, and spectra were recorded every 10 s after mixing for a total of 1043 s measurement time.

EPR Measurements. X-band EPR spectra were recorded on a Bruker EMX EPR spectrometer (9.37 GHz) running WinEPR software. Temperature control was achieved with an Oxford Instruments ESR900 liquid-helium cryostat and an ITC503 controller. Dry O_2 gas was directly bubbled into an 0.50 mM CH_2Cl_2 solution of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]$ for 1 min at –78 °C, resulting in a color change from light yellow to dark forest green, indicating the formation of a mixed-valent Fe(II)Fe(III) intermediate. The solution was then frozen at liquid N_2.

GC/MS Studies. GC/MS analyses were carried out on an HP-5890 gas chromatograph connected to a HP-5971 mass analyzer. Alltech Econo-cap EC-WAX capillary columns of dimensions (30 m $\times$ 0.53 mm $\times$ 1.2 μm) were used for GC/MS studies. The following method was used to effect all separations: initial temperature = 100 °C; initial time = 5 min; temperature ramp = 100 – 250 °C at 25 deg/min. The products were identified by comparing their retention times and mass spectral patterns to those of authentic standards. Response calibrations were measured by running calibration curves with authentic samples and an internal standard of 1,2-dichlorobenzene. A 7.1 mM CH_2Cl_2 solution (1 mL) of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]$ was loaded into a vessel fitted with a rubber septum. Dioxygen was bubbled into the solution for one minute at room temperature and the resulting yellow solution was filtered through 1 cm silica column. The 63.5 mM toluene solution (0.15 mL) of dichlorobenzene was added. All samples were prepared in an anaerobic glove box prior to dried dioxygen bubbling.

Kinetic Isotope Effect Measurement. A 7.8 mM CH_2Cl_2 solution of $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(\mu\text{-}d_1\text{-}BA^{p\text{-}OMe})_2]$ was bubbled with dry O_2 gas at –78 °C for 1 h, warmed to room temperature, and filtered through a 1 cm (diameter, 0.6 cm) dry silica column . ^{1}H-NMR (CD_2Cl_2) was used to determine the product distribution by comparing the integration of 9.85 ppm (s, 1H) and 7.83 ppm (d, *J* = 8.5 Hz, 2H) peaks.

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Table S1. Crystal Data and Structure Refinement Informatin for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA)_2]$ (**1**)

Identification code	$[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA)_2]$ (**1**)	
Empirical formula	C98 H86 Fe2 N2 O8	
Formula weight	1531.39	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 14.6583(18) Å	
	b = 19.801(3) Å	β = 91.968(2)°
	c = 27.365(4) Å	
Volume	7938.2(17) $Å^3$	
Z	4	
Density (calculated)	1.281 Mg/m^3	
Absorption coefficient	0.426 mm^{-1}	
F(000)	3216	
Crystal size	0.20 x 0.20 x 0.08 mm^3	
Theta range for data collection	1.27 to 28.27°.	
Index ranges	$-16 \leq h \leq 19$, $-21 \leq k \leq 25$, $-35 \leq l \leq 36$	
Reflections collected	57047	
Independent reflections	18357 [R(int) = 0.0812]	
Completeness to theta = 28.27°	93.2 %	
Absorption correction	Sadabs	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18357 / 0 / 1007	
Goodness-of-fit on F^2	0.952	
Final R indices [I>2sigma(I)]	R1 = 0.0538, wR2 = 0.1031	
R indices (all data)	R1 = 0.1233, wR2 = 0.1324	
Largest diff. peak and hole	0.508 and -0.615 $eÅ^{-3}$	

Table S2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Thermal Parameters (Å^{2}x 10^3) for [Fe_2(-O_2CAr^{Tol})$_4$(BA)$_2$] (**1**). U(eq) is Defined as One-Third of the Trace of the Orthogonalized U^{ij} Tensor.

	x	y	z	U(eq)
C(1)	6924(3)	6929(2)	6585(1)	69(1)
C(2)	6977(3)	6502(2)	7044(1)	46(1)
C(3)	7676(3)	6580(2)	7389(2)	56(1)
C(4)	7746(3)	6178(2)	7803(1)	59(1)
C(5)	7107(3)	5693(2)	7880(1)	57(1)
C(6)	6414(3)	5612(3)	7545(2)	80(2)
C(7)	6340(3)	6012(2)	7130(2)	71(1)
C(8)	8263(4)	7888(2)	3475(1)	72(1)
C(9)	8214(3)	8346(2)	3031(1)	46(1)
C(10)	8805(3)	8872(3)	2984(2)	75(1)
C(11)	8738(3)	9303(2)	2585(2)	75(1)
C(12)	8083(3)	9206(2)	2226(1)	56(1)
C(13)	7500(3)	8680(2)	2270(1)	68(1)
C(14)	7557(3)	8254(2)	2670(1)	60(1)
C(100)	8046(2)	6153(1)	4794(1)	21(1)
C(101)	8180(2)	5413(1)	4691(1)	21(1)
C(102)	8059(2)	5159(1)	4211(1)	24(1)
C(103)	8129(2)	4466(2)	4129(1)	31(1)
C(104)	8308(2)	4021(2)	4508(1)	33(1)
C(105)	8442(2)	4268(2)	4975(1)	31(1)
C(106)	8388(2)	4957(2)	5078(1)	25(1)
C(107)	8640(2)	5168(2)	5589(1)	26(1)
C(108)	9295(2)	5660(2)	5688(1)	32(1)
C(109)	9593(2)	5797(2)	6164(1)	41(1)
C(110)	9255(2)	5455(2)	6559(1)	45(1)
C(111)	8587(3)	4970(2)	6464(1)	48(1)
C(112)	8278(2)	4828(2)	5987(1)	38(1)
C(113)	9617(3)	5590(2)	7077(1)	68(1)
C(114)	7836(2)	5578(1)	3764(1)	26(1)
C(115)	8439(2)	5563(2)	3383(1)	34(1)
C(116)	8200(3)	5846(2)	2934(1)	44(1)
C(117)	7358(3)	6142(2)	2849(1)	44(1)
C(118)	6771(3)	6175(2)	3235(1)	45(1)
C(119)	7006(2)	5900(2)	3691(1)	35(1)
C(120)	7069(3)	6392(2)	2342(1)	73(1)
C(200)	9408(2)	7595(1)	5312(1)	22(1)
C(201)	10403(2)	7716(1)	5451(1)	23(1)
C(202)	10669(2)	7848(2)	5943(1)	27(1)
C(203)	11594(2)	7932(2)	6064(1)	35(1)
C(204)	12254(2)	7900(2)	5716(1)	34(1)
C(205)	11989(2)	7783(2)	5231(1)	29(1)
C(206)	11077(2)	7692(1)	5090(1)	23(1)
C(207)	10882(2)	7540(2)	4560(1)	24(1)

C(208)	11272(2)	7937(2)	4202(1)	31(1)
C(209)	11166(2)	7775(2)	3711(1)	39(1)
C(210)	10680(2)	7211(2)	3560(1)	41(1)
C(211)	10283(2)	6818(2)	3916(1)	36(1)
C(212)	10379(2)	6983(2)	4407(1)	27(1)
C(213)	10573(3)	7023(2)	3025(1)	71(1)
C(214)	10014(2)	7961(2)	6343(1)	30(1)
C(215)	10143(2)	7640(2)	6794(1)	43(1)
C(216)	9591(3)	7796(2)	7178(1)	55(1)
C(217)	8895(3)	8266(2)	7135(1)	51(1)
C(218)	8759(2)	8572(2)	6685(1)	44(1)
C(219)	9313(2)	8424(2)	6295(1)	36(1)
C(220)	8301(3)	8437(2)	7560(2)	82(2)
C(300)	7322(2)	8655(1)	5297(1)	22(1)
C(301)	7109(2)	9379(1)	5418(1)	24(1)
C(302)	7535(2)	9907(2)	5165(1)	28(1)
C(303)	7317(2)	10576(2)	5278(1)	39(1)
C(304)	6709(2)	10726(2)	5636(1)	46(1)
C(305)	6297(2)	10208(2)	5885(1)	41(1)
C(306)	6474(2)	9533(2)	5782(1)	30(1)
C(307)	5934(2)	9012(2)	6035(1)	30(1)
C(308)	5843(2)	9032(2)	6539(1)	45(1)
C(309)	5301(3)	8569(2)	6771(1)	55(1)
C(310)	4838(2)	8062(2)	6515(1)	45(1)
C(311)	4926(2)	8041(2)	6014(1)	39(1)
C(312)	5455(2)	8515(2)	5778(1)	33(1)
C(313)	4266(3)	7536(2)	6769(2)	67(1)
C(314)	8264(2)	9811(2)	4802(1)	27(1)
C(315)	9008(2)	9393(2)	4891(1)	29(1)
C(316)	9719(2)	9359(2)	4576(1)	32(1)
C(317)	9720(2)	9748(2)	4152(1)	34(1)
C(318)	8979(2)	10163(2)	4055(1)	40(1)
C(319)	8252(2)	10196(2)	4372(1)	37(1)
C(320)	10526(2)	9730(2)	3820(1)	44(1)
C(400)	6004(2)	7216(1)	4760(1)	22(1)
C(401)	5020(2)	7114(2)	4588(1)	24(1)
C(402)	4647(2)	7505(2)	4199(1)	27(1)
C(403)	3751(2)	7382(2)	4034(1)	32(1)
C(404)	3226(2)	6896(2)	4245(1)	36(1)
C(405)	3588(2)	6522(2)	4630(1)	34(1)
C(406)	4483(2)	6617(2)	4810(1)	27(1)
C(407)	4817(2)	6157(2)	5210(1)	28(1)
C(408)	4290(2)	6061(2)	5618(1)	40(1)
C(409)	4536(2)	5590(2)	5974(1)	45(1)
C(410)	5320(2)	5201(2)	5937(1)	37(1)
C(411)	5850(2)	5311(2)	5533(1)	34(1)
C(412)	5599(2)	5776(2)	5176(1)	30(1)
C(413)	5571(3)	4665(2)	6313(1)	57(1)
C(414)	5142(2)	8077(2)	3973(1)	29(1)

C(415)	5544(2)	8589(2)	4253(1)	30(1)
C(416)	5949(2)	9142(2)	4036(1)	37(1)
C(417)	5963(2)	9210(2)	3532(1)	41(1)
C(418)	5558(3)	8699(2)	3256(1)	52(1)
C(419)	5158(2)	8143(2)	3467(1)	45(1)
C(420)	6396(3)	9816(2)	3299(2)	64(1)
Fe(1)	7492(1)	7238(1)	5520(1)	21(1)
Fe(2)	7911(1)	7568(1)	4561(1)	20(1)
N(1)	7410(2)	6690(2)	6183(1)	58(1)
N(2)	7995(3)	8184(2)	3926(1)	41(1)
O(1)	7628(1)	6302(1)	5174(1)	24(1)
O(2)	8344(1)	6577(1)	4492(1)	24(1)
O(3)	8939(1)	7257(1)	5602(1)	26(1)
O(4)	9104(1)	7838(1)	4912(1)	23(1)
O(5)	7475(1)	8255(1)	5653(1)	26(1)
O(6)	7336(1)	8490(1)	4854(1)	24(1)
O(7)	6172(1)	7268(1)	5213(1)	24(1)
O(8)	6597(1)	7238(1)	4435(1)	24(1)

Table S3. Interatomic Distances [Å] and Angles [Deg] for $[Fe_2(\square\text{-}O_2CAr^{Tol})_4(BA)_2]$ (**1**).

