Supporting Information for:

Synthesis, Structure & Diphenylacetylene Reduction Reactivity of a Carbide-Supported Fe_4Mo_2 Carbonyl Cluster: A Higher Fe-Valence Hydride Intermediate for Enhanced Selectivity

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Synthetic & Experimental Details

Reagents and Procedures

All manipulations were performed under an inert atmosphere using Schlenk line or glovebox techniques. HPLC grade solvents were purchased from EMD, Fisher, Macron, or J.T. Baker, and dried through an alumina column system (Pure Process Technology). Deuterated solvent (d^3-acetonitrile) was purchased from Acros Organics and used as received. Diphenylacetylene, $FeCl_3$, NEt_4Br, TfOH and benzo-18-crown-6 were used as received. $[Fe_6(\mu_6\text{-C})(\mu_2\text{-CO})_4(CO)_{12}]^{2-}$,[1] $[Fe_4(\mu_4\text{-C(COOMe)})(CO)_{12}]^-$, $[Fe_4(\mu_4\text{-C})(CO_{13}]$, $[Fe_4(\mu_4\text{-C})(CO)_{12}]^{2-}$ (**1**), KC_8,[2] and Mo(chpt)$(CO)_3$ were prepared according to literature procedures.

Caution: Iron carbonyls are extremely toxic and potassium graphite is pyrophoric. Such materials should be handled carefully in a drybox or well-ventilated fume hood under inert atmosphere.

$[K(benzo\text{-}18\text{-}crown\text{-}6)]_2[Fe_4Mo_2(\mu_6\text{-C})(\mu_2\text{-CO})_2(CO)_{16}]$ (**2**) In an N_2 glovebox atmosphere, solid Mo(chpt)$(CO)_3$ (111.3 mg, 0.4090 mmol) was added into a pressure tube and charged with $[K(benzo\text{-}18\text{-}crown\text{-}6)]_2[Fe_4(\mu_4\text{-C})(CO)_{12}]$ (101.1 mg, 0.0793 mmol) in 1,2-dichloroethane (5 mL) and the solution was stirred for 8 h at 80 °C. The solution was passed through a Celite filter and dried under reduced pressure. The resulting dark-brown oil was washed with pentane and Et_2O and subsequently recrystallized by vapor diffusion of pentane into a DCE solution of the product. X-ray quality crystals were grown by vapor diffusion of Et_2O into a 1:1 DCE/FPh solution of the product at –20 °C. Yield: 83.0 mg (64%). Selected IR peaks (**Figure S1**), solid, ν(CO): 2040(w), 1928(s), 1869(s) cm^{-1}. $^{13}C\{^1H\}$ NMR (125.8 MHz, MeCN-d_3), δ in ppm from TMS: 473.4 ppm (carbide), 147.4, 131.2, 126.8, 121.7, 121.4, 121.1, 118.5, 111.9 ppm (CO). Anal. calcd. for $C_{51}H_{48}O_{30}Fe_4Mo_2K_2$: C, 37.48; H, 2.96; found: C, 36.20; H, 3.48.

Diphenylacetylene Reduction. In an N_2 glovebox atmosphere, sodium (11.5 mg, 0.500 mmol) was stirred into a 5 mL THF solution of perylene (63.1 mg, 0.251 mmol) at –20 °C and allowed to stir for 4 h at room temperature. The resulting dark purple solution was added into a concentrated THF solution of the selected cluster (0.016 mmol), diphenylacetylene (15 equiv) and the proton source (30 equiv). The resulting mixture was stirred for 20 h, solvent evaporated, and the organic products were extracted into hexanes. Serial dilution followed by GCMS analysis was used to determine relative ratios of DPA to *cis*-DPE, *trans*-DPE and DP-Ethane. GCMS analysis utilized a Thermo Scientific Trace GC Ultra GC instrument equipped with an Agilent DB-WAXETR capillary column (30 m × 0.25 mm) with a 0.25 μm film thickness coupled with a Thermo Scientific TSQ Quantum GC MS instrument using EI ionization method. A 1.0 μL aliquot of the diluted sample was injected into the GC using a split/splitless injector with a splitless time of 1.00 min and a flow rate of 0.9 mL/min of helium at an initial temperature of 40 °C, which was maintained for 1.00 min and ramped by 20 °C/min to a final temperature of 260 °C, which was maintained for 10.00 min. Retention times of DP-Ethane, *cis*-DPE, DPA, and *trans*-DPE were 9.58, 9.72, 11.02 and 11.43 min (respectively).

X-ray Photoelectron Spectroscopy

XPS samples of Fe_6, Fe_5Mo and Fe_4Mo_2 (**2**) were prepared by dissolving 2 mg of the analyte into separate polyethylene glycol (PEG)/MeCN (10 mg/mL) solutions. Samples were then dropcast onto silicon wafers to form thin films for measurement. Spectra were recorded using a Kratos Axis Ultra XPS equipped with an Al−Kα X-ray source monochromated to 1486.6 eV. The photoelectron takeoff angle was 0°, and the pressure in the acquisition chamber was on the order of 10−9 Torr for all samples analyzed. Survey scans were obtained under the following conditions: pass energy of 160, 1.000 eV step size, and 300 ms dwell time. Region scans were obtained under the following conditions: pass energy of 20, 0.100 eV step size, and 1500 ms dwell time. All peaks in the spectra for Fe_6, Fe_5Mo and Fe_4Mo_2 were referenced against the PEG C 1*s* peak (286.45 eV) for each dataset.

XPS studies were run without the charge neutralizer gun activated. Iterative survey scans of the Fe_6 sample were taken and showed that peak positions were stable without the charge neutralizer gun turned on. This agrees with previous reports on the conductivity of thin films of PEG and shows that there were no significant charging effects in these thin films.[3] During the course of these studies, it was observed that turning on the charge neutralizer, followed by turning the neutralizer off again, increased the signal in the Fe 2*p* XPS region of any future survey scans taken on these samples. We posit that some rearrangement of the Fe_6 loading in the PEG thin film occurs under the charge neutralizer, causing the surface concentration of Fe to increase. We note that such mobility of Fe_6 clusters is very surprising and warrants further study that is outside the scope of this manuscript.

In modelling the high resolution XPS region data for the transition metals, FeOx and MoOx species were tested for an improved fit. These oxidized metal species are likely the result of trace oxidizing gases in the glovebox atmosphere. When the fit was clearly improved, these species were left in the model as a second species. When calculating atom percents in the sample, the oxide species were ignored.

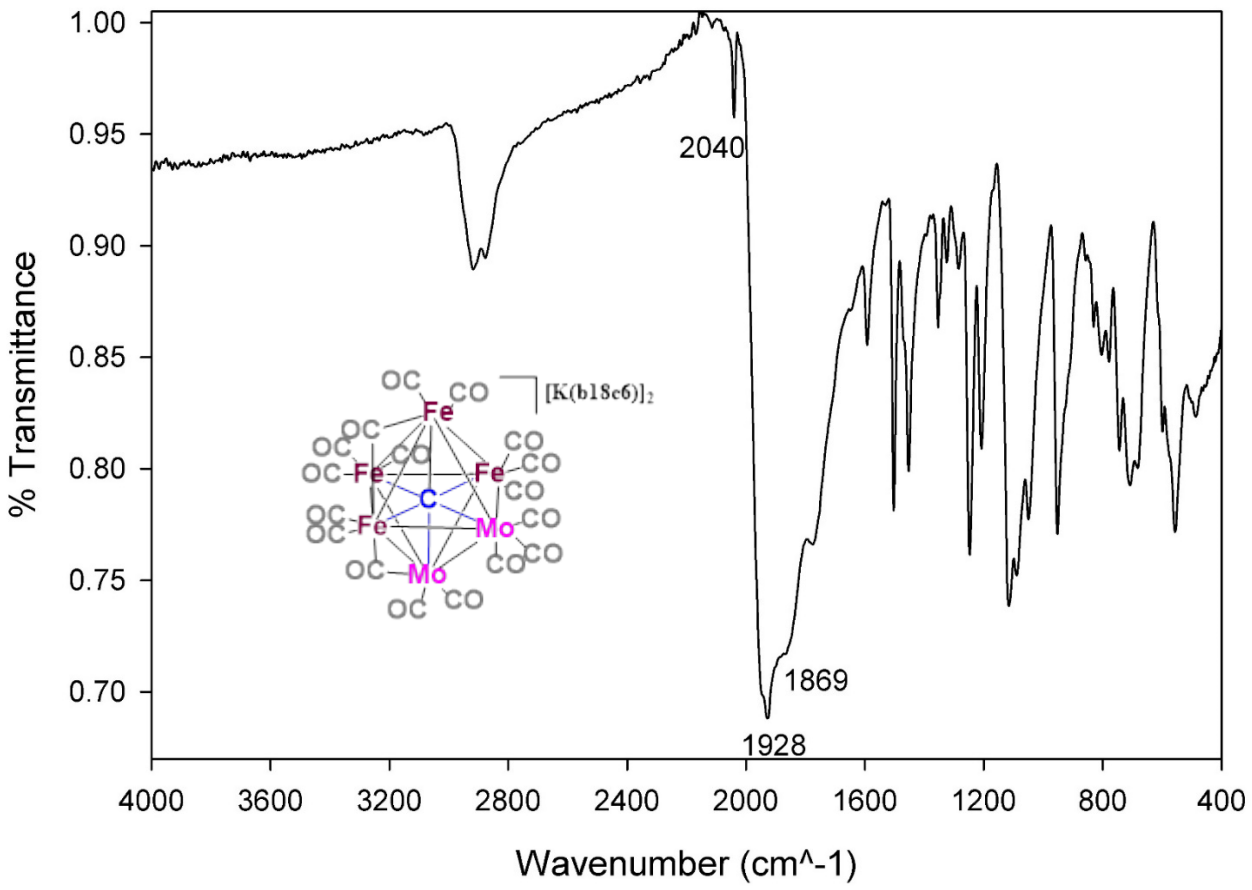


Figure S1. IR spectrum of $[K(benzo\text{-}18\text{-}crown\text{-}6)]_2[Fe_4Mo_2(\mu_6\text{-}C)(\mu_2\text{-}CO)_2(CO)_{16}]$ (**2**) in the solid crystalline state.

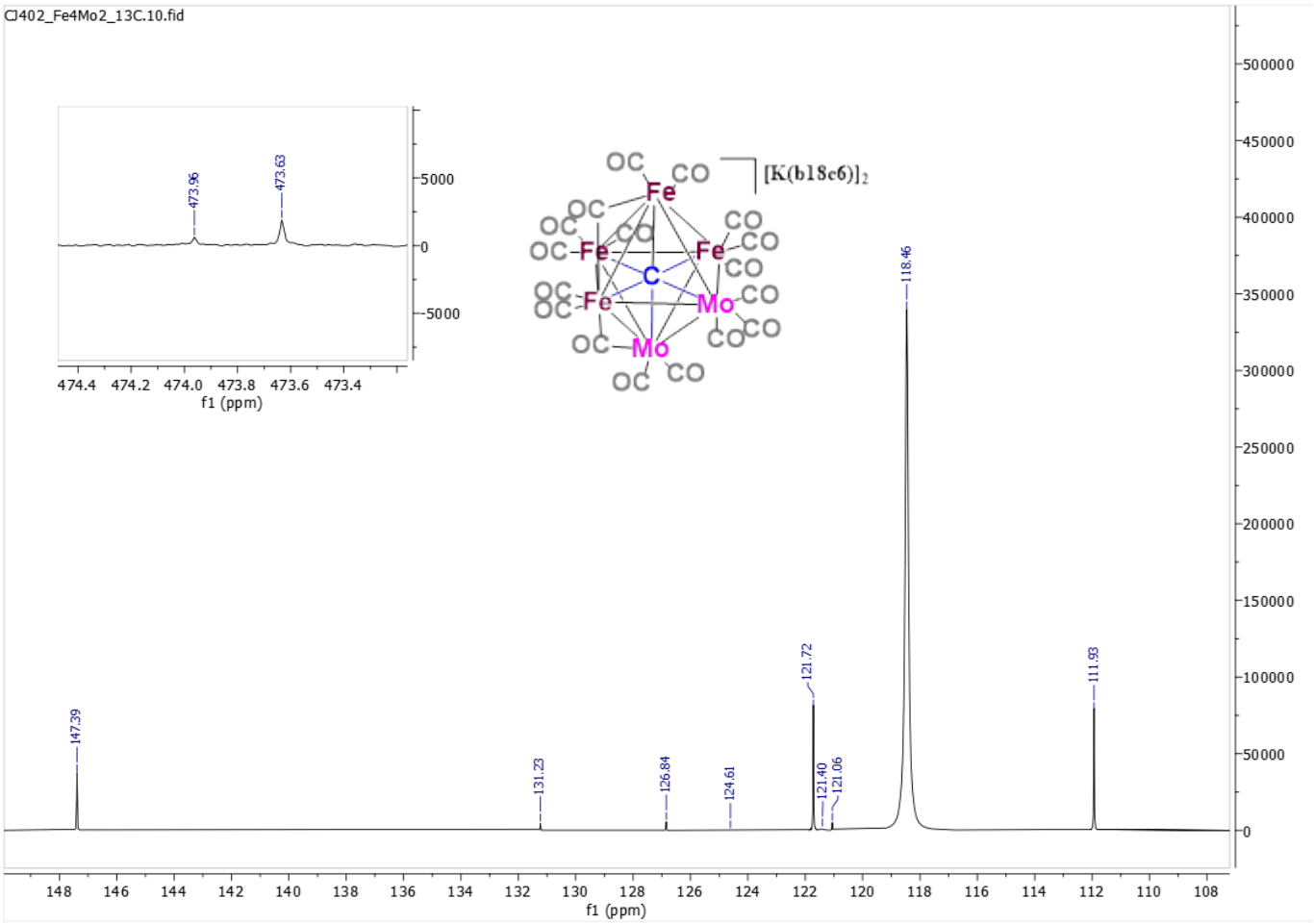


Figure S2. ^{13}C NMR spectrum of **2**, in d_3–MeCN at 25 °C.