C(1)-N(1)	1.415(4)
C(1)-C(2)	1.514(5)
C(2)-C(7)	1.372(5)
C(2)-C(3)	1.377(5)
C(3)-C(4)	1.385(5)
C(4)-C(5)	1.363(5)
C(5)-C(6)	1.355(6)
C(6)-C(7)	1.386(6)
C(8)-N(2)	1.434(5)
C(8)-C(9)	1.517(5)
C(9)-C(10)	1.363(6)
C(9)-C(14)	1.368(5)
C(10)-C(11)	1.387(6)
C(11)-C(12)	1.363(6)
C(12)-C(13)	1.356(6)
C(13)-C(14)	1.382(5)
C(100)-O(1)	1.259(3)
C(100)-O(2)	1.267(3)
C(100)-C(101)	1.506(4)
C(101)-C(102)	1.413(4)
C(101)-C(106)	1.416(4)
C(102)-C(103)	1.395(4)
C(102)-C(114)	1.504(4)
C(103)-C(104)	1.378(4)
C(104)-C(105)	1.378(4)
C(105)-C(106)	1.396(4)
C(106)-C(107)	1.494(4)
C(107)-C(108)	1.387(4)
C(107)-C(112)	1.400(4)
C(108)-C(109)	1.386(4)
C(109)-C(110)	1.383(5)
C(110)-C(111)	1.389(5)
C(110)-C(113)	1.521(5)
C(111)-C(112)	1.396(5)
C(114)-C(119)	1.382(4)
C(114)-C(115)	1.391(4)
C(115)-C(116)	1.385(4)
C(116)-C(117)	1.378(5)
C(117)-C(118)	1.386(5)
C(117)-C(120)	1.520(5)
C(118)-C(119)	1.394(4)
C(200)-O(3)	1.259(3)
C(200)-O(4)	1.264(3)
C(200)-C(201)	1.513(4)
C(201)-C(202)	1.413(4)
C(201)-C(206)	1.422(4)
C(202)-C(203)	1.394(4)

C(202)-C(214)	1.497(4)
C(203)-C(204)	1.381(4)
C(204)-C(205)	1.389(4)
C(205)-C(206)	1.392(4)
C(206)-C(207)	1.499(4)
C(207)-C(212)	1.383(4)
C(207)-C(208)	1.394(4)
C(208)-C(209)	1.387(4)
C(209)-C(210)	1.380(5)
C(210)-C(211)	1.391(5)
C(210)-C(213)	1.515(5)
C(211)-C(212)	1.385(4)
C(214)-C(219)	1.381(4)
C(214)-C(215)	1.394(4)
C(215)-C(216)	1.384(5)
C(216)-C(217)	1.382(5)
C(217)-C(218)	1.380(5)
C(217)-C(220)	1.516(5)
C(218)-C(219)	1.392(4)
C(300)-O(6)	1.256(3)
C(300)-O(5)	1.271(3)
C(300)-C(301)	1.507(4)
C(301)-C(302)	1.411(4)
C(301)-C(306)	1.419(4)
C(302)-C(303)	1.400(4)
C(302)-C(314)	1.495(4)
C(303)-C(304)	1.380(5)
C(304)-C(305)	1.381(5)
C(305)-C(306)	1.392(4)
C(306)-C(307)	1.486(4)
C(307)-C(312)	1.388(4)
C(307)-C(308)	1.391(4)
C(308)-C(309)	1.380(5)
C(309)-C(310)	1.388(5)
C(310)-C(311)	1.381(5)
C(310)-C(313)	1.521(5)
C(311)-C(312)	1.391(4)
C(314)-C(315)	1.384(4)
C(314)-C(319)	1.403(4)
C(315)-C(316)	1.377(4)
C(316)-C(317)	1.393(4)
C(317)-C(318)	1.381(5)
C(317)-C(320)	1.515(4)
C(318)-C(319)	1.399(4)
C(400)-O(7)	1.260(3)
C(400)-O(8)	1.266(3)
C(400)-C(401)	1.517(4)
C(401)-C(406)	1.410(4)
C(401)-C(402)	1.411(4)

C(402)-C(403)	1.395(4)
C(402)-C(414)	1.491(4)
C(403)-C(404)	1.373(4)
C(404)-C(405)	1.379(4)
C(405)-C(406)	1.398(4)
C(406)-C(407)	1.494(4)
C(407)-C(412)	1.378(4)
C(407)-C(408)	1.391(4)
C(408)-C(409)	1.388(5)
C(409)-C(410)	1.390(5)
C(410)-C(411)	1.388(4)
C(410)-C(413)	1.517(5)
C(411)-C(412)	1.385(4)
C(414)-C(415)	1.389(4)
C(414)-C(419)	1.391(4)
C(415)-C(416)	1.389(4)
C(416)-C(417)	1.386(5)
C(417)-C(418)	1.386(5)
C(417)-C(420)	1.509(5)
C(418)-C(419)	1.382(5)
Fe(1)-O(5)	2.046(2)
Fe(1)-O(7)	2.0831(19)
Fe(1)-O(1)	2.0953(19)
Fe(1)-N(1)	2.119(3)
Fe(1)-O(3)	2.1256(19)
Fe(1)-Fe(2)	2.7937(6)
Fe(2)-O(4)	2.0372(19)
Fe(2)-O(8)	2.0512(19)
Fe(2)-O(2)	2.074(2)
Fe(2)-N(2)	2.130(3)
Fe(2)-O(6)	2.1754(19)
N(1)-C(1)-C(2)	116.5(3)
C(7)-C(2)-C(3)	117.1(3)
C(7)-C(2)-C(1)	121.4(4)
C(3)-C(2)-C(1)	121.4(4)
C(2)-C(3)-C(4)	121.9(4)
C(5)-C(4)-C(3)	120.0(4)
C(6)-C(5)-C(4)	118.7(4)
C(5)-C(6)-C(7)	121.5(4)
C(2)-C(7)-C(6)	120.7(4)
N(2)-C(8)-C(9)	116.0(3)
C(10)-C(9)-C(14)	117.8(3)
C(10)-C(9)-C(8)	121.3(4)
C(14)-C(9)-C(8)	120.8(4)
C(9)-C(10)-C(11)	121.1(4)
C(12)-C(11)-C(10)	120.6(4)
C(13)-C(12)-C(11)	118.5(4)
C(12)-C(13)-C(14)	121.1(4)

C(9)-C(14)-C(13)	120.9(4)
O(1)-C(100)-O(2)	124.9(3)
O(1)-C(100)-C(101)	116.9(2)
O(2)-C(100)-C(101)	118.2(2)
C(102)-C(101)-C(106)	119.1(3)
C(102)-C(101)-C(100)	120.5(2)
C(106)-C(101)-C(100)	120.4(3)
C(103)-C(102)-C(101)	119.4(3)
C(103)-C(102)-C(114)	115.4(3)
C(101)-C(102)-C(114)	125.3(3)
C(104)-C(103)-C(102)	121.6(3)
C(103)-C(104)-C(105)	119.2(3)
C(104)-C(105)-C(106)	121.8(3)
C(105)-C(106)-C(101)	119.0(3)
C(105)-C(106)-C(107)	116.5(3)
C(101)-C(106)-C(107)	124.2(3)
C(108)-C(107)-C(112)	117.6(3)
C(108)-C(107)-C(106)	121.7(3)
C(112)-C(107)-C(106)	120.5(3)
C(109)-C(108)-C(107)	121.0(3)
C(110)-C(109)-C(108)	121.9(3)
C(109)-C(110)-C(111)	117.5(3)
C(109)-C(110)-C(113)	121.4(4)
C(111)-C(110)-C(113)	121.1(4)
C(110)-C(111)-C(112)	121.2(3)
C(111)-C(112)-C(107)	120.8(3)
C(119)-C(114)-C(115)	118.7(3)
C(119)-C(114)-C(102)	122.5(3)
C(115)-C(114)-C(102)	118.2(3)
C(116)-C(115)-C(114)	120.5(3)
C(117)-C(116)-C(115)	121.3(3)
C(116)-C(117)-C(118)	117.9(3)
C(116)-C(117)-C(120)	120.8(4)
C(118)-C(117)-C(120)	121.2(4)
C(117)-C(118)-C(119)	121.4(3)
C(114)-C(119)-C(118)	120.0(3)
O(3)-C(200)-O(4)	124.3(3)
O(3)-C(200)-C(201)	117.9(2)
O(4)-C(200)-C(201)	117.7(2)
C(202)-C(201)-C(206)	119.5(3)
C(202)-C(201)-C(200)	120.1(2)
C(206)-C(201)-C(200)	120.4(2)
C(203)-C(202)-C(201)	118.8(3)
C(203)-C(202)-C(214)	117.0(3)
C(201)-C(202)-C(214)	124.0(3)
C(204)-C(203)-C(202)	122.0(3)
C(203)-C(204)-C(205)	119.1(3)
C(204)-C(205)-C(206)	121.4(3)
C(205)-C(206)-C(201)	119.2(3)

C(205)-C(206)-C(207)	116.4(2)
C(201)-C(206)-C(207)	124.4(2)
C(212)-C(207)-C(208)	117.6(3)
C(212)-C(207)-C(206)	122.4(3)
C(208)-C(207)-C(206)	119.8(3)
C(209)-C(208)-C(207)	121.0(3)
C(210)-C(209)-C(208)	121.1(3)
C(209)-C(210)-C(211)	117.9(3)
C(209)-C(210)-C(213)	121.5(3)
C(211)-C(210)-C(213)	120.5(4)
C(212)-C(211)-C(210)	121.1(3)
C(207)-C(212)-C(211)	121.2(3)
C(219)-C(214)-C(215)	117.6(3)
C(219)-C(214)-C(202)	121.7(3)
C(215)-C(214)-C(202)	120.5(3)
C(216)-C(215)-C(214)	120.4(3)
C(217)-C(216)-C(215)	122.2(3)
C(218)-C(217)-C(216)	117.1(3)
C(218)-C(217)-C(220)	121.2(4)
C(216)-C(217)-C(220)	121.7(4)
C(217)-C(218)-C(219)	121.4(4)
C(214)-C(219)-C(218)	121.2(3)
O(6)-C(300)-O(5)	124.8(3)
O(6)-C(300)-C(301)	118.1(2)
O(5)-C(300)-C(301)	117.2(2)
C(302)-C(301)-C(306)	119.8(3)
C(302)-C(301)-C(300)	119.8(3)
C(306)-C(301)-C(300)	120.3(3)
C(303)-C(302)-C(301)	118.9(3)
C(303)-C(302)-C(314)	116.1(3)
C(301)-C(302)-C(314)	124.8(3)
C(304)-C(303)-C(302)	121.2(3)
C(303)-C(304)-C(305)	119.7(3)
C(304)-C(305)-C(306)	121.7(3)
C(305)-C(306)-C(301)	118.6(3)
C(305)-C(306)-C(307)	117.8(3)
C(301)-C(306)-C(307)	123.4(3)
C(312)-C(307)-C(308)	117.3(3)
C(312)-C(307)-C(306)	121.6(3)
C(308)-C(307)-C(306)	120.9(3)
C(309)-C(308)-C(307)	120.8(3)
C(308)-C(309)-C(310)	121.9(3)
C(311)-C(310)-C(309)	117.5(3)
C(311)-C(310)-C(313)	120.4(4)
C(309)-C(310)-C(313)	122.1(3)
C(310)-C(311)-C(312)	120.9(3)
C(307)-C(312)-C(311)	121.6(3)
C(315)-C(314)-C(319)	117.4(3)
C(315)-C(314)-C(302)	122.5(3)

C(319)-C(314)-C(302)	119.9(3)
C(316)-C(315)-C(314)	121.9(3)
C(315)-C(316)-C(317)	121.2(3)
C(318)-C(317)-C(316)	117.7(3)
C(318)-C(317)-C(320)	121.6(3)
C(316)-C(317)-C(320)	120.7(3)
C(317)-C(318)-C(319)	121.4(3)
C(318)-C(319)-C(314)	120.4(3)
O(7)-C(400)-O(8)	125.0(3)
O(7)-C(400)-C(401)	118.0(2)
O(8)-C(400)-C(401)	117.1(2)
C(406)-C(401)-C(402)	120.1(3)
C(406)-C(401)-C(400)	119.9(3)
C(402)-C(401)-C(400)	120.1(3)
C(403)-C(402)-C(401)	118.9(3)
C(403)-C(402)-C(414)	117.6(3)
C(401)-C(402)-C(414)	123.3(3)
C(404)-C(403)-C(402)	121.4(3)
C(403)-C(404)-C(405)	119.5(3)
C(404)-C(405)-C(406)	121.9(3)
C(405)-C(406)-C(401)	118.3(3)
C(405)-C(406)-C(407)	117.1(3)
C(401)-C(406)-C(407)	124.5(3)
C(412)-C(407)-C(408)	117.7(3)
C(412)-C(407)-C(406)	122.4(3)
C(408)-C(407)-C(406)	119.7(3)
C(409)-C(408)-C(407)	121.2(3)
C(408)-C(409)-C(410)	121.0(3)
C(411)-C(410)-C(409)	117.3(3)
C(411)-C(410)-C(413)	121.4(3)
C(409)-C(410)-C(413)	121.3(3)
C(412)-C(411)-C(410)	121.5(3)
C(407)-C(412)-C(411)	121.2(3)
C(415)-C(414)-C(419)	117.3(3)
C(415)-C(414)-C(402)	122.0(3)
C(419)-C(414)-C(402)	120.5(3)
C(414)-C(415)-C(416)	121.2(3)
C(417)-C(416)-C(415)	121.6(3)
C(418)-C(417)-C(416)	116.7(3)
C(418)-C(417)-C(420)	122.0(3)
C(416)-C(417)-C(420)	121.3(4)
C(419)-C(418)-C(417)	122.3(3)
C(418)-C(419)-C(414)	120.8(3)
O(5)-Fe(1)-O(7)	91.56(8)
O(5)-Fe(1)-O(1)	162.40(8)
O(7)-Fe(1)-O(1)	86.80(8)
O(5)-Fe(1)-N(1)	110.51(10)
O(7)-Fe(1)-N(1)	106.29(11)
O(1)-Fe(1)-N(1)	86.71(10)

O(5)-Fe(1)-O(3)	88.95(8)
O(7)-Fe(1)-O(3)	162.03(7)
O(1)-Fe(1)-O(3)	87.31(7)
N(1)-Fe(1)-O(3)	90.30(11)
O(5)-Fe(1)-Fe(2)	86.63(5)
O(7)-Fe(1)-Fe(2)	81.11(5)
O(1)-Fe(1)-Fe(2)	75.79(5)
N(1)-Fe(1)-Fe(2)	160.73(8)
O(3)-Fe(1)-Fe(2)	80.99(5)
O(4)-Fe(2)-O(8)	161.57(8)
O(4)-Fe(2)-O(2)	91.79(8)
O(8)-Fe(2)-O(2)	88.38(8)
O(4)-Fe(2)-N(2)	99.26(12)
O(8)-Fe(2)-N(2)	97.18(12)
O(2)-Fe(2)-N(2)	116.15(10)
O(4)-Fe(2)-O(6)	86.76(7)
O(8)-Fe(2)-O(6)	87.46(7)
O(2)-Fe(2)-O(6)	162.15(7)
N(2)-Fe(2)-O(6)	81.61(10)
O(4)-Fe(2)-Fe(1)	80.33(5)
O(8)-Fe(2)-Fe(1)	81.28(5)
O(2)-Fe(2)-Fe(1)	86.71(5)
N(2)-Fe(2)-Fe(1)	157.10(9)
O(6)-Fe(2)-Fe(1)	75.51(5)
C(1)-N(1)-Fe(1)	122.7(2)
C(8)-N(2)-Fe(2)	119.6(2)
C(100)-O(1)-Fe(1)	129.56(19)
C(100)-O(2)-Fe(2)	117.00(18)
C(200)-O(3)-Fe(1)	120.56(18)
C(200)-O(4)-Fe(2)	125.42(18)
C(300)-O(5)-Fe(1)	118.68(18)
C(300)-O(6)-Fe(2)	126.36(18)
C(400)-O(7)-Fe(1)	122.82(18)
C(400)-O(8)-Fe(2)	123.79(18)

Table S4. Anisotropic Thermal Parameters (Å^{2}x 10^3) for [$Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA)_2$] (**1**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U11	U22	U33	U23	U13	U12
C(1)	98(4)	69(3)	41(2)	16(2)	28(2)	30(3)
C(2)	58(2)	52(2)	29(2)	6(2)	18(2)	10(2)
C(3)	56(3)	54(3)	59(3)	8(2)	17(2)	-9(2)
C(4)	53(3)	82(3)	42(2)	6(2)	0(2)	1(2)
C(5)	61(3)	74(3)	35(2)	19(2)	14(2)	5(2)
C(6)	76(3)	100(4)	65(3)	32(3)	3(3)	-38(3)
C(7)	74(3)	98(4)	40(2)	17(2)	-12(2)	-17(3)
C(8)	136(4)	51(3)	30(2)	9(2)	18(2)	29(3)
C(9)	71(3)	44(2)	24(2)	7(2)	9(2)	15(2)
C(10)	81(3)	96(4)	46(3)	22(2)	-25(2)	-22(3)
C(11)	76(3)	83(4)	67(3)	32(3)	-3(2)	-30(3)
C(12)	64(3)	71(3)	32(2)	23(2)	8(2)	11(2)
C(13)	70(3)	92(4)	40(2)	17(2)	-15(2)	-7(3)
C(14)	72(3)	61(3)	48(3)	9(2)	4(2)	-10(2)
C(100)	15(1)	22(2)	26(2)	1(1)	-5(1)	0(1)
C(101)	17(1)	20(2)	27(2)	3(1)	1(1)	1(1)
C(102)	21(2)	21(2)	29(2)	-1(1)	0(1)	1(1)
C(103)	36(2)	24(2)	33(2)	-6(1)	-2(1)	2(1)
C(104)	37(2)	19(2)	43(2)	2(1)	0(2)	2(1)
C(105)	29(2)	25(2)	38(2)	12(1)	3(1)	3(1)
C(106)	19(2)	26(2)	30(2)	3(1)	2(1)	-1(1)
C(107)	24(2)	27(2)	28(2)	6(1)	-2(1)	5(1)
C(108)	29(2)	36(2)	32(2)	4(1)	-3(1)	4(2)
C(109)	31(2)	50(2)	43(2)	-6(2)	-10(2)	7(2)
C(110)	44(2)	59(3)	31(2)	-5(2)	-5(2)	22(2)
C(111)	54(2)	60(3)	29(2)	15(2)	4(2)	11(2)
C(112)	39(2)	39(2)	38(2)	11(2)	5(2)	2(2)
C(113)	72(3)	96(4)	36(2)	-13(2)	-14(2)	29(3)
C(114)	34(2)	18(2)	26(2)	-4(1)	-4(1)	-1(1)
C(115)	39(2)	30(2)	34(2)	-5(1)	-1(1)	3(2)
C(116)	65(3)	38(2)	31(2)	2(2)	7(2)	-2(2)
C(117)	68(3)	32(2)	30(2)	3(2)	-12(2)	-1(2)
C(118)	50(2)	40(2)	45(2)	7(2)	-14(2)	12(2)
C(119)	38(2)	34(2)	33(2)	1(2)	-1(1)	5(2)
C(120)	104(4)	74(3)	40(2)	19(2)	-18(2)	5(3)
C(200)	25(2)	19(2)	22(1)	-5(1)	1(1)	0(1)
C(201)	25(2)	18(2)	25(2)	4(1)	-4(1)	-3(1)
C(202)	29(2)	26(2)	28(2)	2(1)	-3(1)	-4(1)
C(203)	34(2)	38(2)	31(2)	0(2)	-13(1)	-3(2)
C(204)	24(2)	34(2)	42(2)	0(2)	-8(1)	-4(1)
C(205)	24(2)	26(2)	35(2)	3(1)	0(1)	-1(1)
C(206)	25(2)	15(2)	27(2)	3(1)	-2(1)	-1(1)
C(207)	19(2)	23(2)	30(2)	1(1)	0(1)	5(1)

C(208)	28(2)	32(2)	33(2)	4(1)	1(1)	1(1)
C(209)	38(2)	48(2)	32(2)	10(2)	7(1)	7(2)
C(210)	36(2)	59(3)	29(2)	-7(2)	-2(1)	8(2)
C(211)	31(2)	41(2)	36(2)	-11(2)	-5(1)	1(2)
C(212)	20(2)	28(2)	35(2)	0(1)	2(1)	4(1)
C(213)	73(3)	107(4)	32(2)	-15(2)	2(2)	1(3)
C(214)	30(2)	32(2)	26(2)	-1(1)	-6(1)	-9(1)
C(215)	42(2)	55(2)	33(2)	11(2)	-7(2)	-1(2)
C(216)	66(3)	74(3)	23(2)	11(2)	-1(2)	-15(2)
C(217)	61(3)	57(3)	34(2)	-6(2)	14(2)	-18(2)
C(218)	49(2)	39(2)	46(2)	-8(2)	10(2)	-5(2)
C(219)	47(2)	33(2)	28(2)	-4(1)	2(2)	-4(2)
C(220)	109(4)	89(4)	50(3)	-11(2)	40(3)	-13(3)
C(300)	18(2)	22(2)	26(2)	0(1)	2(1)	-2(1)
C(301)	26(2)	21(2)	25(2)	-1(1)	-1(1)	1(1)
C(302)	27(2)	20(2)	36(2)	-1(1)	0(1)	2(1)
C(303)	42(2)	24(2)	52(2)	-1(2)	8(2)	-1(2)
C(304)	45(2)	29(2)	65(3)	-11(2)	12(2)	7(2)
C(305)	41(2)	36(2)	46(2)	-9(2)	12(2)	8(2)
C(306)	29(2)	30(2)	30(2)	-3(1)	1(1)	3(1)
C(307)	25(2)	33(2)	33(2)	-1(1)	6(1)	6(1)
C(308)	51(2)	51(2)	32(2)	-3(2)	3(2)	-3(2)
C(309)	63(3)	73(3)	28(2)	8(2)	11(2)	4(2)
C(310)	37(2)	52(2)	45(2)	13(2)	10(2)	5(2)
C(311)	27(2)	47(2)	41(2)	1(2)	5(1)	-2(2)
C(312)	28(2)	43(2)	30(2)	0(2)	8(1)	3(2)
C(313)	56(3)	82(3)	65(3)	30(2)	20(2)	-3(2)
C(314)	29(2)	17(2)	36(2)	-1(1)	4(1)	-4(1)
C(315)	35(2)	18(2)	34(2)	-1(1)	3(1)	-3(1)
C(316)	30(2)	23(2)	43(2)	-3(1)	5(1)	-1(1)
C(317)	35(2)	26(2)	41(2)	-5(2)	7(2)	-4(2)
C(318)	54(2)	33(2)	35(2)	10(2)	8(2)	-2(2)
C(319)	38(2)	33(2)	42(2)	6(2)	0(2)	5(2)
C(320)	46(2)	40(2)	47(2)	1(2)	17(2)	-5(2)
C(400)	26(2)	15(2)	26(2)	0(1)	0(1)	2(1)
C(401)	21(2)	25(2)	28(2)	-6(1)	0(1)	1(1)
C(402)	23(2)	29(2)	28(2)	-6(1)	-1(1)	3(1)
C(403)	28(2)	30(2)	37(2)	-6(1)	-6(1)	5(1)
C(404)	19(2)	34(2)	53(2)	-8(2)	-9(1)	1(2)
C(405)	21(2)	31(2)	49(2)	-4(2)	4(1)	-2(1)
C(406)	23(2)	24(2)	35(2)	-4(1)	5(1)	1(1)
C(407)	23(2)	26(2)	36(2)	1(1)	1(1)	-5(1)
C(408)	30(2)	39(2)	50(2)	4(2)	10(2)	3(2)
C(409)	42(2)	51(2)	42(2)	11(2)	16(2)	1(2)
C(410)	41(2)	35(2)	36(2)	6(2)	-1(2)	-7(2)
C(411)	30(2)	28(2)	44(2)	4(2)	-2(1)	-1(1)
C(412)	24(2)	26(2)	39(2)	0(1)	2(1)	-5(1)
C(413)	65(3)	55(3)	50(2)	17(2)	8(2)	4(2)
C(414)	25(2)	34(2)	26(2)	1(1)	-3(1)	8(1)

C(415)	28(2)	35(2)	26(2)	2(1)	0(1)	4(1)
C(416)	31(2)	35(2)	43(2)	9(2)	-2(2)	-2(2)
C(417)	29(2)	48(2)	46(2)	21(2)	0(2)	5(2)
C(418)	55(2)	74(3)	27(2)	21(2)	-3(2)	2(2)
C(419)	51(2)	55(3)	28(2)	1(2)	-5(2)	-3(2)
C(420)	57(3)	66(3)	68(3)	38(2)	7(2)	-1(2)
Fe(1)	24(1)	21(1)	19(1)	1(1)	1(1)	-1(1)
Fe(2)	21(1)	20(1)	19(1)	2(1)	0(1)	0(1)
N(1)	84(3)	58(2)	32(2)	17(2)	26(2)	27(2)
N(2)	65(2)	34(2)	26(2)	6(1)	13(1)	1(2)
O(1)	25(1)	23(1)	25(1)	-2(1)	1(1)	0(1)
O(2)	23(1)	21(1)	28(1)	1(1)	1(1)	-2(1)
O(3)	27(1)	25(1)	27(1)	3(1)	0(1)	-3(1)
O(4)	24(1)	22(1)	24(1)	2(1)	-3(1)	1(1)
O(5)	28(1)	25(1)	26(1)	0(1)	2(1)	1(1)
O(6)	26(1)	22(1)	24(1)	-1(1)	0(1)	1(1)
O(7)	23(1)	25(1)	24(1)	-1(1)	-2(1)	-2(1)
O(8)	22(1)	26(1)	23(1)	-1(1)	0(1)	0(1)

Table S5. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters (Å^2 x 10^3) for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA)_2]$ (**1**).

	x	y	z	U(eq)
H(1A)	6273	6975	6481	83
H(2B)	7152	7387	6669	83
H(3)	8122	6919	7341	67
H(4)	8240	6240	8032	71
H(5)	7147	5417	8164	68
H(6)	5969	5273	7595	96
H(7)	5844	5946	6903	85
H(8A)	7871	7489	3407	86
H(9B)	8899	7723	3520	86
H(10)	9271	8944	3228	90
H(11)	9152	9670	2562	90
H(12)	8037	9500	1952	67
H(13)	7044	8602	2021	81
H(14)	7135	7893	2695	72
H(15)	8052	4297	3806	37
H(16)	8338	3549	4447	39
H(17)	8576	3962	5235	37
H(18)	9542	5906	5425	39
H(19)	10042	6137	6220	50
H(20)	8336	4731	6729	57
H(21)	7817	4497	5932	46
H(22A)	9274	5320	7308	102
H(23B)	9547	6070	7153	102
H(24C)	10265	5467	7104	102
H(25)	9021	5357	3431	41
H(26)	8623	5835	2679	53
H(27)	6195	6390	3187	55
H(28)	6595	5933	3951	42
H(29A)	7436	6787	2259	110
H(30B)	6422	6518	2338	110
H(31C)	7162	6033	2102	110
H(32)	11776	8014	6395	41
H(33)	12880	7957	5807	40
H(34)	12441	7765	4991	34
H(35)	11615	8326	4297	37
H(36)	11434	8056	3473	47
H(37)	9939	6430	3821	43
H(38)	10095	6709	4643	33
H(39A)	10882	7359	2826	106
H(40B)	9923	7010	2928	106
H(41C)	10844	6577	2972	106
H(42)	10612	7313	6837	52