X-ray Experimental

Structure 1

Crystals grew as small, dark brown plates by slow evaporation from fluorobenzene. The data had approximate dimensions; 0.12×0.09×0.04 mm. The data were collected on a Rigaku Oxford Diffraction SuperNova Dual Source diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418Å) with collimating mirror monochromators. A total of 1215 frames of data were collected using ω-scans with a scan range of 1° and a counting time of 12.5 seconds per frame with a detector offset of ± 41.3° and 37.5 seconds per frame with a detector offset of 108.3°. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in **Tables S1-S6**. Data collection, unit cell refinement and data reduction were performed using Rigaku Oxford Diffraction CrysAlisPro V 1.171.38.43f.[2] The structure was solved by direct methods using SHELXT[3] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/3.[4] Structure analysis was aided by use of the programs PLATON[5] and OLEX2.[6] The hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2×U_{eq} of the attached atom (1.5×U_{eq} for methyl hydrogen atoms).

The complex resides around a crystallographic inversion center at 0, 1, ½. The complex consists of three iron-carbonyl clusters interspersed with six benzo-18-crown-6 potassium ion complexes. The central iron carbonyl cluster is disordered around a crystallographic inversion center. There are also five molecules of fluorobenzene per complex. All fluorobenzene molecules were disordered. The disorder was modeled in the same manner for each. The site occupancy factors for one component was set to 1–*x*, while the alternate site occupancy factor was set to *x*. A common isotropic displacement parameter was refined for all atoms of the disordered group while refining the variable *x*. Upon convergence of *x*, the site occupancy factors were fixed and the displacement parameters were refined with restraints applied to make the displacement parameters similar for all atoms in the molecule and for the displacement parameters to remain approximately isotropic. Near the end of the refinement process, the geometry of the phenyl rings was idealized using the AFIX 66 constraint.

The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.023*P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_W(F^2)$ refined to 0.157, with R(F) equal to 0.0702 and a goodness of fit, S, = 0.937. Definitions used for calculating R(F), $R_W(F^2)$ and the goodness of fit, S, are given below.[7] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[8] All figures were generated using SHELXTL/PC.[9] Tables of positional and

thermal parameters, bond lengths and angles, torsion angles and figures are found below as **Tables S1-S6**. **Structure 2**.

Crystals grew as dark brown plates by vapor diffusion of diethyl ether into a fluorobenzene solution. The data crystal had approximate dimensions; 0.29×0.22×0.18 mm. The data were collected on a Rigaku AFC12 diffractometer with a Saturn 724+ CCD using a graphite monochromator with MoKα radiation (λ = 0.71073 Å). A total of 1420 frames of data were collected using ω-scans with a scan range of 0.5°. The data were collected at 100 K using a Rigaku XStream Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in **Tables S7-S12**. Data reduction were performed using the Rigaku Americas Corporation's Crystal Clear version 1.40.[10] The structure was solved by direct methods using SHELXT[2] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2018/8.[4] Structure analysis was aided by use of the programs PLATON[5] and OLEX2.[6] The hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to $1.2 \times U_{eq}$ of the attached atom.

The structure resides around an approximate, non-crystallographic inversion center near 0.39, 0.75, 0.89. The structure consists of two (benzo-18-crown-6)K moities and one $Fe_4Mo_2(CO)_{18}C$ complex. The $Fe_4Mo_2(CO)_{18}C$ complex is disordered about two orientations with site occupancies of 0.58 for one composed of Mo1, Mo2, Fe1, Fe2, Fe3 and Fe4 with carbonyl group labels appended by an A, while the second complex has a site occupancy of 0.42 with labels appended by a B. The site occupancy factors were refined by setting the site occupancy for one component to the variable *x*, while the site occupancy for the alternate component was set to (1–*x*). The displacement parameters were refined with similarity restraints while refining the variable *x*. Upon convergence of the variable *x*, the displacement parameters were allowed to refine. The refinement was plagued by very high correlation coefficients of atoms related by the approximate inversion center. Generous use of displacement parameter restraints and bond length restraints were used throughout the refinement. In severe cases, where atoms could not be refined anisotropically, these atoms were refined isotropically.

An alternate model was initially proposed in the much more common space group, *P21/n*. In this space group, the metal complex was disordered around a crystallographic inversion center requiring the site occupancy factors for the two components to be equal to ½. The class of reflections, 0 k 0, where k is odd have two very weak reflections with I > 2 sigma I, 0 1 0 and 0 9 0. However, it is not uncommon for some reflections to have intensity above noise level with a strongly scattering crystal. However, we think the correct space group is *Pn* because the agreement factors in *Pn* are dramatically lower than those using the model in *P21/n*. The model in *P21/n* has $R_1 = 0.0707$, with a $wR_2 = 0.159$ compared with $R_1 = 0.0249$ and $wR_2 = 0.0619$.

The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0309*P)^2 + (1.7063*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_W(F^2)$ refined to 0.0619, with R(F) equal to 0.0249 and a goodness of fit, S, = 1.03. Definitions used for calculating R(F), $R_W(F^2)$ and the goodness of fit, S, are given below.[7] The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[8] All figures were generated using SHELXTL/PC.[9] Tables of positional and thermal parameters, bond lengths and angles, torsion angles and figures are found below as **Tables S7-S12**.

Analysis of Crystallographic Structures

Structure 1

Similar to previous reports on the structure of tetra-iron–carbide clusters, the crystal structure data for **1** (**Figure S3**) revealed a four-coordinate carbide encompassed by four Fe atoms fixed in a butterfly geometry. The asymmetric unit of the crystal structure (in *P-1*) contains 1.5 $[Fe_4(\mu_4\text{-}C)(CO)_{12}]^{2-}$ units and three $[K(benzo\text{-}18\text{-}crown\text{-}6)]^+$, where the carbide of the half-occupied Fe_4 unit (s.o.f. = 0.5) is located near an inversion center. In comparison to the previously reported structure for the hexa-iron cluster $(NEt_4)_2[Fe_6(\mu_6\text{-}C)(\mu_2\text{-}CO)_4(CO)_{12}]$, the average Fe–Fe and Fe–$C_{carbide}$ contacts are slightly compressed from 2.66(6) Å and 1.88(1) Å (respectively) in the six-iron cluster, to 2.62(4) Å, 1.87(11) Å in **1**. Additionally, several O_{CO} atoms exhibit close contacts with the crowned K ion (avg 2.83 ± 0.18 Å for O_{CO}–K ≤ 3 Å) in the case of **1**.

Structure 2

The structure of **2** in **Figure S4** (in *P*2*n*) exhibits an inversion center near the carbide, despite the *cis* orientation of the molybdenum atoms. The crowned K cations exhibit close contact with carbonyl oxygen atoms (avg 2.80 ± 0.14 Å for O_{CO}–K ≤ 3 Å) similar to that observed in previous structures.

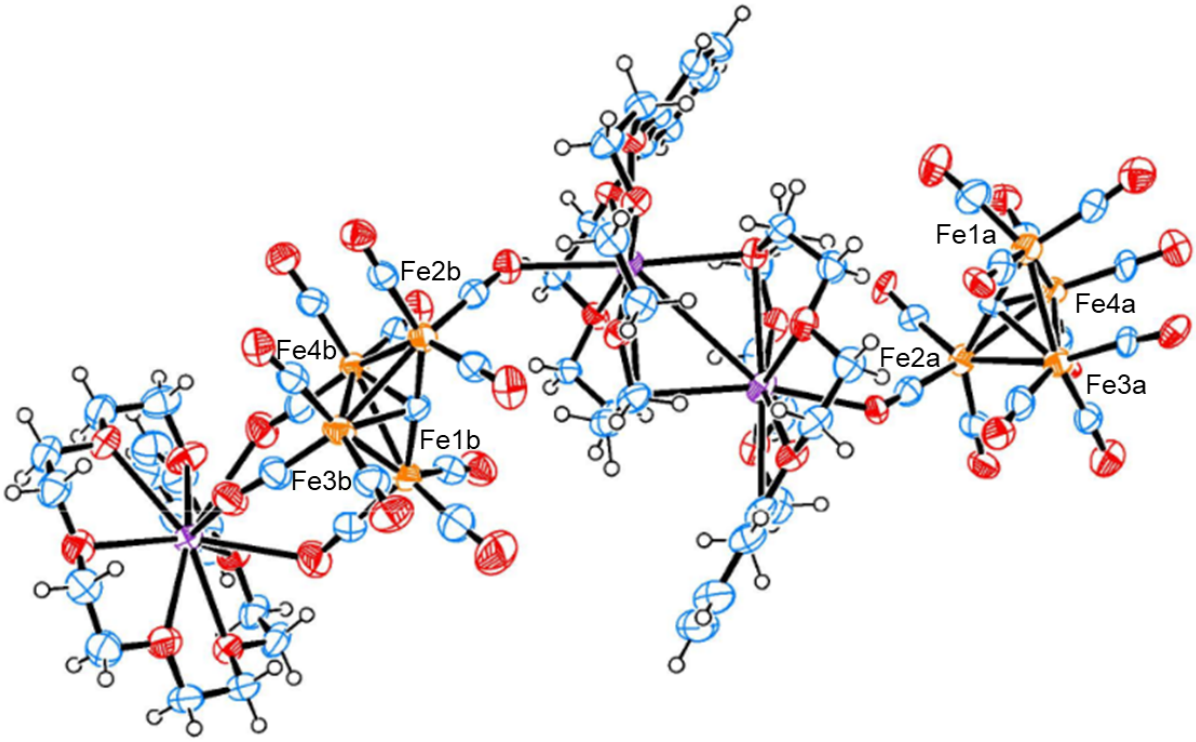


Figure S3. Full thermal ellipsoid plot (50% ellipsoids) of $[K(benzo\text{-}18\text{-}crown\text{-}6)]_2[Fe_4(\mu_4\text{-}C)(CO)_{12}]$ (**1**) ($Z = 2$).