H(43)	9694	7573	7482	65
H(44)	8278	8889	6640	53
H(45)	9206	8647	5991	43
H(46A)	7708	8212	7516	123
H(47B)	8210	8927	7574	123
H(48C)	8600	8283	7866	123
H(49)	7593	10933	5105	47
H(50)	6574	11182	5711	56
H(51)	5883	10315	6133	49
H(52)	6157	9368	6727	54
H(53)	5244	8598	7115	65
H(54)	4621	7698	5829	46
H(55)	5490	8497	5432	40
H(56A)	3694	7464	6581	101
H(57B)	4130	7696	7098	101
H(58C)	4606	7111	6794	101
H(59)	9030	9122	5178	35
H(60)	10218	9065	4649	38
H(61)	8962	10431	3767	48
H(62)	7746	10482	4295	45
H(63A)	10374	9979	3518	66
H(64B)	10669	9260	3739	66
H(65C)	11057	9938	3986	66
H(66)	3500	7640	3769	38
H(67)	2618	6818	4127	43
H(68)	3218	6190	4777	41
H(69)	3752	6321	5652	47
H(70)	4163	5533	6248	54
H(71)	6398	5060	5502	41
H(72)	5972	5834	4902	36
H(73A)	5463	4216	6172	85
H(74B)	5195	4722	6600	85
H(75C)	6217	4710	6412	85
H(76)	5542	8560	4599	36
H(77)	6222	9481	4237	44
H(78)	5554	8730	2910	62
H(79)	4890	7802	3265	54
H(80A)	6368	9764	2942	96
H(81B)	7035	9852	3413	96
H(82C)	6067	10226	3389	96
H(84)	7290(40)	8410(30)	3870(20)	160(20)
H(85)	8300(40)	8500(30)	3968(18)	100(20)
H(1B)	7169	6274	6102	69
H(1C)	8000	6616	6295	69

Table S6. Crystal data and structure refinement for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot 0.5CH_2Cl_2$ **(2)**.

Identification code	$[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot 0.5CH_2Cl_2$ **(2)**.	
Empirical formula	C100.50 H91 Cl Fe2 N2 O10	
Formula weight	1633.90	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 14.353(9) Å	α = 70.78(3)°.
	b = 16.211(9) Å	β = 89.83(3)°.
	c = 19.993(12) Å	γ= 76.08(3)°.
Volume	4249(4) Å^3	
Z	2	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.435 mm^{-1}	
F(000)	1714	
Crystal size	0.20 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.47 to 28.29°	
Index ranges	-18 ≤ h ≤ 17, -20 ≤ k ≤ 11, -26 ≤ l ≤ 25	
Reflections collected	26166	
Independent reflections	18658 [R(int) = 0.0213]	
Completeness to theta = 28.29°	88.3 %	
Absorption correction	Sadabs	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18658 / 0 / 1064	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0578, wR2 = 0.1583	
R indices (all data)	R1 = 0.0918, wR2 = 0.1790	
Largest diff. peak and hole	1.184 and -0.318 eÅ^{-3}	

Table S7. Atomic Coordinates (x 10^4) and Equivalent Isotropic Thermal Parameters (Å^2 x 10^3) for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot 0.5CH_2Cl_2$ **(2)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	7341(1)	9024(1)	7790(1)	20(1)
Fe(2)	7338(1)	10788(1)	7023(1)	23(1)
C(10)	7059(3)	7400(2)	9011(2)	52(1)
C(11)	7084(3)	6414(2)	9360(2)	40(1)
C(12)	7701(3)	5729(3)	9201(3)	64(1)
C(13)	7695(3)	4824(2)	9512(2)	56(1)
C(14)	7030(3)	4613(2)	9984(2)	43(1)
C(15)	6409(4)	5291(3)	10155(3)	63(1)
C(16)	6438(3)	6182(2)	9839(2)	49(1)
C(17)	7505(3)	3058(2)	10112(2)	51(1)
C(20)	7092(3)	12757(3)	6077(3)	57(1)
C(21)	7460(3)	13572(2)	5719(2)	47(1)
C(22)	7468(4)	13910(3)	4992(3)	64(1)
C(23)	7833(4)	14639(3)	4671(3)	77(2)
C(24)	8203(4)	15054(3)	5072(3)	61(1)
C(25)	8190(3)	14742(3)	5796(2)	55(1)
C(26)	7810(3)	14008(3)	6104(2)	54(1)
C(27)	9119(6)	16087(4)	5136(4)	109(3)
C(100)	7708(2)	10197(2)	8574(2)	23(1)
C(101)	7953(2)	10365(2)	9243(2)	26(1)
C(102)	7604(2)	9925(2)	9885(2)	30(1)
C(103)	7861(3)	10064(3)	10505(2)	40(1)
C(104)	8465(3)	10614(3)	10496(2)	47(1)
C(105)	8802(3)	11050(3)	9868(2)	43(1)
C(106)	8554(2)	10944(2)	9232(2)	33(1)
C(107)	6892(2)	9370(2)	9951(2)	29(1)
C(108)	6982(3)	8583(2)	10531(2)	37(1)
C(109)	6263(3)	8126(2)	10646(2)	39(1)
C(110)	5436(3)	8431(2)	10184(2)	35(1)
C(111)	5366(2)	9201(2)	9590(2)	32(1)
C(112)	6073(2)	9660(2)	9481(2)	29(1)
C(113)	4634(3)	7958(3)	10325(2)	42(1)
C(114)	8970(2)	11429(2)	8586(2)	33(1)
C(115)	8917(3)	12344(3)	8411(2)	55(1)
C(116)	9337(4)	12796(3)	7823(3)	64(1)
C(117)	9813(3)	12361(3)	7389(2)	45(1)
C(118)	9874(2)	11447(2)	7571(2)	35(1)
C(119)	9470(2)	10998(2)	8156(2)	30(1)
C(120)	10245(3)	12859(3)	6734(3)	66(1)
C(200)	5512(2)	10428(2)	7495(2)	24(1)
C(201)	4442(2)	10691(2)	7551(2)	25(1)
C(202)	3909(2)	10041(2)	7699(2)	27(1)
C(203)	2909(2)	10309(2)	7716(2)	32(1)

C(204)	2453(2)	11199(3)	7606(2)	38(1)
C(205)	3973(2)	11601(2)	7449(2)	31(1)
C(206)	2977(2)	11835(2)	7476(2)	38(1)
C(207)	4313(2)	9058(2)	7816(2)	26(1)
C(208)	4894(2)	8756(2)	7353(2)	30(1)
C(209)	5195(2)	7844(3)	7450(2)	37(1)
C(210)	4937(3)	7203(2)	8024(2)	39(1)
C(211)	4366(2)	7508(2)	8494(2)	36(1)
C(212)	4049(2)	8420(2)	8391(2)	30(1)
C(213)	5273(3)	6210(3)	8129(3)	58(1)
C(214)	4477(2)	12326(2)	7356(2)	32(1)
C(215)	5262(2)	12208(2)	7819(2)	34(1)
C(216)	5682(3)	12907(2)	7760(2)	41(1)
C(217)	5329(3)	13754(3)	7243(2)	47(1)
C(218)	4555(3)	13870(3)	6787(2)	52(1)
C(219)	4131(3)	13169(2)	6835(2)	44(1)
C(220)	5778(4)	14520(3)	7190(3)	73(2)
C(300)	7003(2)	9616(2)	6234(2)	26(1)
C(301)	6873(2)	9472(2)	5536(2)	31(1)
C(302)	7170(2)	8604(3)	5498(2)	35(1)
C(303)	7102(3)	8478(3)	4844(2)	45(1)
C(304)	6748(3)	9197(3)	4237(2)	52(1)
C(305)	6432(3)	10054(3)	4272(2)	48(1)
C(306)	6474(2)	10217(3)	4915(2)	37(1)
C(307)	6045(2)	11150(3)	4905(2)	38(1)
C(308)	5423(2)	11322(3)	5400(2)	41(1)
C(309)	4982(3)	12191(3)	5362(2)	47(1)
C(310)	5135(3)	12932(3)	4824(2)	51(1)
C(311)	5758(3)	12759(3)	4325(2)	53(1)
C(312)	6204(3)	11897(3)	4363(2)	45(1)
C(313)	4667(4)	13865(3)	4796(3)	74(2)
C(314)	7602(3)	7779(2)	6115(2)	39(1)
C(315)	7166(4)	7059(3)	6320(2)	60(1)
C(316)	7647(5)	6253(3)	6887(3)	78(2)
C(317)	8534(5)	6155(3)	7208(3)	70(2)
C(318)	9029(6)	5271(3)	7767(3)	116(3)
C(319)	8920(4)	6872(3)	6999(2)	65(1)
C(320)	8473(3)	7668(3)	6470(2)	46(1)
C(400)	9187(2)	9299(2)	7339(1)	23(1)
C(401)	10258(2)	8969(2)	7308(2)	24(1)
C(402)	10792(2)	8206(2)	7865(2)	27(1)
C(403)	11778(2)	7905(2)	7832(2)	32(1)
C(404)	12239(2)	8341(2)	7268(2)	34(1)
C(405)	11712(2)	9086(2)	6725(2)	30(1)
C(406)	10722(2)	9408(2)	6733(2)	26(1)
C(407)	10220(2)	10186(2)	6100(2)	26(1)
C(408)	9383(2)	10194(2)	5747(2)	26(1)
C(409)	8968(2)	10897(2)	5138(2)	31(1)
C(410)	9371(2)	11620(2)	4847(2)	33(1)

C(411)	10211(3)	11613(2)	5198(2)	38(1)
C(412)	10631(2)	10913(2)	5815(2)	34(1)
C(413)	8945(3)	12366(3)	4164(2)	46(1)
C(414)	10361(2)	7732(2)	8515(2)	28(1)
C(415)	9880(2)	8190(2)	8933(2)	30(1)
C(416)	9523(2)	7748(2)	9555(2)	37(1)
C(417)	9649(3)	6824(3)	9779(2)	50(1)
C(418)	10136(3)	6363(3)	9359(2)	57(1)
C(419)	10491(3)	6804(2)	8739(2)	44(1)
C(420)	9269(4)	6337(3)	10469(3)	74(2)
C(1S)	7229(9)	5425(7)	2032(5)	83(4)
Cl(1)	8138(2)	5800(2)	2267(2)	107(1)
Cl(2)	7226(3)	4317(2)	2500(3)	126(1)
N(1)	7413(3)	7653(2)	8332(2)	53(1)
N(2)	7818(2)	11931(2)	6425(2)	39(1)
O(1)	7831(1)	9391(1)	8615(1)	24(1)
O(2)	7399(1)	10872(1)	8022(1)	26(1)
O(3)	5988(1)	9683(1)	7927(1)	25(1)
O(4)	5863(1)	10966(1)	7020(1)	27(1)
O(5)	6820(2)	9059(2)	6788(1)	28(1)
O(6)	7305(2)	10296(2)	6211(1)	28(1)
O(7)	8711(1)	8710(1)	7504(1)	24(1)
O(8)	8846(1)	10128(1)	7205(1)	24(1)
O(9)	8578(4)	15758(2)	4711(2)	103(2)
O(10)	6938(2)	3760(2)	10320(2)	63(1)

Table S8. Interatomic distances [Å] and angles [Deg] for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot 0.5CH_2Cl_2$ **(2)**.

Fe(1)-O(7)	2.039(2)
Fe(1)-O(3)	2.044(2)
Fe(1)-O(1)	2.102(2)
Fe(1)-N(1)	2.105(3)
Fe(1)-O(5)	2.120(2)
Fe(1)-Fe(2)	2.7638(17)
Fe(2)-O(6)	2.036(2)
Fe(2)-O(2)	2.049(2)
Fe(2)-O(4)	2.067(2)
Fe(2)-N(2)	2.119(3)
Fe(2)-O(8)	2.143(2)
C(10)-N(1)	1.413(5)
C(10)-C(11)	1.510(5)
C(11)-C(16)	1.358(5)
C(11)-C(12)	1.369(5)
C(12)-C(13)	1.395(5)
C(13)-C(14)	1.362(5)
C(14)-O(10)	1.363(4)
C(14)-C(15)	1.378(6)
C(15)-C(16)	1.383(5)
C(17)-O(10)	1.412(5)
C(20)-N(2)	1.443(5)
C(20)-C(21)	1.500(5)
C(21)-C(26)	1.370(6)
C(21)-C(22)	1.375(6)
C(22)-C(23)	1.371(6)
C(23)-C(24)	1.382(7)
C(24)-O(9)	1.365(5)
C(24)-C(25)	1.368(6)
C(25)-C(26)	1.386(6)
C(27)-O(9)	1.452(8)
C(100)-O(1)	1.251(4)
C(100)-O(2)	1.260(3)
C(100)-C(101)	1.509(4)
C(101)-C(102)	1.405(4)
C(101)-C(106)	1.414(5)
C(102)-C(103)	1.397(5)
C(102)-C(107)	1.493(5)
C(103)-C(104)	1.381(5)
C(104)-C(105)	1.372(5)
C(105)-C(106)	1.395(5)
C(106)-C(114)	1.482(5)
C(107)-C(112)	1.391(5)
C(107)-C(108)	1.392(5)
C(108)-C(109)	1.385(5)
C(109)-C(110)	1.390(5)

C(110)-C(111)	1.393(5)
C(110)-C(113)	1.509(5)
C(111)-C(112)	1.373(5)
C(114)-C(119)	1.375(5)
C(114)-C(115)	1.392(5)
C(115)-C(116)	1.386(6)
C(116)-C(117)	1.374(6)
C(117)-C(118)	1.385(5)
C(117)-C(120)	1.512(5)
C(118)-C(119)	1.369(5)
C(200)-O(4)	1.257(3)
C(200)-O(3)	1.261(3)
C(200)-C(201)	1.505(4)
C(201)-C(202)	1.403(4)
C(201)-C(205)	1.412(4)
C(202)-C(203)	1.399(4)
C(202)-C(207)	1.497(5)
C(203)-C(204)	1.376(5)
C(204)-C(206)	1.377(5)
C(205)-C(206)	1.394(5)
C(205)-C(214)	1.485(5)
C(207)-C(208)	1.374(4)
C(207)-C(212)	1.392(4)
C(208)-C(209)	1.383(5)
C(209)-C(210)	1.390(5)
C(210)-C(211)	1.381(5)
C(210)-C(213)	1.508(5)
C(211)-C(212)	1.383(5)
C(214)-C(219)	1.392(5)
C(214)-C(215)	1.395(5)
C(215)-C(216)	1.378(5)
C(216)-C(217)	1.395(5)
C(217)-C(218)	1.376(6)
C(217)-C(220)	1.506(6)
C(218)-C(219)	1.389(6)
C(300)-O(5)	1.251(4)
C(300)-O(6)	1.267(4)
C(300)-C(301)	1.507(4)
C(301)-C(302)	1.396(5)
C(301)-C(306)	1.419(5)
C(302)-C(303)	1.396(5)
C(302)-C(314)	1.488(5)
C(303)-C(304)	1.369(6)
C(304)-C(305)	1.378(6)
C(305)-C(306)	1.400(5)
C(306)-C(307)	1.483(6)
C(307)-C(308)	1.382(5)
C(307)-C(312)	1.400(5)
C(308)-C(309)	1.375(6)

C(309)-C(310)	1.388(5)
C(310)-C(311)	1.389(6)
C(310)-C(313)	1.483(6)
C(311)-C(312)	1.367(6)
C(314)-C(320)	1.383(6)
C(314)-C(315)	1.398(5)
C(315)-C(316)	1.436(7)
C(316)-C(317)	1.379(8)
C(317)-C(319)	1.349(7)
C(317)-C(318)	1.506(7)
C(319)-C(320)	1.379(5)
C(400)-O(8)	1.250(4)
C(400)-O(7)	1.262(4)
C(400)-C(401)	1.509(4)
C(401)-C(406)	1.399(4)
C(401)-C(402)	1.415(4)
C(402)-C(403)	1.390(4)
C(402)-C(414)	1.494(4)
C(403)-C(404)	1.379(5)
C(404)-C(405)	1.383(5)
C(405)-C(406)	1.394(4)
C(406)-C(407)	1.492(4)
C(407)-C(408)	1.391(4)
C(407)-C(412)	1.396(4)
C(408)-C(409)	1.379(4)
C(409)-C(410)	1.387(5)
C(410)-C(411)	1.391(5)
C(410)-C(413)	1.505(5)
C(411)-C(412)	1.388(5)
C(414)-C(415)	1.372(5)
C(414)-C(419)	1.386(5)
C(415)-C(416)	1.381(5)
C(416)-C(417)	1.380(5)
C(417)-C(418)	1.381(6)
C(417)-C(420)	1.521(5)
C(418)-C(419)	1.378(5)
C(1S)-Cl(1)	1.693(13)
C(1S)-Cl(2)	1.733(12)
O(7)-Fe(1)-O(3)	164.59(8)
O(7)-Fe(1)-O(1)	90.63(9)
O(3)-Fe(1)-O(1)	86.72(9)
O(7)-Fe(1)-N(1)	91.45(13)
O(3)-Fe(1)-N(1)	103.96(13)
O(1)-Fe(1)-N(1)	100.63(12)
O(7)-Fe(1)-O(5)	88.93(9)
O(3)-Fe(1)-O(5)	89.22(9)
O(1)-Fe(1)-O(5)	163.08(8)
N(1)-Fe(1)-O(5)	96.30(12)

O(7)-Fe(1)-Fe(2)	85.15(7)
O(3)-Fe(1)-Fe(2)	79.45(7)
O(1)-Fe(1)-Fe(2)	81.07(7)
N(1)-Fe(1)-Fe(2)	176.22(10)
O(5)-Fe(1)-Fe(2)	82.04(7)
O(6)-Fe(2)-O(2)	162.11(9)
O(6)-Fe(2)-O(4)	88.06(9)
O(2)-Fe(2)-O(4)	90.59(9)
O(6)-Fe(2)-N(2)	95.36(11)
O(2)-Fe(2)-N(2)	101.23(11)
O(4)-Fe(2)-N(2)	116.05(11)
O(6)-Fe(2)-O(8)	87.06(9)
O(2)-Fe(2)-O(8)	88.14(9)
O(4)-Fe(2)-O(8)	159.96(8)
N(2)-Fe(2)-O(8)	83.77(11)
O(6)-Fe(2)-Fe(1)	80.28(7)
O(2)-Fe(2)-Fe(1)	81.87(7)
O(4)-Fe(2)-Fe(1)	82.38(7)
N(2)-Fe(2)-Fe(1)	161.07(8)
O(8)-Fe(2)-Fe(1)	77.64(7)
N(1)-C(10)-C(11)	116.9(3)
C(16)-C(11)-C(12)	117.1(3)
C(16)-C(11)-C(10)	119.1(3)
C(12)-C(11)-C(10)	123.7(3)
C(11)-C(12)-C(13)	123.0(4)
C(14)-C(13)-C(12)	118.5(4)
C(13)-C(14)-O(10)	124.6(3)
C(13)-C(14)-C(15)	119.3(3)
O(10)-C(14)-C(15)	116.1(3)
C(14)-C(15)-C(16)	120.7(4)
C(11)-C(16)-C(15)	121.4(4)
N(2)-C(20)-C(21)	115.7(3)
C(26)-C(21)-C(22)	117.2(4)
C(26)-C(21)-C(20)	121.2(4)
C(22)-C(21)-C(20)	121.5(4)
C(23)-C(22)-C(21)	121.1(5)
C(22)-C(23)-C(24)	120.6(5)
O(9)-C(24)-C(25)	123.7(5)
O(9)-C(24)-C(23)	116.8(4)
C(25)-C(24)-C(23)	119.5(4)
C(24)-C(25)-C(26)	118.5(4)
C(21)-C(26)-C(25)	123.0(4)
O(1)-C(100)-O(2)	125.2(3)
O(1)-C(100)-C(101)	116.9(3)
O(2)-C(100)-C(101)	117.9(3)
C(102)-C(101)-C(106)	119.8(3)
C(102)-C(101)-C(100)	119.8(3)
C(106)-C(101)-C(100)	120.4(3)
C(103)-C(102)-C(101)	119.2(3)

C(103)-C(102)-C(107)	116.0(3)
C(101)-C(102)-C(107)	124.6(3)
C(104)-C(103)-C(102)	120.9(3)
C(105)-C(104)-C(103)	120.0(3)
C(104)-C(105)-C(106)	121.3(3)
C(105)-C(106)-C(101)	118.8(3)
C(105)-C(106)-C(114)	117.3(3)
C(101)-C(106)-C(114)	123.9(3)
C(112)-C(107)-C(108)	117.5(3)
C(112)-C(107)-C(102)	121.8(3)
C(108)-C(107)-C(102)	120.4(3)
C(109)-C(108)-C(107)	120.9(3)
C(108)-C(109)-C(110)	121.2(3)
C(109)-C(110)-C(111)	117.6(3)
C(109)-C(110)-C(113)	121.4(3)
C(111)-C(110)-C(113)	121.0(3)
C(112)-C(111)-C(110)	121.1(3)
C(111)-C(112)-C(107)	121.6(3)
C(119)-C(114)-C(115)	116.8(3)
C(119)-C(114)-C(106)	122.5(3)
C(115)-C(114)-C(106)	120.6(3)
C(116)-C(115)-C(114)	121.0(4)
C(117)-C(116)-C(115)	121.5(4)
C(116)-C(117)-C(118)	117.2(3)
C(116)-C(117)-C(120)	121.6(4)
C(118)-C(117)-C(120)	121.2(4)
C(119)-C(118)-C(117)	121.4(3)
C(118)-C(119)-C(114)	122.1(3)
O(4)-C(200)-O(3)	124.8(3)
O(4)-C(200)-C(201)	117.6(3)
O(3)-C(200)-C(201)	117.6(3)
C(202)-C(201)-C(205)	119.9(3)
C(202)-C(201)-C(200)	120.5(3)
C(205)-C(201)-C(200)	119.7(3)
C(203)-C(202)-C(201)	119.3(3)
C(203)-C(202)-C(207)	115.2(3)
C(201)-C(202)-C(207)	125.4(3)
C(204)-C(203)-C(202)	120.6(3)
C(203)-C(204)-C(206)	120.1(3)
C(206)-C(205)-C(201)	118.7(3)
C(206)-C(205)-C(214)	116.9(3)
C(201)-C(205)-C(214)	124.3(3)
C(204)-C(206)-C(205)	121.3(3)
C(208)-C(207)-C(212)	118.3(3)
C(208)-C(207)-C(202)	122.5(3)
C(212)-C(207)-C(202)	119.1(3)
C(207)-C(208)-C(209)	120.8(3)
C(208)-C(209)-C(210)	121.4(3)
C(211)-C(210)-C(209)	117.6(3)

C(211)-C(210)-C(213)	121.4(3)
C(209)-C(210)-C(213)	121.0(4)
C(210)-C(211)-C(212)	121.2(3)
C(211)-C(212)-C(207)	120.8(3)
C(219)-C(214)-C(215)	118.1(3)
C(219)-C(214)-C(205)	120.5(3)
C(215)-C(214)-C(205)	121.2(3)
C(216)-C(215)-C(214)	120.8(3)
C(215)-C(216)-C(217)	121.1(4)
C(218)-C(217)-C(216)	118.0(4)
C(218)-C(217)-C(220)	121.1(4)
C(216)-C(217)-C(220)	120.8(4)
C(217)-C(218)-C(219)	121.6(4)
C(218)-C(219)-C(214)	120.4(4)
O(5)-C(300)-O(6)	124.9(3)
O(5)-C(300)-C(301)	118.5(3)
O(6)-C(300)-C(301)	116.6(3)
C(302)-C(301)-C(306)	119.9(3)
C(302)-C(301)-C(300)	119.8(3)
C(306)-C(301)-C(300)	120.3(3)
C(301)-C(302)-C(303)	119.7(3)
C(301)-C(302)-C(314)	124.2(3)
C(303)-C(302)-C(314)	116.0(3)
C(304)-C(303)-C(302)	120.7(4)
C(303)-C(304)-C(305)	120.0(3)
C(304)-C(305)-C(306)	121.6(4)
C(305)-C(306)-C(301)	117.9(4)
C(305)-C(306)-C(307)	117.4(3)
C(301)-C(306)-C(307)	124.6(3)
C(308)-C(307)-C(312)	117.2(4)
C(308)-C(307)-C(306)	121.6(3)
C(312)-C(307)-C(306)	121.1(3)
C(309)-C(308)-C(307)	121.4(3)
C(308)-C(309)-C(310)	121.5(4)
C(309)-C(310)-C(311)	117.1(4)
C(309)-C(310)-C(313)	121.0(4)
C(311)-C(310)-C(313)	121.9(4)
C(312)-C(311)-C(310)	121.6(4)
C(311)-C(312)-C(307)	121.2(4)
C(320)-C(314)-C(315)	117.8(4)
C(320)-C(314)-C(302)	121.8(3)
C(315)-C(314)-C(302)	120.3(4)
C(314)-C(315)-C(316)	118.2(5)
C(317)-C(316)-C(315)	122.2(4)
C(319)-C(317)-C(316)	117.3(5)
C(319)-C(317)-C(318)	123.0(6)
C(316)-C(317)-C(318)	119.7(5)
C(317)-C(319)-C(320)	122.4(5)
C(319)-C(320)-C(314)	122.0(4)