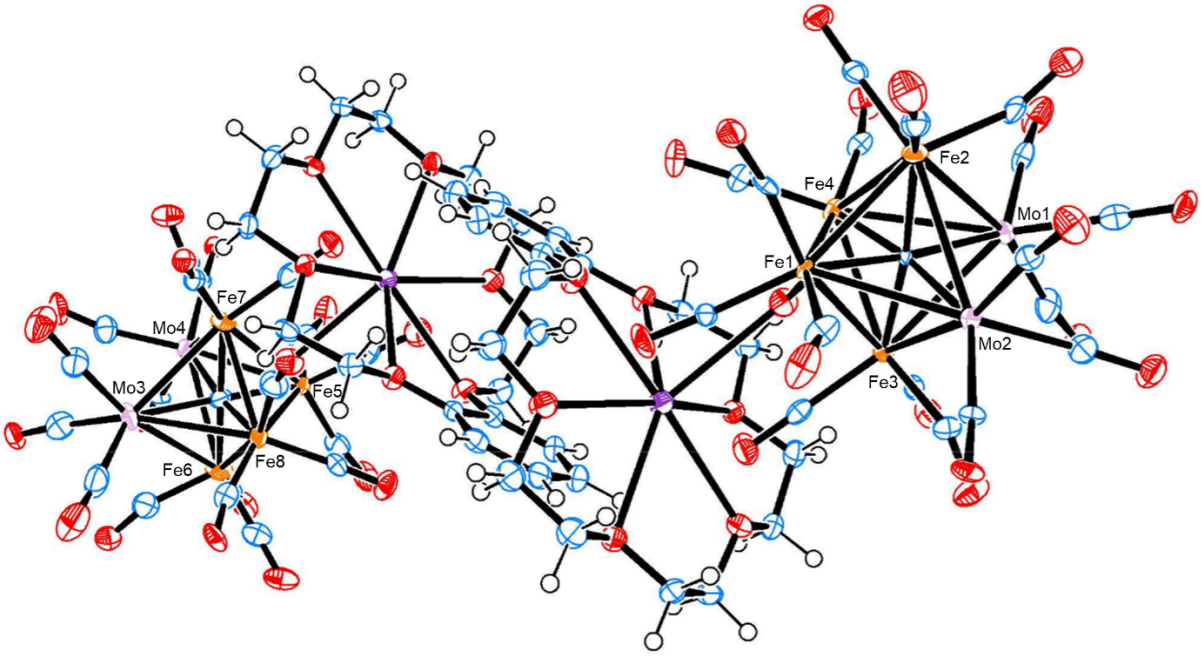


Figure S4. Thermal ellipsoid plot (50% ellipsoids) of $[K(benzo\text{-}18\text{-}crown\text{-}6)]_2[Fe_4Mo_2(\mu_6\text{-}C)(\mu_2\text{-}CO)_2(CO)_{16}]$ (**2**) ($Z = 2$).

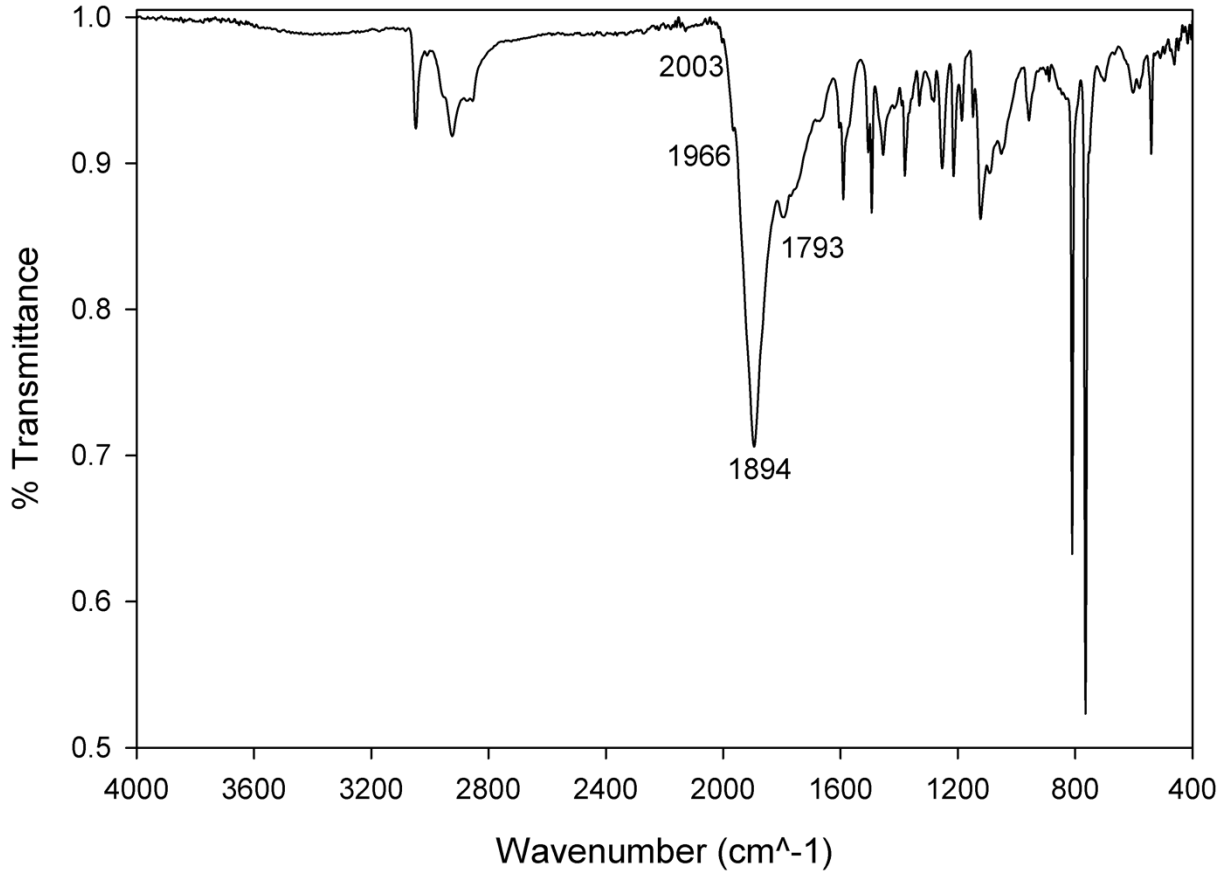


Figure S5. IR spectrum following two electron reduction of **2** with Na_2per in THF to generate $Fe_4Mo_2^{4-}$.

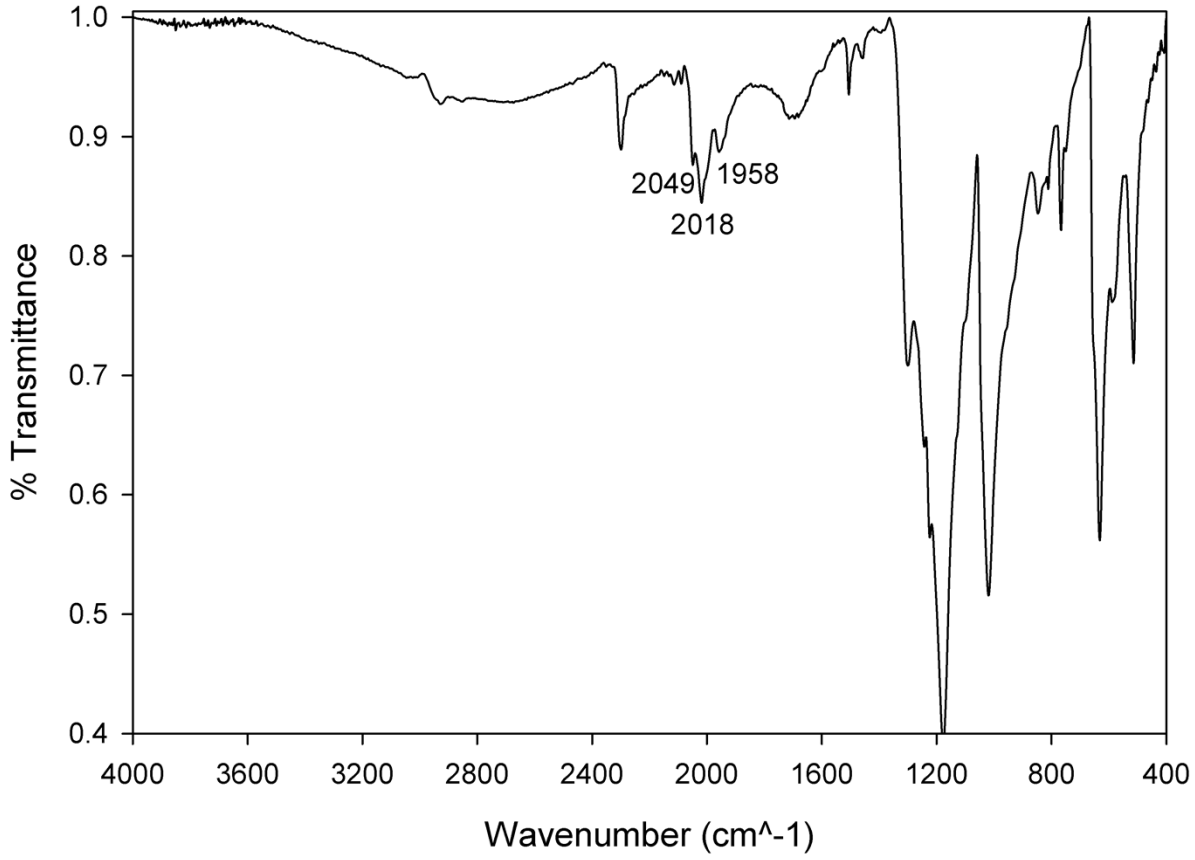


Figure S6. IR spectrum following protonation of $Fe_4Mo_2^{4-}$ with TfOH in MeCN to generate $H_2Fe_4Mo_2^{2-}$.

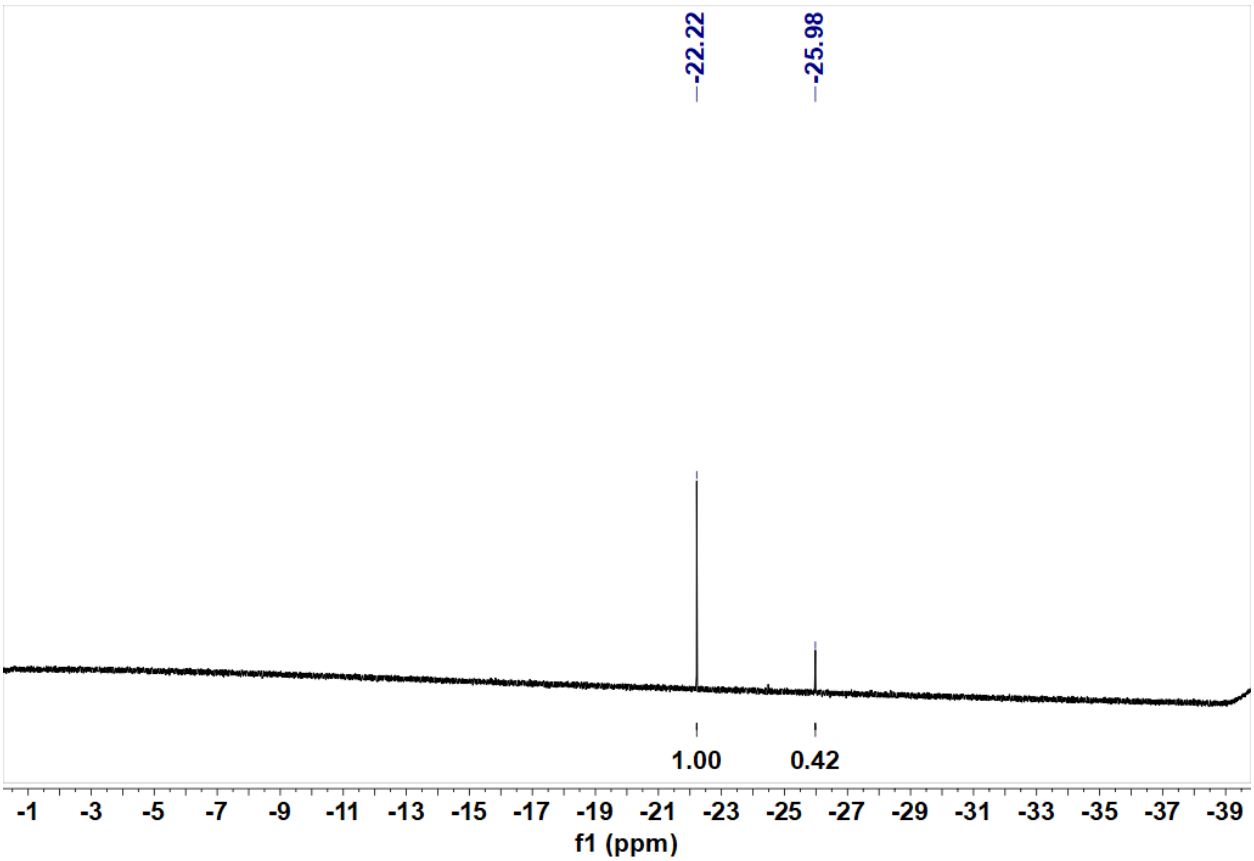


Figure S7. ^{1}H NMR spectrum of the full hydride region after reduction of **2** with Na_2per (THF) and protonation with TfOH in d_3–MeCN at 25 °C.