O(8)-C(400)-O(7)	125.4(3)
O(8)-C(400)-C(401)	117.7(3)
O(7)-C(400)-C(401)	116.9(3)
C(406)-C(401)-C(402)	120.0(3)
C(406)-C(401)-C(400)	120.6(3)
C(402)-C(401)-C(400)	119.5(3)
C(403)-C(402)-C(401)	119.1(3)
C(403)-C(402)-C(414)	117.6(3)
C(401)-C(402)-C(414)	123.1(3)
C(404)-C(403)-C(402)	121.1(3)
C(403)-C(404)-C(405)	119.5(3)
C(404)-C(405)-C(406)	121.5(3)
C(405)-C(406)-C(401)	118.9(3)
C(405)-C(406)-C(407)	116.7(3)
C(401)-C(406)-C(407)	124.4(3)
C(408)-C(407)-C(412)	117.7(3)
C(408)-C(407)-C(406)	122.5(3)
C(412)-C(407)-C(406)	119.7(3)
C(409)-C(408)-C(407)	121.3(3)
C(408)-C(409)-C(410)	121.5(3)
C(409)-C(410)-C(411)	117.4(3)
C(409)-C(410)-C(413)	121.6(3)
C(411)-C(410)-C(413)	121.0(3)
C(412)-C(411)-C(410)	121.6(3)
C(411)-C(412)-C(407)	120.5(3)
C(415)-C(414)-C(419)	118.1(3)
C(415)-C(414)-C(402)	121.2(3)
C(419)-C(414)-C(402)	120.5(3)
C(414)-C(415)-C(416)	121.5(3)
C(417)-C(416)-C(415)	120.6(3)
C(416)-C(417)-C(418)	117.9(3)
C(416)-C(417)-C(420)	120.5(4)
C(418)-C(417)-C(420)	121.6(4)
C(419)-C(418)-C(417)	121.5(4)
C(418)-C(419)-C(414)	120.4(4)
Cl(1)-C(1S)-Cl(2)	116.4(6)
C(10)-N(1)-Fe(1)	119.2(2)
C(20)-N(2)-Fe(2)	117.3(2)
C(100)-O(1)-Fe(1)	122.37(19)
C(100)-O(2)-Fe(2)	123.32(19)
C(200)-O(3)-Fe(1)	124.31(19)
C(200)-O(4)-Fe(2)	120.20(19)
C(300)-O(5)-Fe(1)	119.4(2)
C(300)-O(6)-Fe(2)	125.66(19)
C(400)-O(7)-Fe(1)	119.99(19)
C(400)-O(8)-Fe(2)	124.49(19)
C(24)-O(9)-C(27)	116.6(4)
C(14)-O(10)-C(17)	117.6(3)

Table S9. Anisotropic Thermal Parameters ($Å^2$x 10^3) for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot$-$0.5CH_2Cl_2$ **(2)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U11	U22	U33	U23	U13	U12
Fe(1)	20(1)	19(1)	19(1)	-2(1)	2(1)	-6(1)
Fe(2)	23(1)	22(1)	21(1)	-1(1)	3(1)	-8(1)
C(10)	80(3)	28(2)	43(2)	-5(2)	23(2)	-18(2)
C(11)	51(2)	25(2)	36(2)	0(2)	9(2)	-8(2)
C(12)	72(3)	31(2)	80(3)	-6(2)	46(3)	-16(2)
C(13)	58(3)	24(2)	73(3)	-3(2)	30(2)	-7(2)
C(14)	51(2)	25(2)	45(2)	0(2)	14(2)	-12(2)
C(15)	77(3)	40(2)	75(3)	-20(2)	44(3)	-23(2)
C(16)	61(3)	29(2)	56(2)	-12(2)	23(2)	-11(2)
C(17)	63(3)	24(2)	59(3)	-5(2)	17(2)	-12(2)
C(20)	40(2)	31(2)	78(3)	11(2)	-2(2)	-7(2)
C(21)	43(2)	24(2)	59(2)	3(2)	6(2)	-5(2)
C(22)	85(3)	45(2)	61(3)	-11(2)	11(2)	-23(2)
C(23)	125(5)	48(3)	51(3)	-3(2)	21(3)	-33(3)
C(24)	88(3)	26(2)	66(3)	-7(2)	35(3)	-19(2)
C(25)	66(3)	35(2)	62(3)	-14(2)	20(2)	-12(2)
C(26)	54(2)	45(2)	48(2)	2(2)	13(2)	-14(2)
C(27)	179(7)	71(4)	124(5)	-57(4)	87(5)	-86(5)
C(100)	17(1)	25(2)	26(2)	-7(1)	3(1)	-5(1)
C(101)	26(2)	26(2)	24(1)	-10(1)	-2(1)	-1(1)
C(102)	33(2)	31(2)	25(2)	-9(1)	0(1)	-5(1)
C(103)	47(2)	45(2)	25(2)	-12(2)	0(2)	-10(2)
C(104)	57(2)	56(2)	35(2)	-23(2)	-2(2)	-17(2)
C(105)	49(2)	46(2)	42(2)	-22(2)	-1(2)	-19(2)
C(106)	35(2)	30(2)	33(2)	-12(1)	-1(1)	-5(1)
C(107)	32(2)	32(2)	23(2)	-11(1)	4(1)	-5(1)
C(108)	39(2)	40(2)	25(2)	-6(2)	0(1)	-6(2)
C(109)	48(2)	35(2)	27(2)	-2(2)	6(2)	-10(2)
C(110)	41(2)	39(2)	26(2)	-13(2)	11(1)	-13(2)
C(111)	34(2)	36(2)	25(2)	-10(1)	4(1)	-6(1)
C(112)	34(2)	29(2)	21(1)	-8(1)	4(1)	-3(1)
C(113)	45(2)	46(2)	36(2)	-12(2)	10(2)	-18(2)
C(114)	31(2)	30(2)	40(2)	-12(2)	-2(1)	-9(1)
C(115)	66(3)	37(2)	71(3)	-27(2)	21(2)	-19(2)
C(116)	77(3)	26(2)	87(3)	-12(2)	23(3)	-20(2)
C(117)	36(2)	34(2)	54(2)	-1(2)	3(2)	-10(2)
C(118)	25(2)	37(2)	42(2)	-11(2)	1(1)	-12(1)
C(119)	25(2)	27(2)	36(2)	-8(1)	-3(1)	-10(1)
C(120)	52(3)	43(2)	81(3)	8(2)	19(2)	-13(2)
C(200)	23(1)	27(2)	22(1)	-7(1)	1(1)	-8(1)
C(201)	21(1)	29(2)	18(1)	-2(1)	1(1)	-4(1)
C(202)	24(2)	35(2)	18(1)	-2(1)	1(1)	-7(1)

C(203)	25(2)	42(2)	26(2)	-4(1)	1(1)	-11(1)
C(204)	20(2)	50(2)	36(2)	-6(2)	3(1)	-4(2)
C(205)	28(2)	32(2)	23(2)	-1(1)	4(1)	-4(1)
C(206)	28(2)	37(2)	34(2)	-3(2)	2(1)	4(1)
C(207)	22(1)	32(2)	22(1)	-5(1)	-2(1)	-12(1)
C(208)	24(2)	42(2)	26(2)	-9(1)	0(1)	-14(1)
C(209)	29(2)	48(2)	41(2)	-21(2)	5(1)	-15(2)
C(210)	35(2)	36(2)	48(2)	-15(2)	-4(2)	-14(2)
C(211)	35(2)	36(2)	36(2)	-3(2)	2(1)	-17(2)
C(212)	27(2)	34(2)	28(2)	-6(1)	4(1)	-12(1)
C(213)	66(3)	40(2)	75(3)	-26(2)	5(2)	-15(2)
C(214)	34(2)	26(2)	30(2)	-6(1)	8(1)	-3(1)
C(215)	33(2)	29(2)	34(2)	-7(1)	5(1)	-4(1)
C(216)	47(2)	40(2)	40(2)	-17(2)	10(2)	-16(2)
C(217)	65(3)	34(2)	50(2)	-17(2)	20(2)	-21(2)
C(218)	67(3)	26(2)	51(2)	-3(2)	7(2)	-7(2)
C(219)	48(2)	31(2)	40(2)	-1(2)	3(2)	-2(2)
C(220)	104(4)	48(3)	79(3)	-25(3)	25(3)	-38(3)
C(300)	20(1)	35(2)	22(1)	-7(1)	1(1)	-10(1)
C(301)	26(2)	51(2)	20(1)	-8(1)	4(1)	-22(2)
C(302)	36(2)	56(2)	25(2)	-17(2)	8(1)	-28(2)
C(303)	45(2)	72(3)	34(2)	-27(2)	12(2)	-34(2)
C(304)	51(2)	96(4)	26(2)	-26(2)	9(2)	-44(2)
C(305)	39(2)	85(3)	21(2)	-6(2)	0(1)	-35(2)
C(306)	26(2)	61(2)	24(2)	-5(2)	3(1)	-26(2)
C(307)	24(2)	57(2)	23(2)	3(2)	-4(1)	-14(2)
C(308)	25(2)	57(2)	28(2)	5(2)	-3(1)	-13(2)
C(309)	31(2)	65(3)	32(2)	-2(2)	0(2)	-8(2)
C(310)	40(2)	56(2)	39(2)	3(2)	-6(2)	-3(2)
C(311)	44(2)	62(3)	34(2)	10(2)	0(2)	-14(2)
C(312)	35(2)	61(3)	27(2)	4(2)	3(1)	-13(2)
C(313)	73(3)	57(3)	59(3)	5(2)	11(2)	5(3)
C(314)	61(2)	39(2)	30(2)	-20(2)	17(2)	-26(2)
C(315)	84(3)	62(3)	63(3)	-41(2)	43(2)	-46(3)
C(316)	135(5)	34(2)	89(4)	-34(3)	76(4)	-47(3)
C(317)	116(5)	39(2)	56(3)	-19(2)	25(3)	-15(3)
C(318)	204(8)	36(3)	81(4)	-10(3)	44(5)	4(4)
C(319)	105(4)	33(2)	48(2)	-13(2)	-5(2)	0(2)
C(320)	71(3)	33(2)	37(2)	-15(2)	-4(2)	-12(2)
C(400)	22(1)	28(2)	18(1)	-8(1)	2(1)	-8(1)
C(401)	20(1)	26(2)	27(2)	-11(1)	2(1)	-7(1)
C(402)	23(2)	29(2)	28(2)	-10(1)	0(1)	-5(1)
C(403)	24(2)	35(2)	34(2)	-11(2)	-1(1)	-3(1)
C(404)	18(2)	45(2)	38(2)	-17(2)	0(1)	-3(1)
C(405)	24(2)	38(2)	31(2)	-12(1)	6(1)	-12(1)
C(406)	23(2)	31(2)	28(2)	-13(1)	3(1)	-9(1)
C(407)	25(2)	28(2)	27(2)	-9(1)	7(1)	-8(1)
C(408)	23(2)	28(2)	28(2)	-9(1)	7(1)	-8(1)
C(409)	26(2)	36(2)	29(2)	-11(1)	4(1)	-6(1)

C(410)	39(2)	29(2)	28(2)	-7(1)	5(1)	-5(1)
C(411)	47(2)	30(2)	39(2)	-9(2)	10(2)	-19(2)
C(412)	34(2)	35(2)	34(2)	-11(2)	3(1)	-14(2)
C(413)	55(2)	37(2)	38(2)	-1(2)	0(2)	-12(2)
C(414)	22(2)	25(2)	32(2)	-4(1)	-2(1)	-5(1)
C(415)	28(2)	25(2)	30(2)	-1(1)	-3(1)	-4(1)
C(416)	34(2)	35(2)	33(2)	-3(2)	2(1)	-2(2)
C(417)	52(2)	37(2)	44(2)	7(2)	8(2)	-8(2)
C(418)	68(3)	23(2)	66(3)	3(2)	19(2)	-8(2)
C(419)	46(2)	27(2)	55(2)	-10(2)	10(2)	-5(2)
C(420)	81(3)	53(3)	60(3)	15(2)	26(3)	-11(3)
C(1S)	113(9)	67(6)	38(5)	-13(5)	8(5)	28(6)
Cl(1)	79(2)	103(2)	149(3)	-56(2)	47(2)	-22(2)
Cl(2)	120(3)	74(2)	196(4)	-67(3)	9(3)	-16(2)
N(1)	87(3)	31(2)	40(2)	-6(1)	11(2)	-21(2)
N(2)	37(2)	27(1)	44(2)	-2(1)	5(1)	-9(1)
O(1)	25(1)	25(1)	25(1)	-9(1)	1(1)	-6(1)
O(2)	25(1)	24(1)	25(1)	-4(1)	1(1)	-4(1)
O(3)	22(1)	25(1)	23(1)	-4(1)	-1(1)	-5(1)
O(4)	23(1)	28(1)	25(1)	-2(1)	4(1)	-8(1)
O(5)	27(1)	35(1)	20(1)	-4(1)	4(1)	-13(1)
O(6)	26(1)	35(1)	21(1)	-5(1)	2(1)	-12(1)
O(7)	21(1)	25(1)	28(1)	-9(1)	4(1)	-7(1)
O(8)	24(1)	21(1)	25(1)	-5(1)	1(1)	-3(1)
O(9)	183(5)	53(2)	91(3)	-21(2)	68(3)	-70(3)
O(10)	81(2)	26(1)	76(2)	-7(1)	44(2)	-20(1)

Table S10. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal parameters (Å^2 x 10^3) for $[Fe_2(\mu\text{-}O_2CAr^{Tol})_4(BA^{p\text{-}OMe})_2]\cdot 0.5CH_2Cl_2$ **(2)**.

	x	y	z	U(eq)
H(10A)	6383	7756	8970	62
H(10B)	7435	7575	9332	62
H(12)	8155	5878	8864	76
H(13)	8144	4365	9397	67
H(15)	5957	5146	10494	75
H(16)	5996	6641	9959	59
H(17A)	7350	3181	9606	77
H(17B)	7370	2483	10391	77
H(17C)	8188	3022	10195	77
H(20A)	6657	12889	6434	69
H(20B)	6703	12656	5717	69
H(22)	7217	13632	4708	77
H(23)	7830	14861	4168	92
H(25)	8436	15022	6081	66
H(26)	7790	13798	6606	64
H(27A)	8682	16365	5424	163
H(27B)	9420	16536	4822	163
H(27C)	9618	15581	5449	163
H(103)	7618	9776	10939	47
H(104)	8648	10690	10923	56
H(105)	9211	11432	9867	51
H(108)	7543	8357	10852	44
H(109)	6338	7594	11049	47
H(111)	4819	9412	9256	39
H(112)	6001	10188	9075	35
H(11A)	4817	7425	10756	62
H(11B)	4517	7771	9921	62
H(11C)	4046	8371	10389	62
H(115)	8589	12665	8700	66
H(116)	9294	13420	7719	77
H(118)	10202	11125	7283	42
H(119)	9536	10368	8269	35
H(12A)	9741	13168	6342	99
H(12B)	10748	12427	6601	99
H(12C)	10526	13304	6836	99
H(203)	2543	9874	7804	39
H(204)	1774	11374	7620	46
H(206)	2654	12447	7402	45
H(208)	5092	9179	6961	36
H(209)	5586	7653	7118	44
H(211)	4187	7084	8896	44
H(212)	3647	8615	8717	36
H(21A)	5587	5883	8610	88

H(21B)	5732	6120	7780	88
H(21C)	4719	5981	8065	88
H(215)	5510	11639	8179	40
H(216)	6220	12810	8078	49
H(218)	4304	14442	6432	62
H(219)	3601	13266	6511	52
H(22A)	6167	14618	6781	109
H(22B)	6190	14370	7626	109
H(22C)	5270	15071	7130	109
H(303)	7303	7887	4819	54
H(304)	6719	9106	3793	62
H(305)	6180	10546	3848	57
H(308)	5298	10830	5773	49
H(309)	4564	12285	5714	56
H(311)	5877	13252	3949	64
H(312)	6629	11803	4015	55
H(31A)	5094	14258	4597	110
H(31B)	4537	13867	5277	110
H(31C)	4059	14088	4496	110
H(315)	6569	7103	6091	72
H(316)	7342	5771	7045	94
H(31D)	9535	4931	7558	174
H(31E)	8558	4919	7946	174
H(31F)	9317	5388	8159	174
H(319)	9521	6827	7224	78
H(320)	8773	8154	6346	56
H(403)	12140	7391	8203	39
H(404)	12914	8130	7253	41
H(405)	12033	9384	6338	36
H(408)	9092	9706	5929	31
H(409)	8391	10886	4912	37
H(411)	10504	12099	5010	45
H(412)	11202	10928	6044	40
H(41A)	9217	12203	3761	70
H(41B)	9095	12926	4160	70
H(41C)	8244	12456	4124	70
H(415)	9791	8826	8791	36
H(416)	9189	8083	9832	45
H(418)	10228	5727	9502	69
H(419)	10828	6470	8462	53
H(42A)	9807	6013	10834	111
H(42B)	8943	5906	10393	111
H(42C)	8813	6778	10626	111
H(1S1)	7250	5496	1521	100
H(1S2)	6611	5822	2085	100
H(1A)	7085	7457	8044	64
H(1B)	8048	7338	8379	64
H(2A)	8218	12046	6724	46

H(2B) 8184 11783 6083 46Figures

Figure S1. ORTEP drawings of [Fe_2(μ-O_2CAr^{Tol})$_4$(BA)$_2$] (**1**) showing 50% probability thermal ellipsoids. Front view (top). Side view (bottom). For clarity, hydrogen atoms are omitted.

Figure S2. Zero-field Mössbauer spectrum (experimental data (|), calculated fit (—)) recorded at 4.2 K of the solid sample of [Fe_2(μ-O_2CAr^{Tol})$_4$(BA)$_2$] (**1**). See Table 1 for derived Mössbauer parameters.

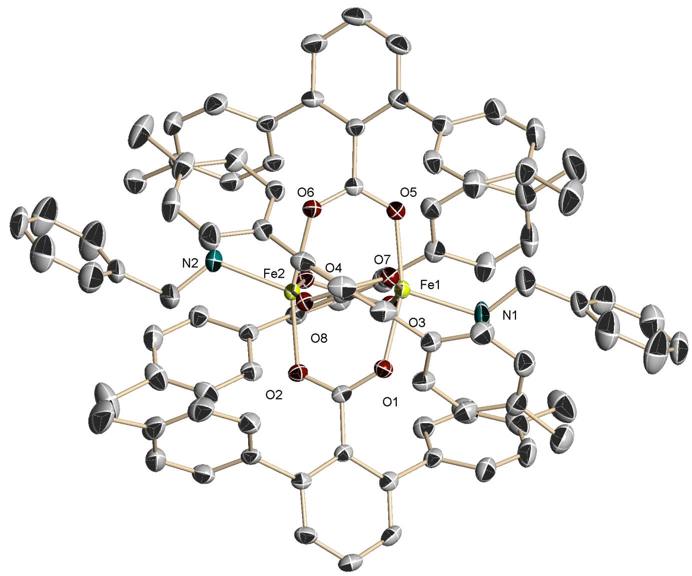
Figure S3. Zero-field Mössbauer spectrum (experimental data (|), calculated fit (—)) recorded at 4.2 K of a solid sample of [Fe_2(μ-O_2CAr^{Tol})$_4$($BA^{p\text{-}OMe}$)$_2$] (**2**). See Table 1 for derived Mössbauer parameters.

Figure S4. Plots of the effective magnetic moment (μ_{eff}) per molecule versus temperature (filled circles) and molar susceptibility (χ_M) versus temperature (unfilled circles) for [Fe_2(μ-O_2CAr^{Tol})$_4$(BA)$_2$] (**1**).

Figure S5. Cyclic voltammograms of [Fe_2(μ-O_2CAr^{Tol})$_4$($BA^{p\text{-}OMe}$)$_2$] (**2**) in CH_2Cl_2 with 0.5 M (Bu_4N)PF_6 as supporting electrolyte and (top) a scan rate of 25 mV/s or (bottom) variable scan rates. The inset in the top panel is a cyclic voltammogram of the reference couple ferrocene/ferricinium ion. The inset in the bottom panel plots current as a function of (scan rate)$^{1/2}$.

Figure S6. Resonance Raman spectra of the frozen solution of intermediates derived from the oxygenation of [Fe_2(μ-O_2CAr^{Tol})$_4$($BA^{p\text{-}OMe}$)$_2$] **(2)** with $^{16}O_2$ (top spectrum) and $^{18}O_2$ (bottom spectrum) at -78 °C. The asterisk indicates a solvent band.

Figure S7. ^{1}H NMR spectrum of oxidation product mixture of [Fe_2(μ-O_2CAr^{Tol})$_4$(α-d_1-$BA^{p\text{-}OMe}$)$_2$] in CH_2Cl_2 solution at –78 °C.



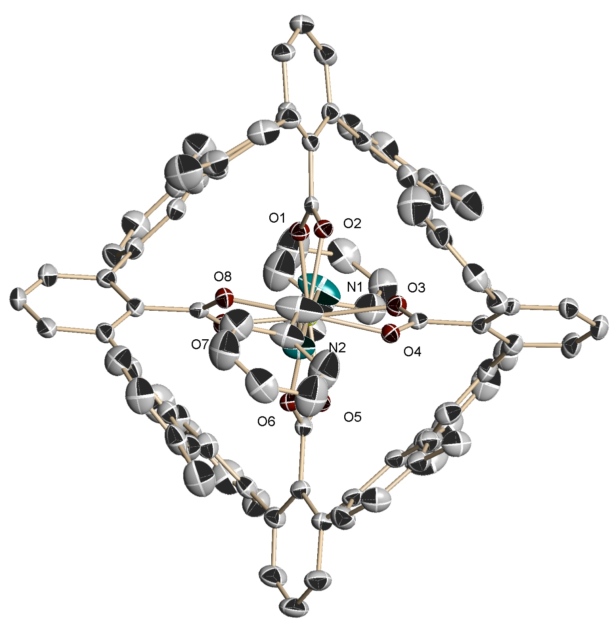


Figure S1. Sungho *et al*.

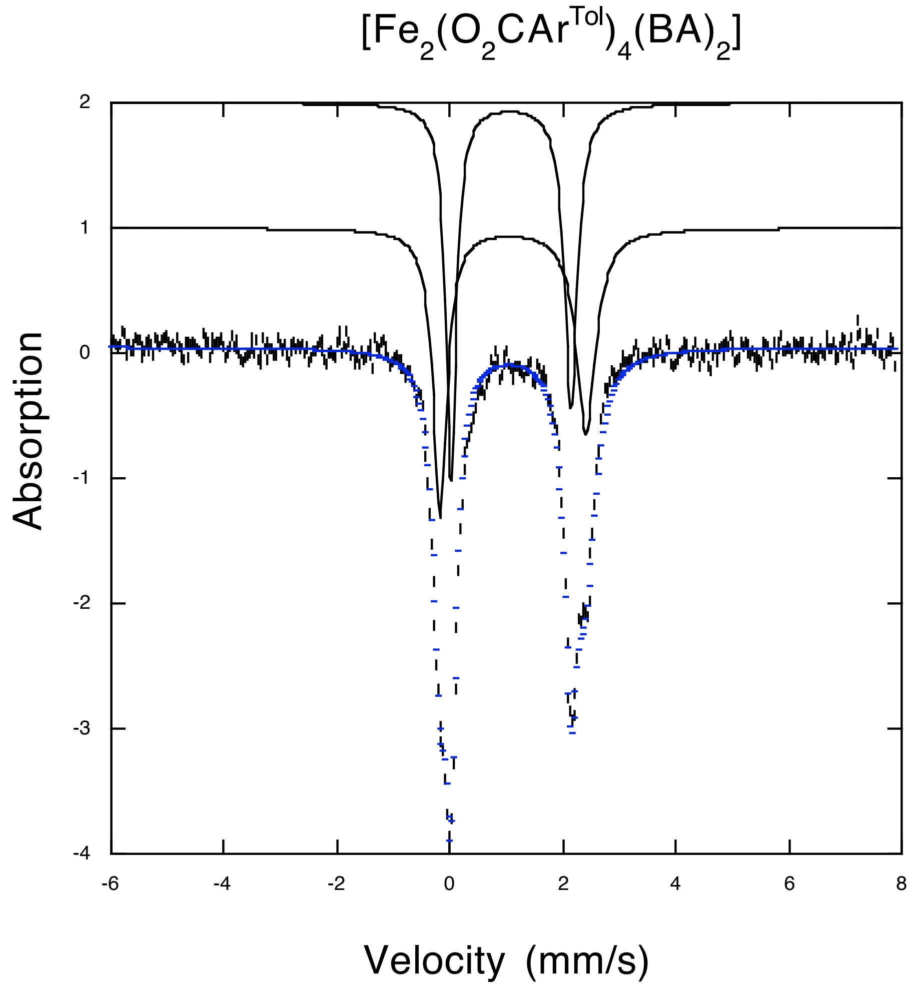


Figure S2. Sungho *et al*.