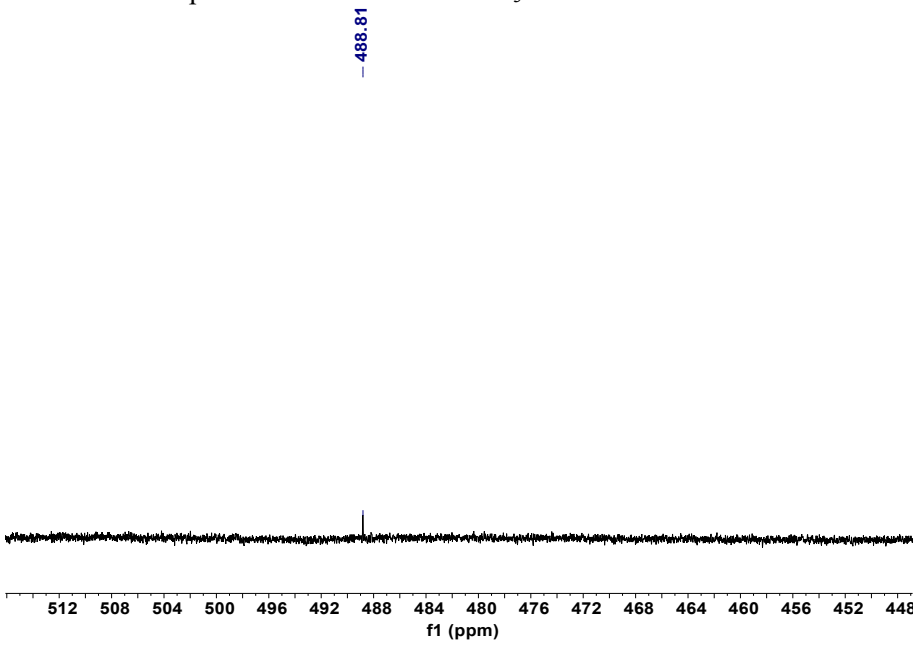


Figure S8. ^{13}C NMR spectrum of the carbide region after reduction of **2** with KC_8 in d_3–MeCN at 25 °C.

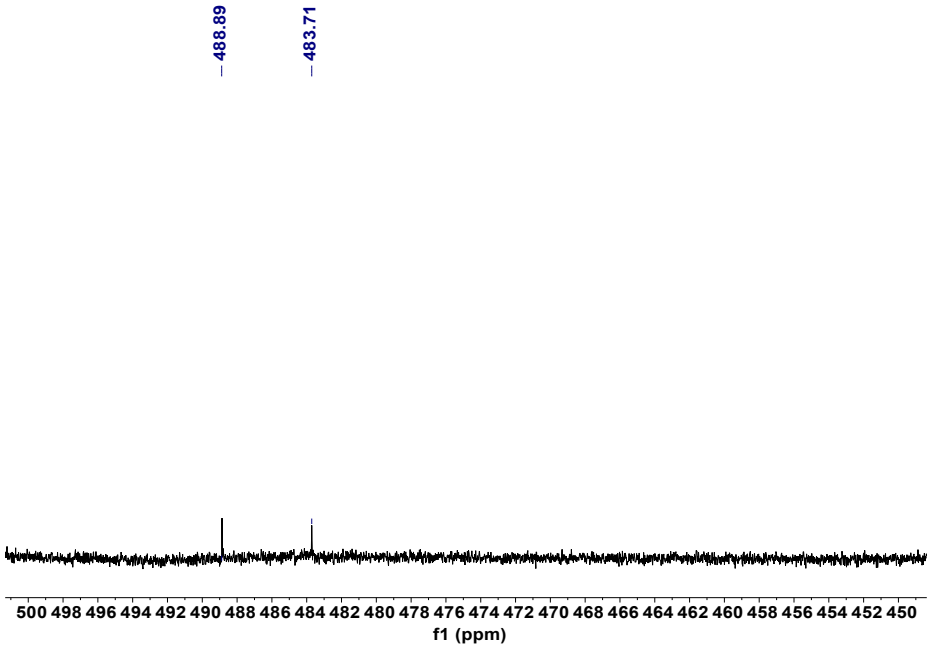


Figure S9. ^{13}C NMR spectrum of the carbide region after reduction of **2** with KC_8 and reaction with DPA in d_3–MeCN at 25 °C for 18 h.

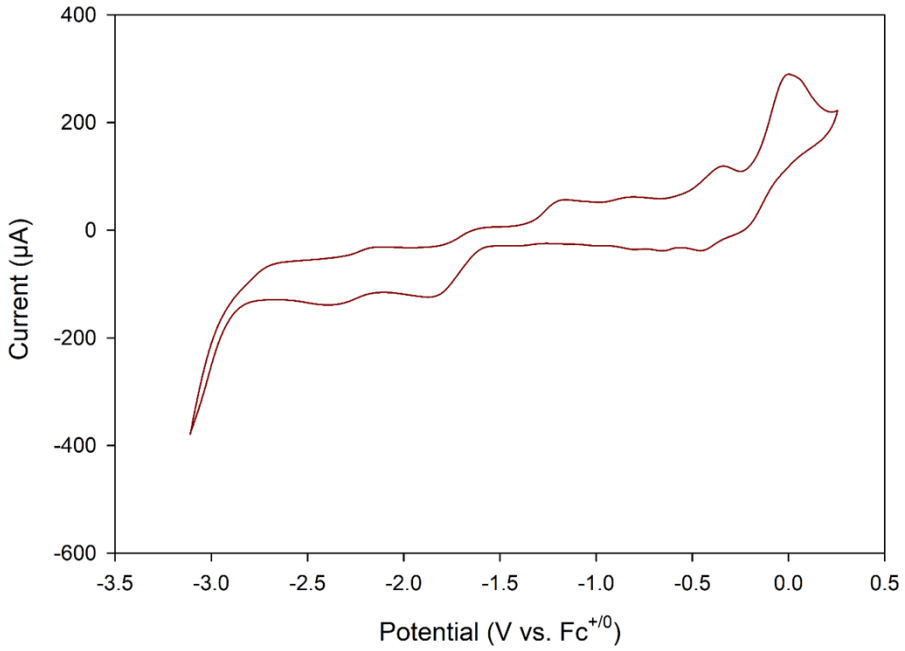


Figure S10. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_4Mo_2 in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **100 mV/s**.

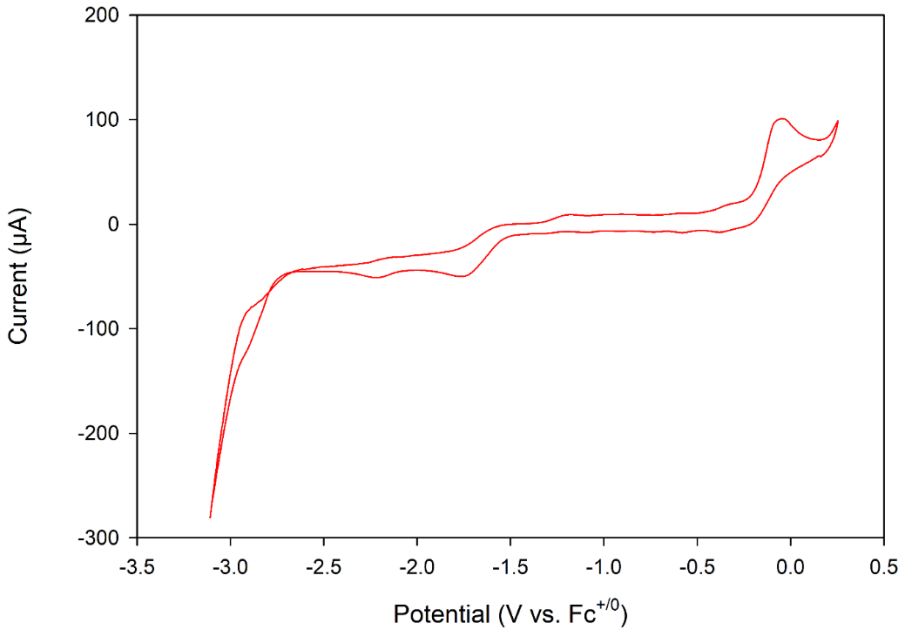


Figure S11. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_4Mo_2 in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **10 mV/s**.

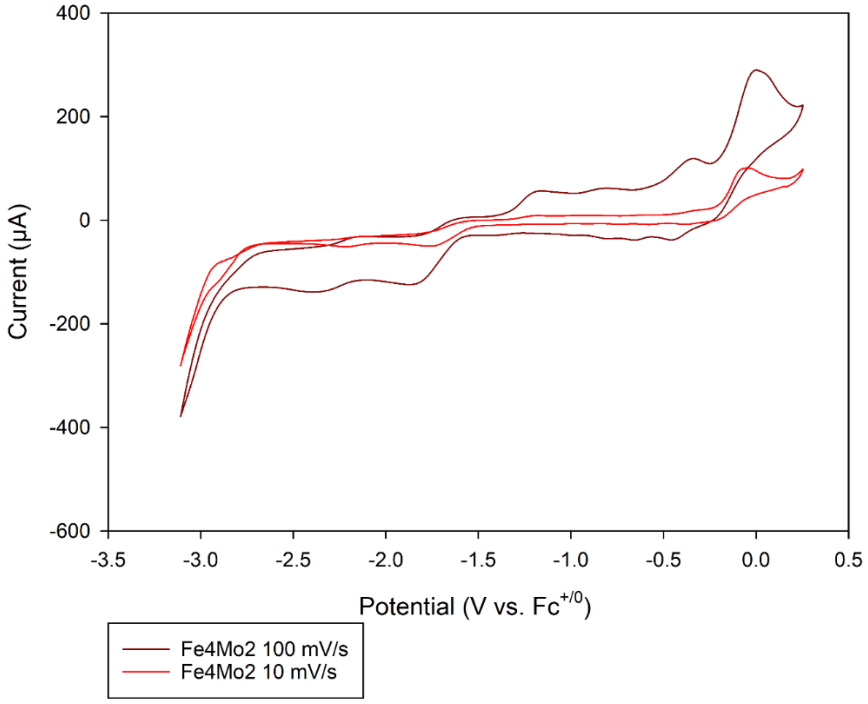


Figure S12. Comparison of scan rate effect on the cyclic voltammograms (vs Fc/Fc^{+}) of 5 mM of Fe_4Mo_2 in MeCN containing 0.2 M $TBAPF_6$. WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference.

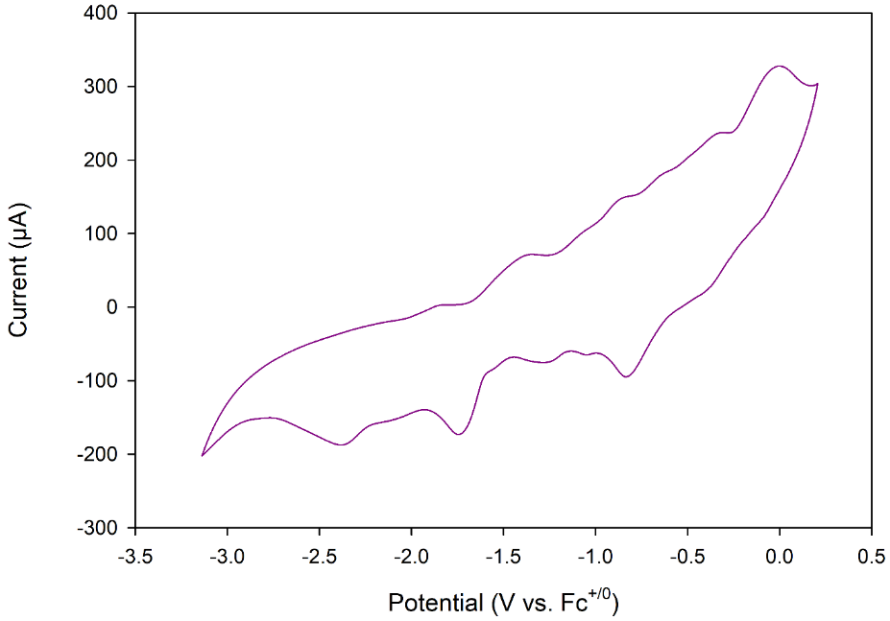


Figure S13. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_5Mo in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **100 mV/s**.

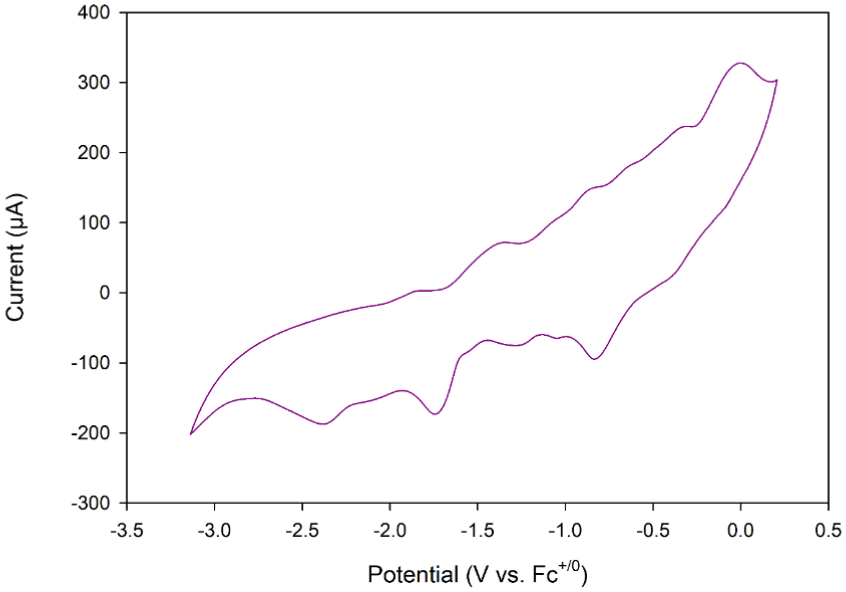
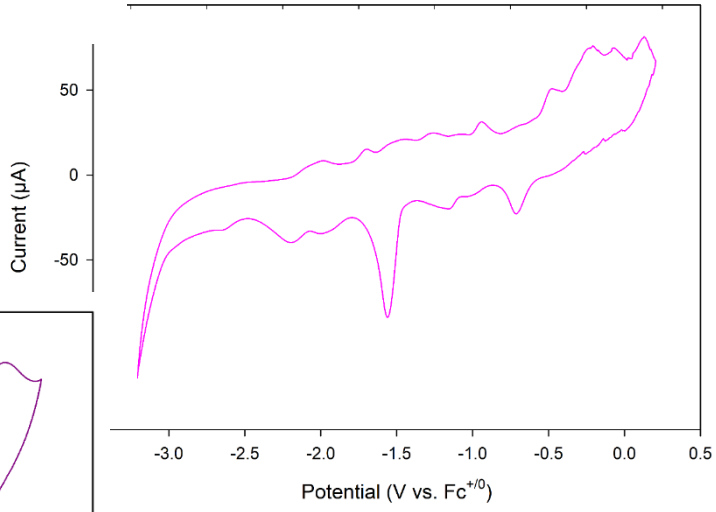


Figure S14. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_5Mo in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **10 mV/s**.



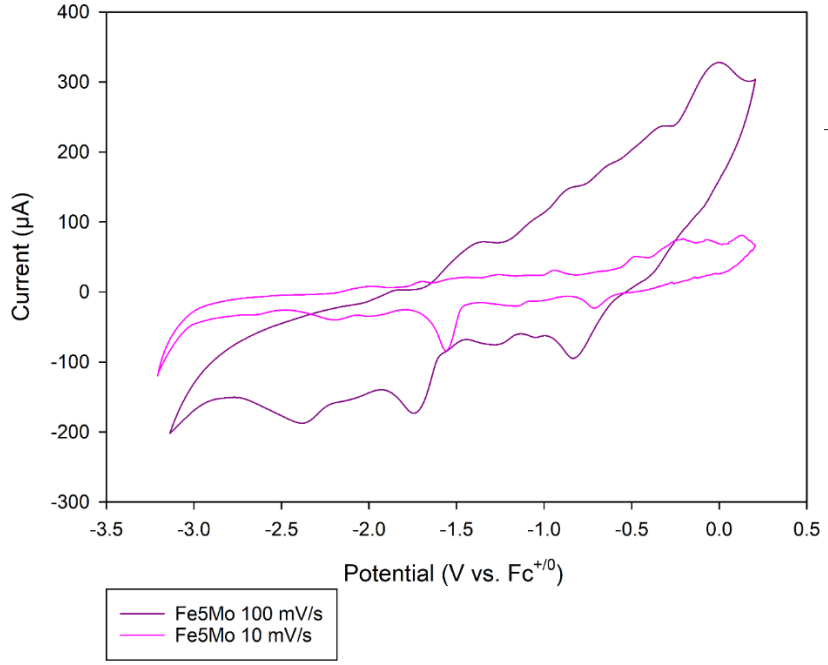


Figure S15. Comparison of the scan rate effect on the cyclic voltammograms (vs Fc/Fc^{+}) of 5 mM of Fe_5Mo in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference.

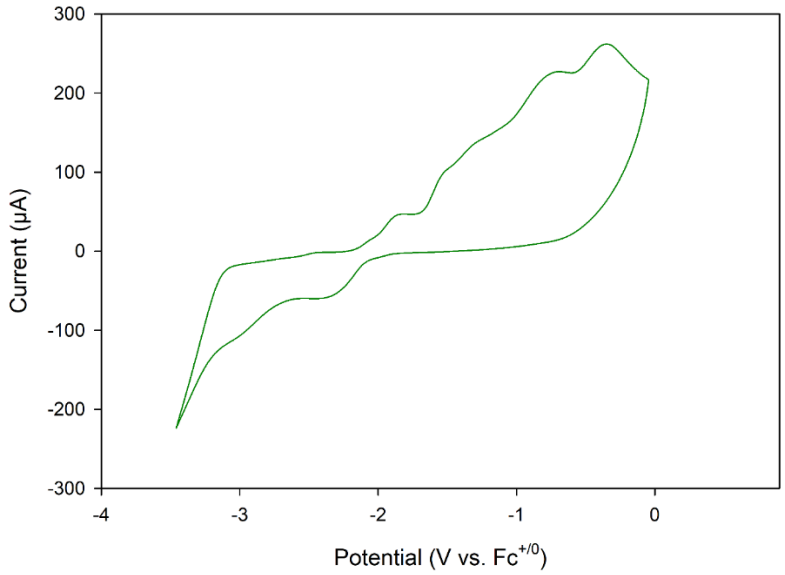


Figure S16. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_6 in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **100 mV/s**.

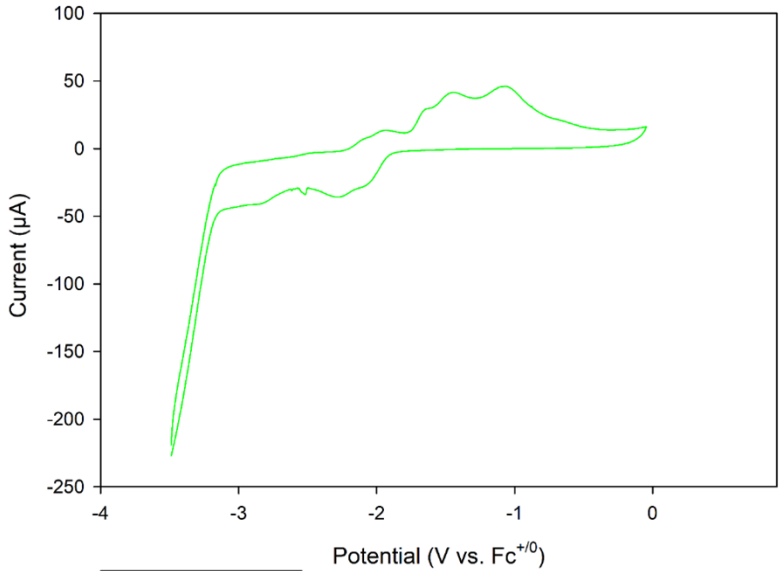


Figure S17. Cyclic voltammogram (vs Fc/Fc^{+}) of 5 mM of Fe_6 in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **10 mV/s**.

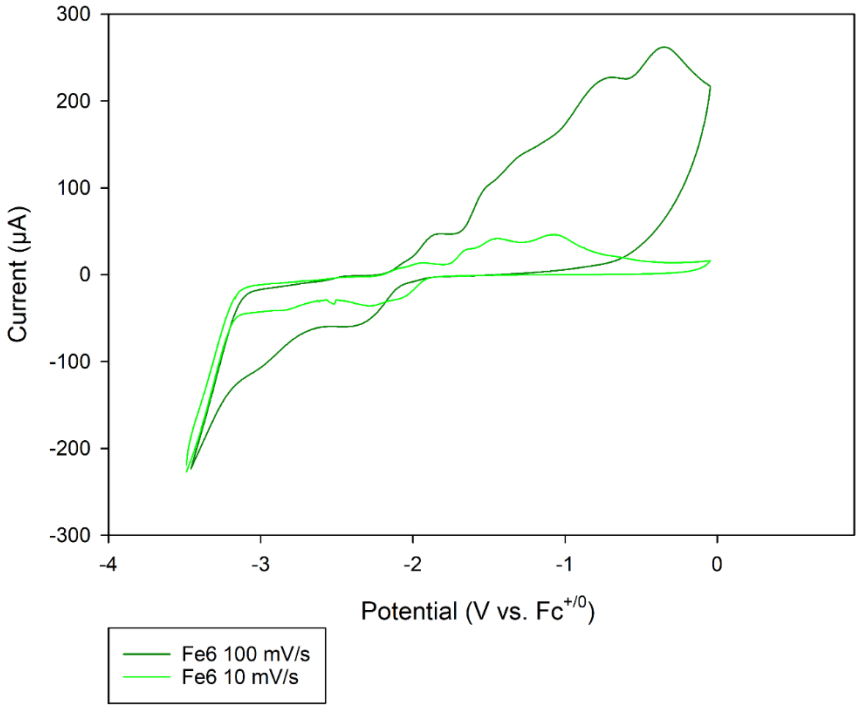


Figure S18. Comparison of scan rate effect on the cyclic voltammograms (vs Fc/Fc^{+}) of 5 mM of Fe_6 in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference.

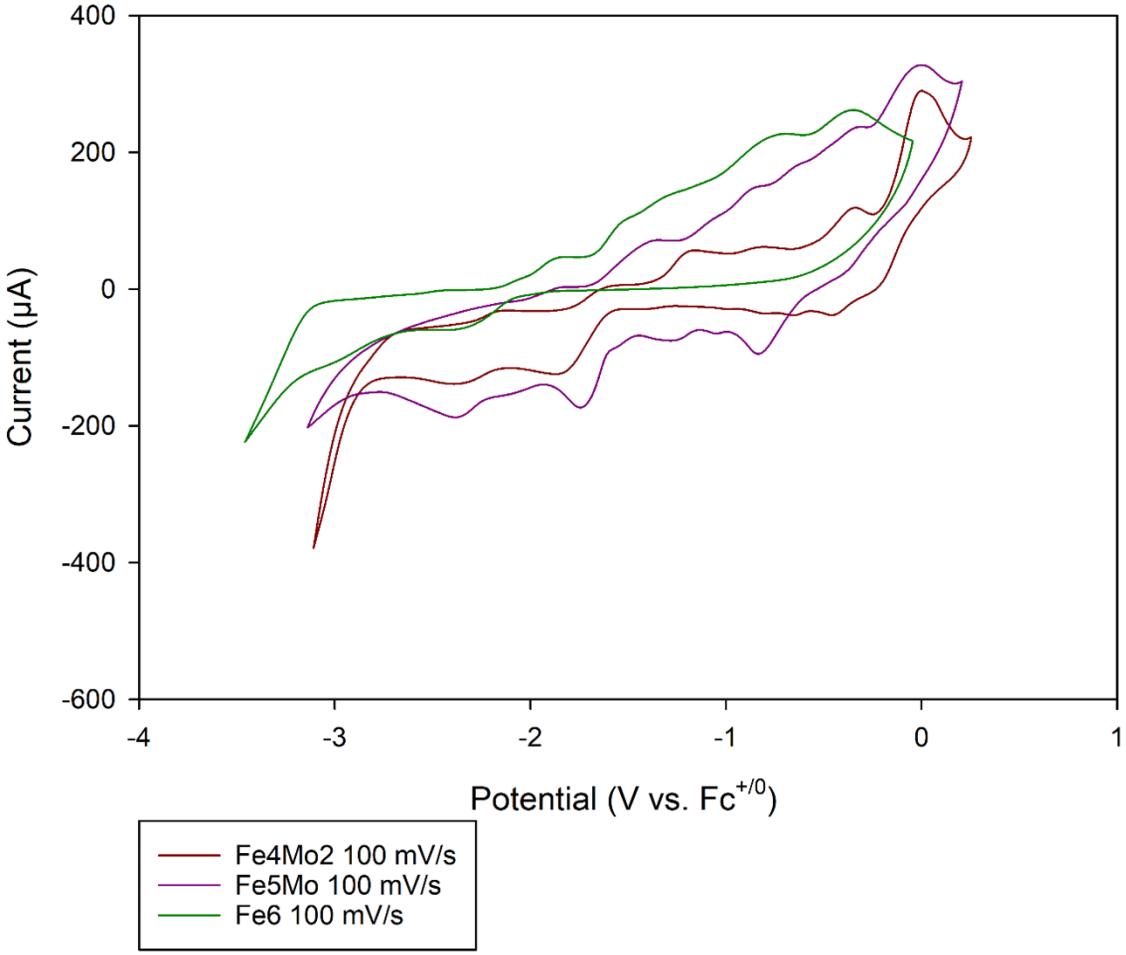


Figure S19. Comparison of the cyclic voltammograms (vs Fc/Fc^{+}) of 5 mM of cluster in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **100 mV/s**.