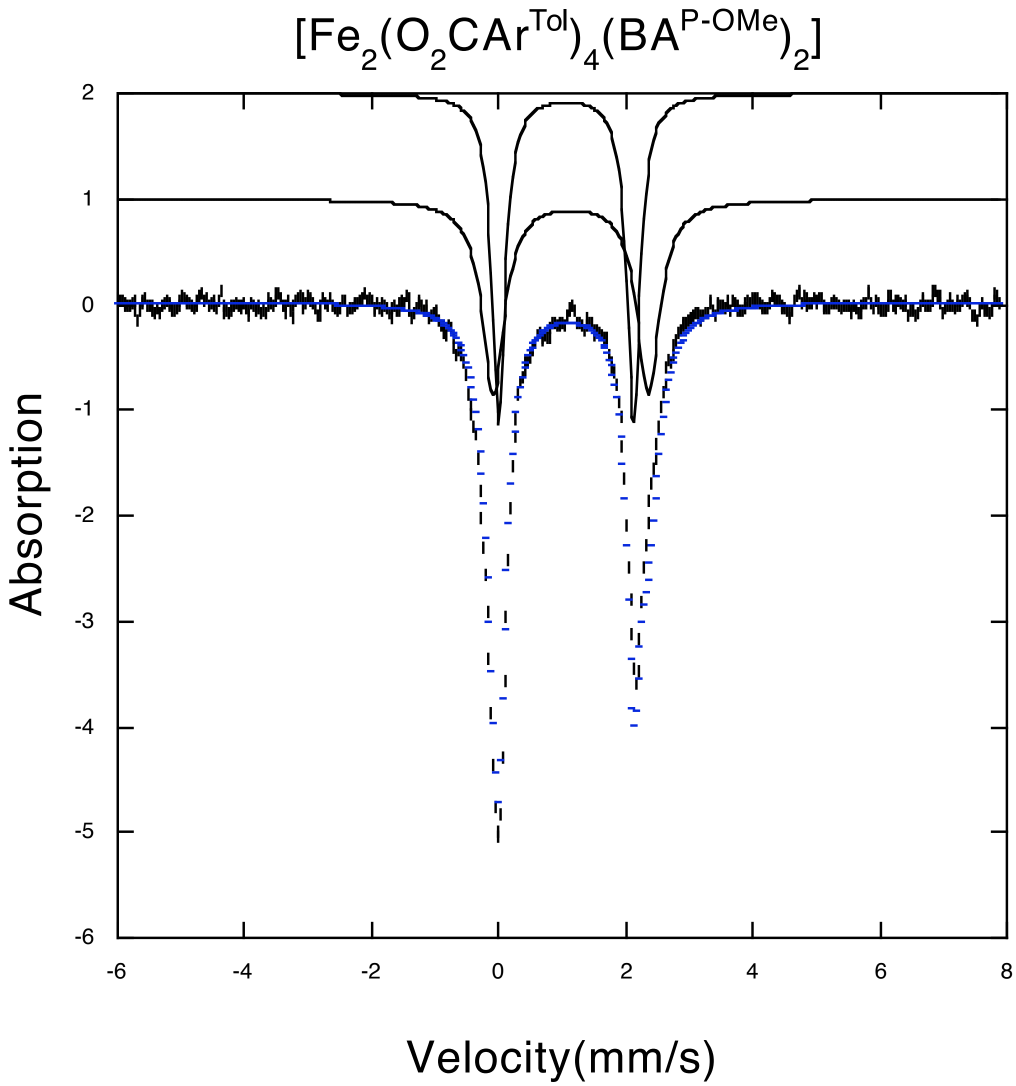


Figure S3. Sungho *et al*.

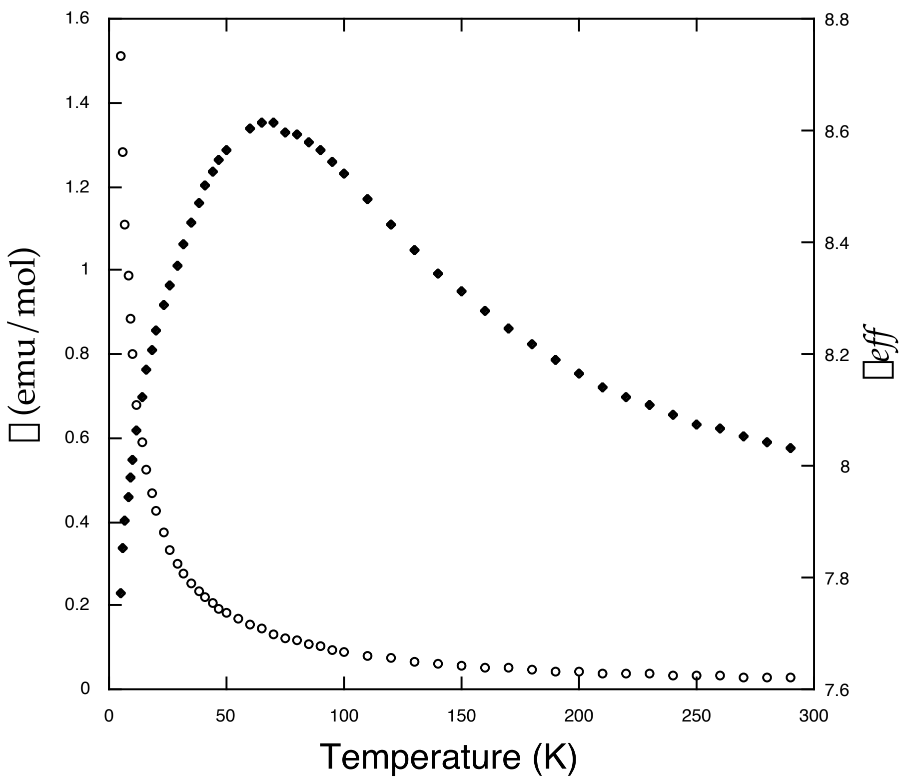


Figure S4. Sungho *et al*.

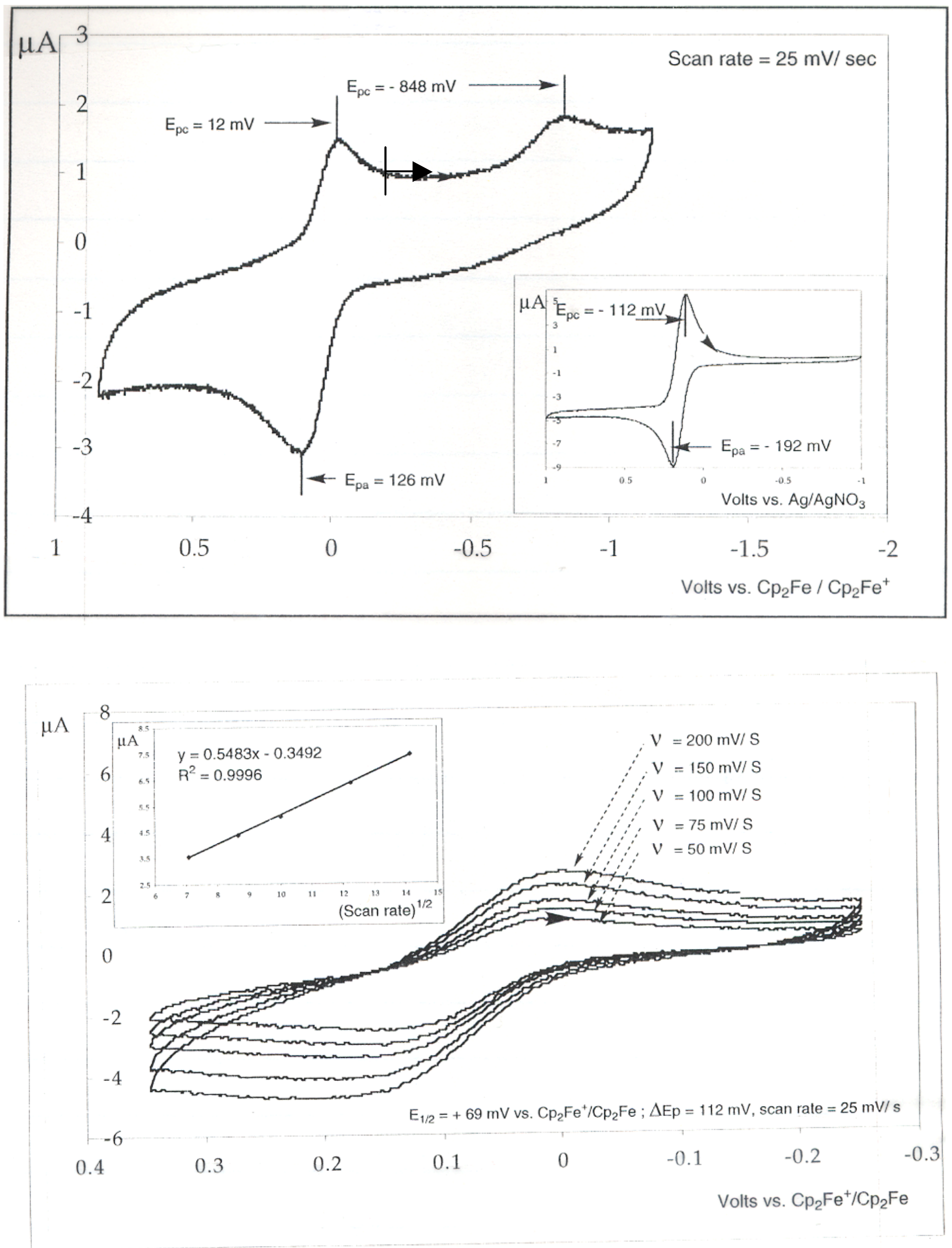


Figure S5. Sungho *et al*.

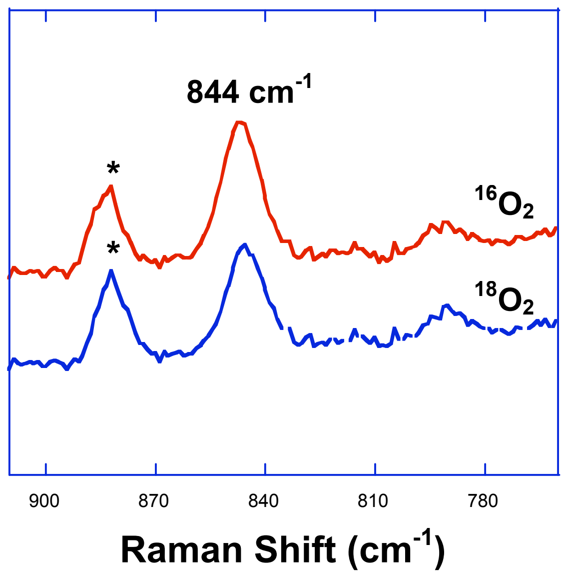


Figure S6. Sungho *et al*.

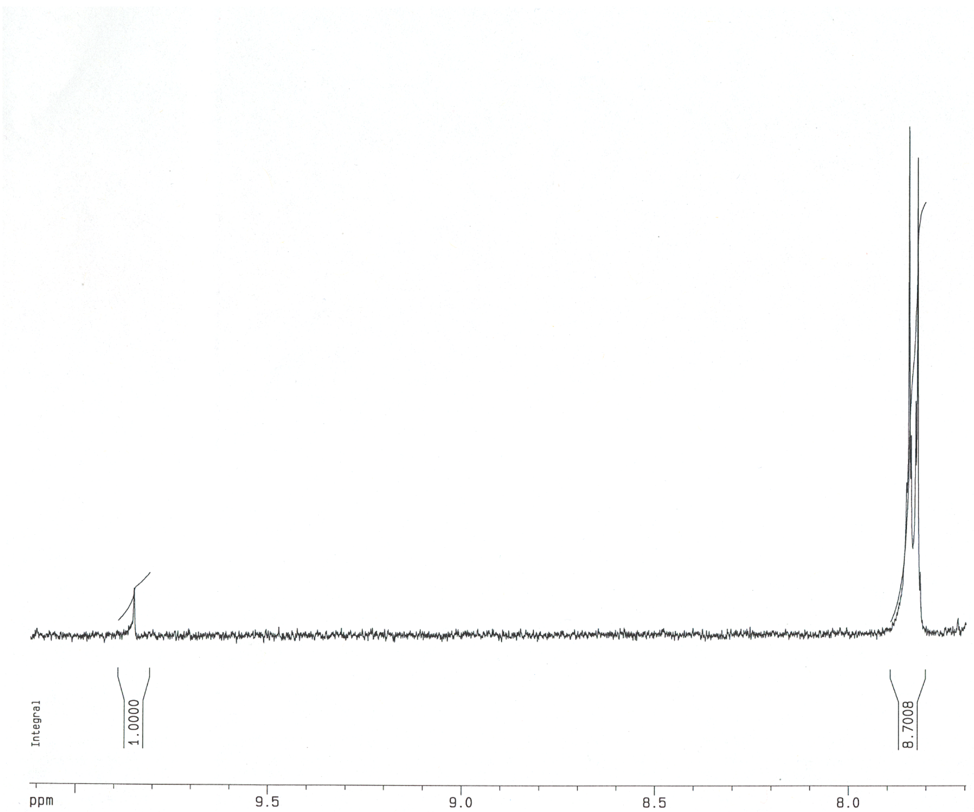


Figure S7. Sungho *et al*.