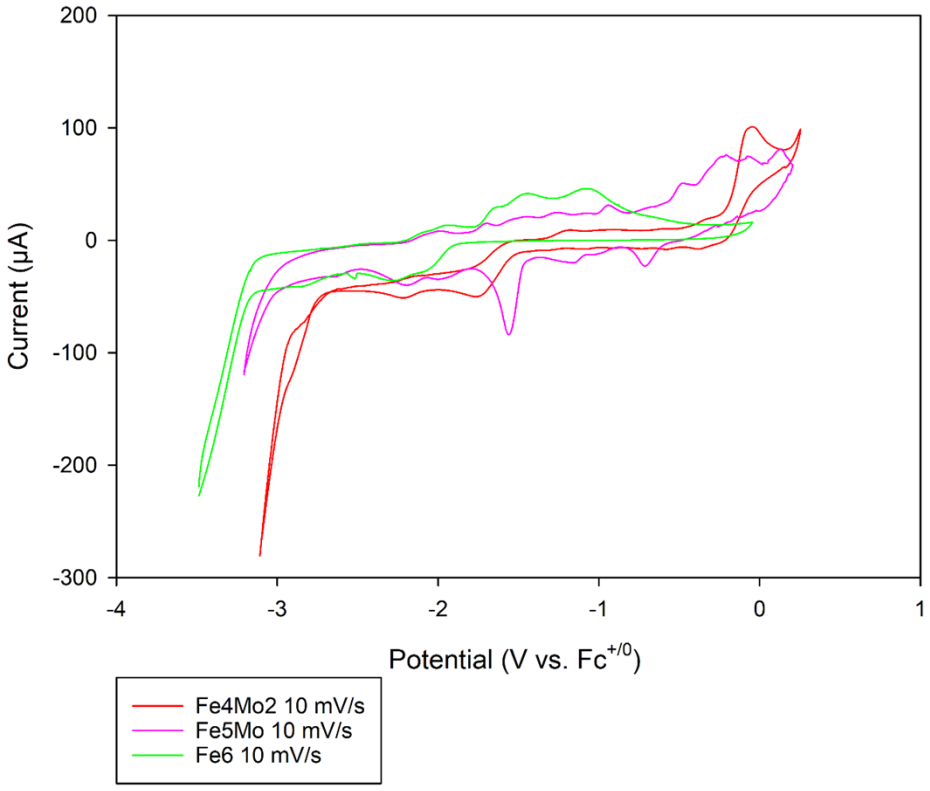


Figure S20. Comparison of cyclic voltammograms (vs Fc/Fc^+) of 5 mM of cluster in MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **10 mV/s**.

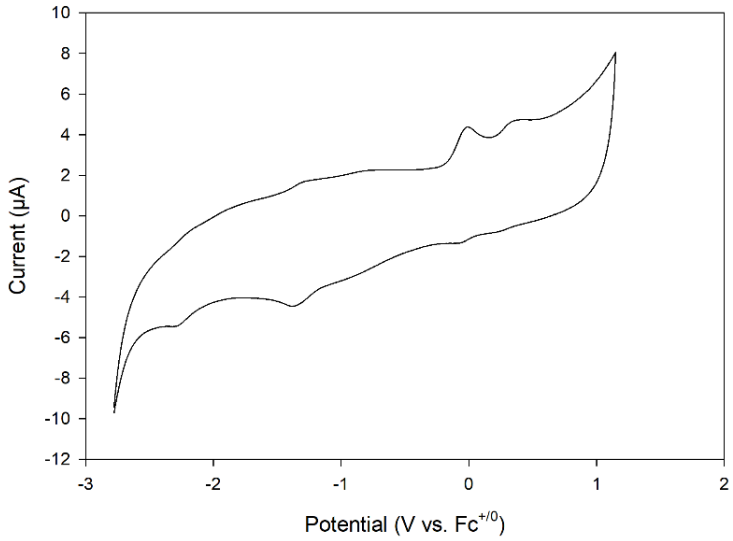


Figure S21. Cyclic voltammogram (vs Fc/Fc^+) of MeCN containing 0.2 M $TBAPF_6$. Experiment conditions: Experiment conditions: WE, glassy carbon; CE, Pt wire; RE, Ag wire quasi-reference; scan rate: **100 mV/s**.

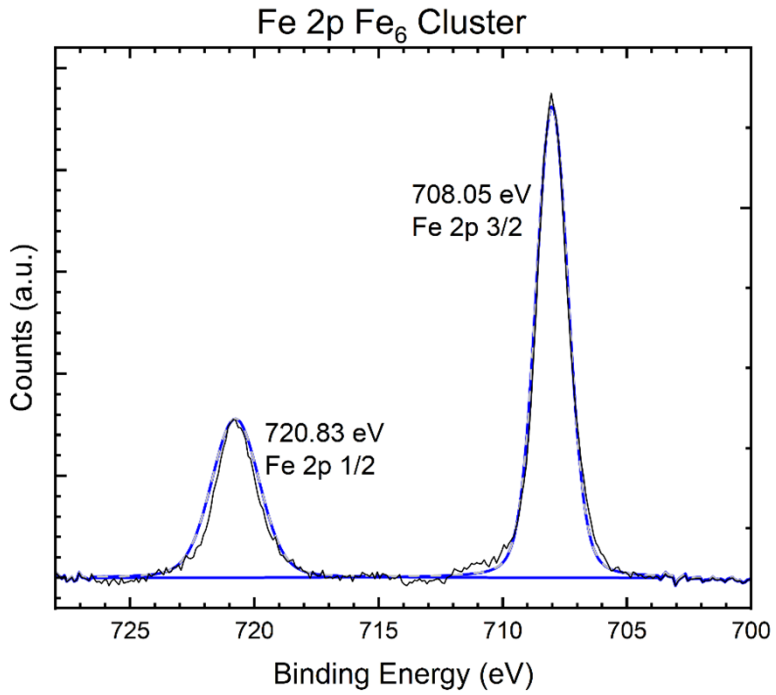


Figure S22. High-resolution X-ray photo-electron spectrum (XPS) of the iron 2*p* region of Fe_6.

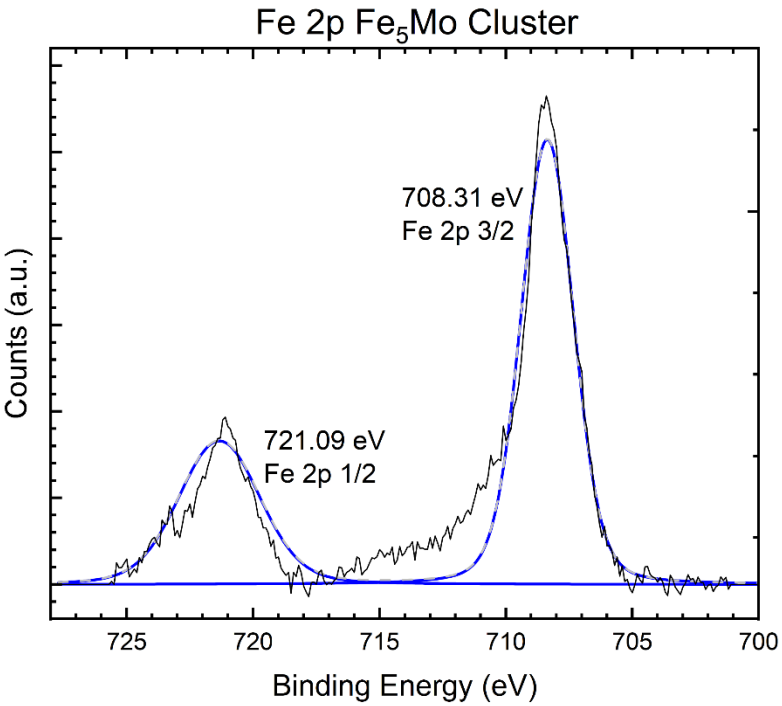


Figure S23. High-resolution X-ray photo-electron spectrum (XPS) of the iron 2*p* region of Fe_5Mo.

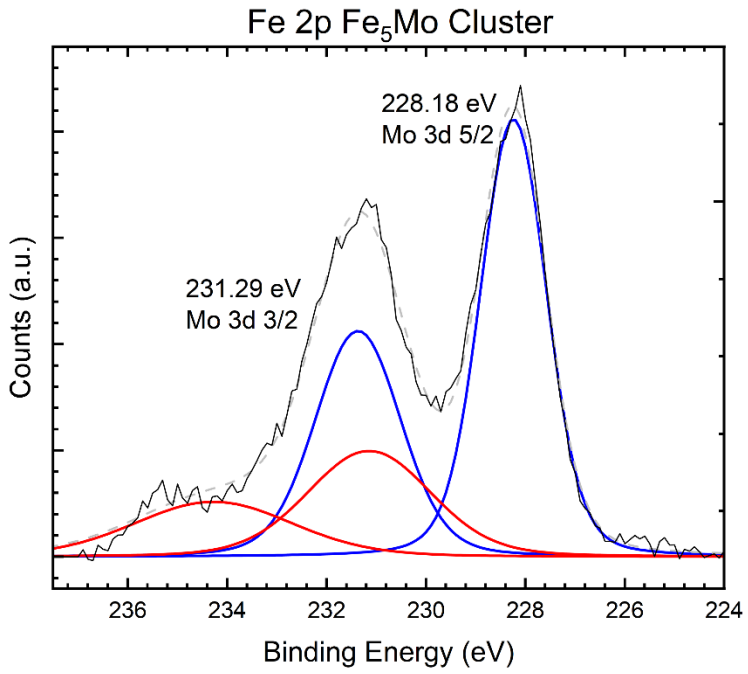


Figure S24. High-resolution X-ray photo-electron spectrum (XPS) of the molybdenum 3*d* region of Fe_5Mo.

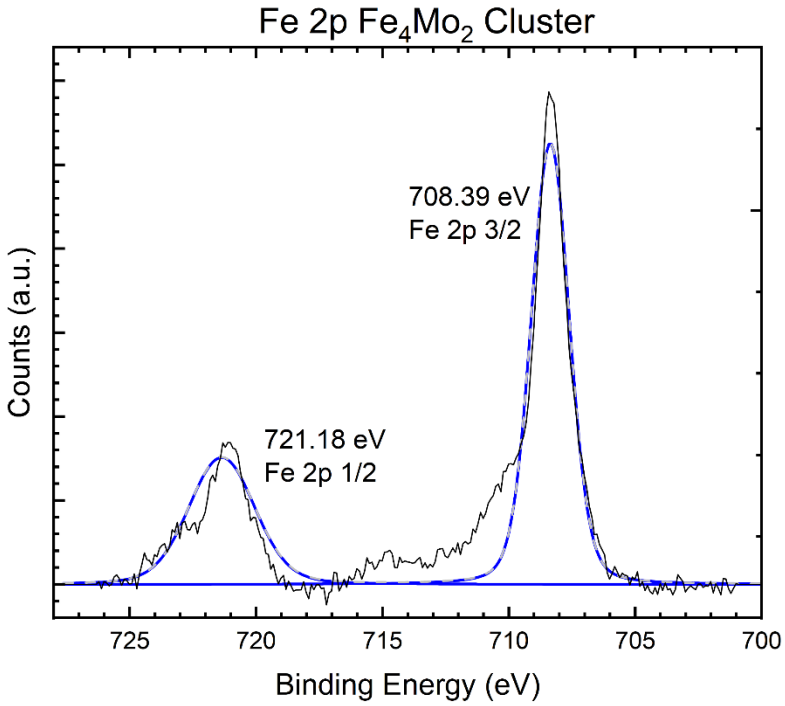


Figure S25. High-resolution X-ray photo-electron spectrum (XPS) of the iron 2*p* region of Fe_4Mo_2.

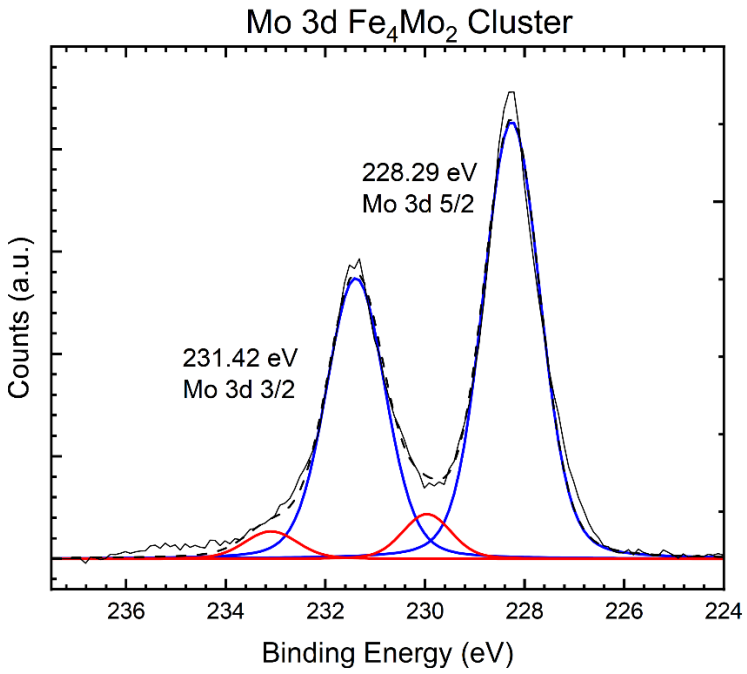


Figure S26. High-resolution X-ray photo-electron spectrum (XPS) of the molybdenum 3*d* region of Fe_4Mo_2.

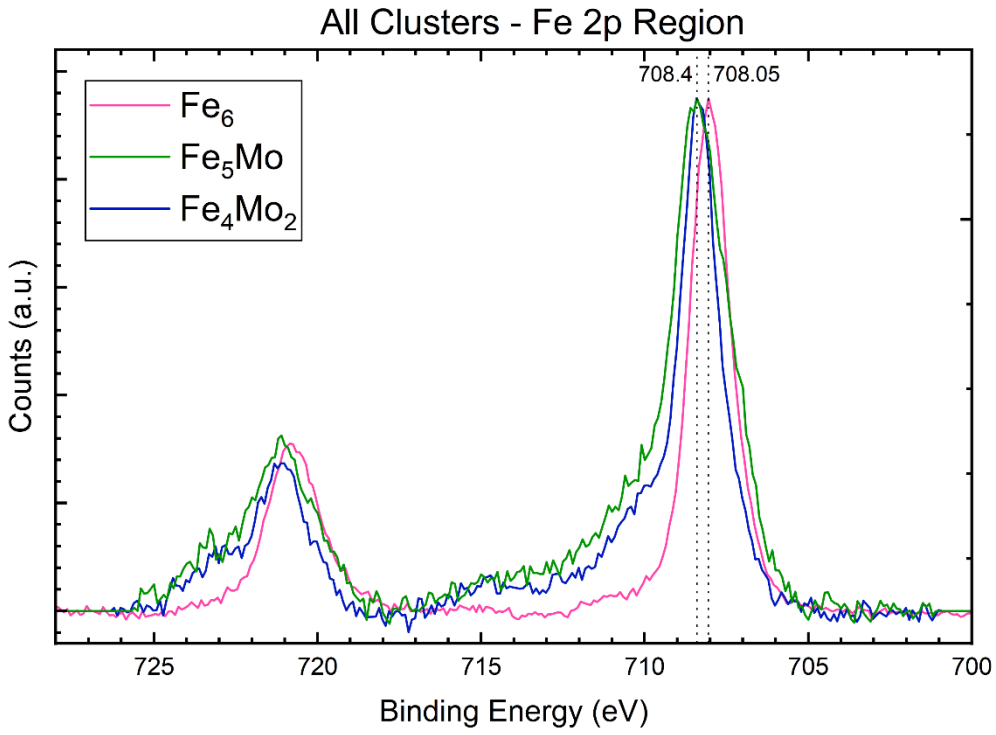


Figure S27. High-resolution X-ray photo-electron spectrum (XPS) of the iron 2*p* regions of Fe_6 (pink), Fe_5Mo (green) and Fe_4Mo_2 (blue).

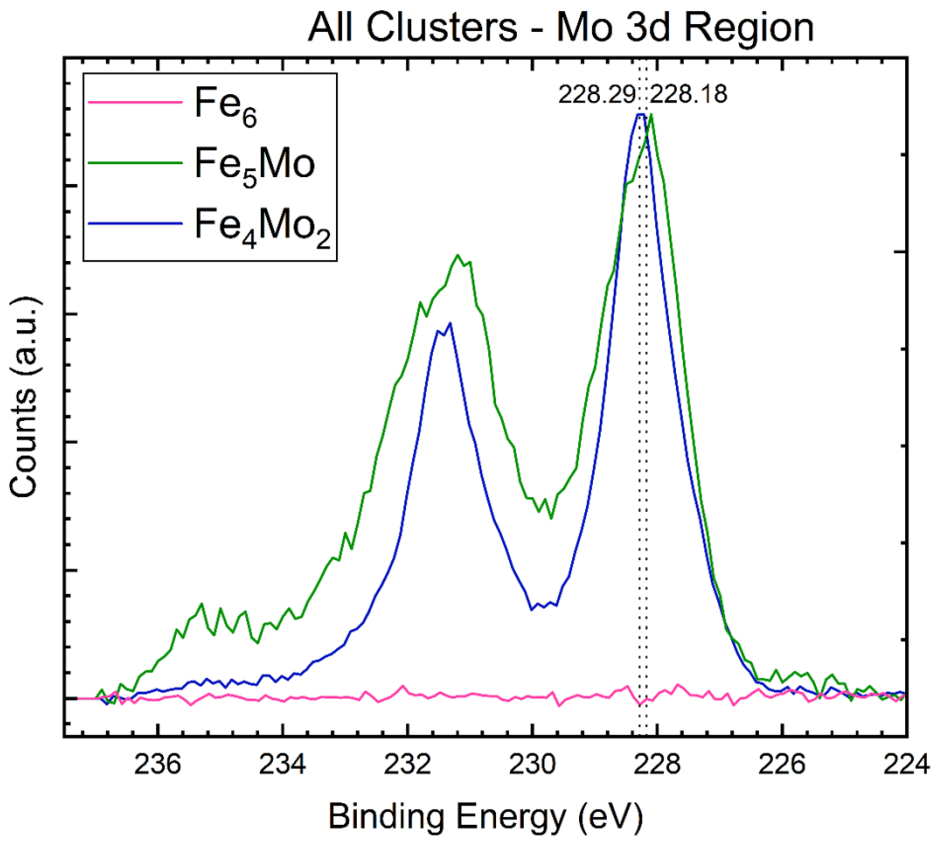


Figure S28. High-resolution X-ray photo-electron spectrum (XPS) of the molybdenum 3*d* regions of Fe_6 (pink), Fe_5Mo (green) and Fe_4Mo_2 (blue).

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

Identification code	$[Fe_4]^{2-}$	
Empirical formula	C82.50 H84.50 F2.50 Fe6 K3 O36	
Formula weight	2151.90	
Temperature	100.15 K	
Wavelength	1.54184 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.2695(7) Å	a= 113.941(6)°.
	b = 20.7691(14) Å	b= 101.028(5)°.
	c = 22.4933(12) Å	g = 95.660(6)°.
Volume	4630.9(6) $Å^3$	
Z	2	
Density (calculated)	1.543 Mg/m^3	
Absorption coefficient	9.323 mm^{-1}	
F(000)	2206	
Crystal size	0.12 x 0.089 x 0.038 mm^3	
Theta range for data collection	3.896 to 69.080°.	
Index ranges	-13<=h<=11, -25<=k<=24, -27<=l<=24	
Reflections collected	33287	
Independent reflections	16876 [R(int) = 0.1168]	
Completeness to theta = 67.684°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.79418	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16876 / 1551 / 1450	
Goodness-of-fit on F^2	0.941	
Final R indices [I>2sigma(I)]	R1 = 0.0695, wR2 = 0.1270	
R indices (all data)	R1 = 0.1498, wR2 = 0.1553	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.691 and -0.592 $e.Å^{-3}$	

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

	x	y	z	U(eq)
Fe1B	8294(1)	7509(1)	8561(1)	37(1)
Fe3B	7322(1)	6422(1)	8739(1)	40(1)
Fe2B	6925(1)	5679(1)	7423(1)	48(1)
Fe4B	9156(1)	6311(1)	8229(1)	44(1)
K2	4680(1)	8728(1)	8011(1)	34(1)
K1	3183(1)	8159(1)	6072(1)	40(1)
K3	7770(1)	3606(1)	8190(1)	43(1)
O7	3104(4)	8844(2)	8813(2)	32(1)
O8	3006(4)	7534(2)	7750(2)	38(1)
O9	4368(4)	7467(2)	6759(2)	37(1)
O10	6599(4)	8509(3)	7446(2)	38(1)
O11	6683(4)	9844(2)	8511(2)	38(1)
O12	4789(4)	9941(2)	9156(2)	35(1)
C17	2720(6)	9490(3)	9057(3)	32(2)
C18	2242(6)	8206(3)	8671(3)	35(2)
C19	2860(6)	7583(4)	8382(3)	38(2)
C20	3505(6)	6922(3)	7398(3)	37(2)
C21	3517(6)	6876(4)	6725(3)	38(2)
C22	5569(6)	7305(4)	6699(4)	44(2)
C23	6377(6)	7967(4)	6778(3)	44(2)
C24	7425(6)	9147(4)	7576(4)	46(2)
C25	7757(6)	9602(4)	8309(4)	45(2)
C26	6899(6)	10237(4)	9216(3)	44(2)
C27	5778(6)	10542(4)	9364(3)	40(2)
C28	3639(6)	10089(3)	9244(3)	34(2)
C29	3374(6)	10778(4)	9491(3)	43(2)
C30	2175(6)	10852(4)	9540(4)	46(2)
C31	1267(6)	10258(4)	9358(3)	42(2)
C32	1537(6)	9569(4)	9109(3)	37(2)
O1	3267(4)	7002(3)	4930(2)	43(1)
C1	4415(6)	6906(4)	4801(3)	45(2)

O2	1239(4)	7011(3)	5481(2)	46(1)
C2	2340(6)	6359(4)	4687(4)	51(2)
O3	1164(4)	8319(3)	6536(2)	46(1)
C3	1140(7)	6594(4)	4776(4)	54(2)
O4	3313(4)	9394(2)	7351(2)	38(1)
C4	102(6)	7232(4)	5592(4)	52(2)
O5	4768(4)	9444(2)	6431(2)	41(1)
C5	272(6)	7679(4)	6326(4)	49(2)
O6	4837(4)	8172(2)	5320(2)	39(1)
C6	1264(6)	8816(4)	7196(4)	49(2)
C7	2072(6)	9506(4)	7349(4)	45(2)
C8	4130(6)	10008(4)	7426(3)	43(2)
C9	4180(7)	10020(4)	6774(4)	45(2)
C10	4973(6)	9440(4)	5819(4)	46(2)
C11	5643(6)	8850(4)	5520(3)	44(2)
C12	5253(6)	7553(4)	5019(3)	39(2)
C13	6411(6)	7538(4)	4904(3)	50(2)
C14	6739(7)	6863(5)	4582(4)	58(2)
C15	5917(8)	6236(5)	4375(4)	71(3)
C16	4744(7)	6261(4)	4499(4)	60(2)
O3B	6165(4)	8187(3)	8727(2)	45(1)
O2B	10172(4)	8506(3)	9797(2)	48(1)
O11B	11278(5)	7128(3)	9389(3)	53(1)
O9B	7071(5)	5008(3)	8745(3)	57(1)
O7B	8709(5)	7307(3)	10133(3)	52(1)
O1B	9121(4)	7943(3)	7606(3)	57(2)
O12B	9491(5)	4940(3)	8269(3)	57(1)
O13	6033(5)	3745(3)	8993(3)	62(2)
O14	8603(5)	4125(3)	9595(2)	53(1)
O15	10132(5)	3484(3)	8750(3)	53(1)
O16	9302(5)	3000(3)	7364(3)	54(1)
O17	6747(5)	2502(3)	6894(2)	50(1)
O18	5152(4)	2867(3)	7749(2)	48(1)
C33	5111(7)	3173(5)	8881(4)	57(2)
C34	6599(8)	4270(5)	9688(4)	65(2)
C35	7711(7)	4054(5)	9949(4)	61(2)

C36	9717(7)	3931(4)	9825(4)	55(2)
C37	10592(7)	4003(4)	9423(4)	58(2)
C38	10953(7)	3486(4)	8347(4)	56(2)
C39	10447(7)	2881(5)	7665(4)	61(2)
C40	8742(7)	2437(4)	6710(4)	59(2)
C41	7481(7)	2543(4)	6457(4)	56(2)
C42	5510(7)	2538(4)	6663(4)	57(2)
C43	4752(7)	2341(4)	7064(4)	56(2)
C44	4619(7)	2730(4)	8206(4)	52(2)
C45	3622(7)	2168(5)	8011(5)	64(2)
C46	3183(8)	2059(5)	8509(5)	74(3)
C47	3706(9)	2479(5)	9170(5)	79(3)
C48	4672(8)	3054(5)	9367(5)	73(3)
O10B	10348(5)	6349(3)	7187(3)	66(2)
O8B	4903(5)	6745(3)	8931(3)	58(2)
O5B	4244(5)	5478(3)	7039(3)	68(2)
O6B	7018(6)	4188(3)	7213(3)	76(2)
C3B	7025(6)	7926(4)	8670(3)	41(2)
C2B	9432(6)	8111(4)	9320(4)	37(2)
O4B	7256(7)	5781(4)	6202(3)	99(2)
C1B	8796(6)	7777(4)	7994(4)	40(2)
C0B	7591(6)	6604(4)	7982(3)	39(2)
C7B	8181(6)	6969(4)	9568(4)	42(2)
C8B	5869(6)	6607(4)	8834(4)	42(2)
C9B	7163(7)	5569(4)	8721(4)	49(2)
C11B	10395(7)	6827(4)	8943(4)	42(2)
C5B	5310(8)	5573(4)	7208(4)	53(2)
C12B	9336(7)	5482(4)	8227(4)	50(2)
C10B	9844(7)	6324(4)	7584(4)	50(2)
C6B	7009(8)	4786(4)	7299(4)	60(2)
C4B	7151(9)	5715(5)	6697(5)	70(3)
Fe1A	-274(2)	9049(1)	5020(1)	39(1)
Fe3A	-1188(2)	10185(1)	5104(1)	39(1)
Fe2A	1131(2)	10868(1)	5730(1)	44(1)
Fe4A	521(2)	9888(1)	4485(1)	41(1)
O1A	-1095(16)	9001(9)	6168(6)	44(4)

O2A	-1825(9)	7814(5)	3803(5)	51(3)
O12A	-1264(16)	8932(10)	3190(9)	58(4)
O9A	-1690(30)	11354(13)	4770(16)	70(9)
O8A	-3440(20)	9072(11)	4137(11)	38(5)
O3A	1914(19)	8464(10)	5147(12)	38(4)
O11A	1044(17)	11089(11)	4144(8)	44(6)
O10A	2790(9)	9330(5)	4286(5)	47(2)
O7A	-2208(10)	10511(6)	6261(6)	57(3)
O5A	1033(9)	12283(4)	5768(5)	59(3)
C1A	-780(20)	8986(16)	5698(14)	36(6)
C2A	-1280(40)	8280(13)	4270(30)	47(7)
O4A	3690(20)	10772(12)	5778(14)	51(6)
C3A	1108(17)	8679(13)	5095(11)	42(5)
C0A	434(10)	9947(6)	5371(6)	27(3)
C8A	-2442(15)	9508(8)	4518(8)	36(4)
C7A	-1810(20)	10388(12)	5797(11)	39(5)
C9A	-1382(13)	10893(8)	4904(7)	40(3)
C12A	-532(15)	9345(9)	3728(8)	43(4)
C11A	804(13)	10623(8)	4296(7)	36(4)
C10A	1860(30)	9542(14)	4386(13)	50(7)
C5A	1080(40)	11715(12)	5740(30)	45(7)
C4A	2749(17)	10865(12)	5763(12)	46(5)
C6A	1010(30)	10973(18)	6531(7)	58(8)
O6A	1015(14)	11010(9)	7055(5)	62(4)
F1D	1186(9)	3821(6)	6492(5)	116(4)
C1D	1951(13)	4194(8)	7096(6)	79(4)
C2D	1800(16)	4877(8)	7502(8)	83(5)
C3D	2643(17)	5290(9)	8119(8)	82(4)
C4D	3636(16)	5019(11)	8330(7)	75(3)
C5D	3786(14)	4335(12)	7924(8)	73(3)
C6D	2944(13)	3923(9)	7307(7)	70(4)
F1DA	4232(15)	5253(10)	8930(8)	117(5)
C1DA	3440(30)	4953(19)	8319(10)	76(4)
C6DA	3810(20)	4356(19)	7883(14)	71(4)
C5DA	3130(20)	3985(14)	7216(12)	64(8)
C4DA	2090(20)	4210(14)	6986(9)	84(6)

C3DA	1730(20)	4806(14)	7422(13)	64(8)
C2DA	2400(30)	5178(15)	8089(12)	86(6)
F1E	-2139(11)	5120(10)	4709(8)	80(5)
C1E	-1002(13)	5039(13)	4879(8)	53(4)
C2E	-350(15)	5360(14)	5551(8)	50(4)
C3E	852(15)	5272(15)	5732(10)	53(4)
C4E	1402(13)	4862(14)	5240(12)	55(4)
C5E	749(16)	4541(14)	4568(11)	54(4)
C6E	-452(16)	4629(13)	4387(8)	54(4)
F1EA	1650(20)	5391(14)	6059(12)	76(6)
C1EA	720(20)	5250(20)	5501(13)	54(4)
C6EA	900(20)	4839(18)	4870(17)	55(4)
C5EA	-50(30)	4640(18)	4296(13)	53(4)
C4EA	-1180(30)	4850(20)	4353(13)	52(5)
C3EA	-1350(20)	5260(20)	4984(16)	53(4)
C2EA	-400(30)	5460(20)	5558(12)	52(4)
F1F	10074(10)	513(6)	7824(6)	131(4)
C1F	9269(9)	933(6)	7922(5)	83(3)
C2F	8350(10)	875(6)	7383(4)	84(3)
C3F	7438(9)	1281(7)	7497(5)	85(3)
C4F	7443(10)	1746(6)	8149(6)	87(3)
C5F	8361(12)	1804(6)	8689(5)	86(3)
C6F	9274(10)	1398(6)	8575(4)	83(3)
F1FA	6663(17)	2051(10)	9315(9)	174(7)
C1FA	7325(14)	1875(8)	8855(7)	80(3)
C2FA	8566(14)	1845(8)	9016(6)	82(4)
C3FA	9152(10)	1537(9)	8507(8)	84(3)
C4FA	8497(14)	1259(8)	7838(7)	83(3)
C5FA	7256(13)	1288(8)	7676(6)	87(3)
C6FA	6670(10)	1596(8)	8185(8)	81(3)

Table S3. Bond lengths (Å) and angles (°) for **1**.

Fe1B-Fe3B	2.6198(15)	K1-O1	2.740(5)
Fe1B-Fe4B	2.6337(16)	K1-O2	2.745(5)
Fe1B-C3B	1.749(7)	K1-O3	2.675(5)
Fe1B-C2B	1.799(7)	K1-O4	2.943(5)
Fe1B-C1B	1.746(7)	K1-C4	3.534(7)
Fe1B-C0B	1.784(7)	K1-O5	2.779(5)
Fe3B-Fe2B	2.6437(17)	K1-O6	2.751(4)
Fe3B-Fe4B	2.5352(16)	K1-C9	3.494(7)
Fe3B-C0B	1.956(7)	K1-C10	3.475(7)
Fe3B-C7B	1.755(8)	K1-O3A	2.62(2)
Fe3B-C8B	1.751(7)	K1-C3A	3.45(2)
Fe3B-C9B	1.747(7)	K3-O9B	2.922(5)
Fe2B-Fe4B	2.6468(18)	K3-O12B	3.143(6)
Fe2B-C0B	1.796(7)	K3-O13	2.867(6)
Fe2B-C5B	1.759(8)	K3-O14	2.815(5)
Fe2B-C6B	1.776(8)	K3-O15	2.802(5)
Fe2B-C4B	1.728(9)	K3-O16	2.789(5)
Fe4B-C0B	1.974(7)	K3-O17	2.802(5)
Fe4B-C11B	1.769(8)	K3-O18	2.965(5)
Fe4B-C12B	1.752(7)	K3-O6B	2.941(6)
Fe4B-C10B	1.777(7)	O7-C17	1.377(7)
K2-O7	2.726(4)	O7-C18	1.444(7)
K2-O8	2.742(5)	O8-C19	1.427(7)
K2-O9	2.893(5)	O8-C20	1.434(7)
K2-O10	2.696(4)	O9-C21	1.449(7)
K2-O11	2.760(5)	O9-C22	1.443(7)
K2-O12	2.748(5)	O10-C23	1.420(8)
K2-C19	3.444(7)	O10-C24	1.431(8)
K2-C20	3.441(7)	O11-C25	1.438(7)
K2-C26	3.520(7)	O11-C26	1.415(7)
K2-O4	2.776(4)	O12-C27	1.439(7)
K2-C8	3.471(7)	O12-C28	1.393(7)
K2-O3B	2.731(5)	C17-C28	1.398(9)
K1-O9	2.760(4)	C17-C32	1.381(9)

C18-H18A	0.99	C1-C16	1.360(10)
C18-H18B	0.99	O2-C3	1.441(8)
C18-C19	1.500(8)	O2-C4	1.435(8)
C19-H19A	0.99	C2-H2A	0.99
C19-H19B	0.99	C2-H2B	0.99
C20-H20A	0.99	C2-C3	1.504(10)
C20-H20B	0.99	O3-C5	1.431(8)
C20-C21	1.479(8)	O3-C6	1.398(8)
C21-H21A	0.99	C3-H3A	0.99
C21-H21B	0.99	C3-H3B	0.99
C22-H22A	0.99	O4-C7	1.439(7)
C22-H22B	0.99	O4-C8	1.428(8)
C22-C23	1.497(10)	C4-H4A	0.99
C23-H23A	0.99	C4-H4B	0.99
C23-H23B	0.99	C4-C5	1.491(10)
C24-H24A	0.99	O5-C9	1.439(8)
C24-H24B	0.99	O5-C10	1.435(7)
C24-C25	1.477(9)	C5-H5A	0.99
C25-H25A	0.99	C5-H5B	0.99
C25-H25B	0.99	O6-C11	1.445(7)
C26-H26A	0.99	O6-C12	1.366(8)
C26-H26B	0.99	C6-H6A	0.99
C26-C27	1.503(9)	C6-H6B	0.99
C27-H27A	0.99	C6-C7	1.491(10)
C27-H27B	0.99	C7-H7A	0.99
C28-C29	1.396(9)	C7-H7B	0.99
C29-H29	0.95	C8-H8A	0.99
C29-C30	1.394(9)	C8-H8B	0.99
C30-H30	0.95	C8-C9	1.489(9)
C30-C31	1.384(9)	C9-H9A	0.99
C31-H31	0.95	C9-H9B	0.99
C31-C32	1.398(9)	C10-H10A	0.99
C32-H32	0.95	C10-H10B	0.99
O1-C1	1.394(8)	C10-C11	1.494(9)
O1-C2	1.446(8)	C11-H11A	0.99
C1-C12	1.406(10)	C11-H11B	0.99

C12-C13	1.379(9)	C36-C37	1.496(10)
C13-H13	0.95	C37-H37A	0.99
C13-C14	1.415(10)	C37-H37B	0.99
C14-H14	0.95	C38-H38A	0.99
C14-C15	1.370(12)	C38-H38B	0.99
C15-H15	0.95	C38-C39	1.489(10)
C15-C16	1.404(11)	C39-H39A	0.99
C16-H16	0.95	C39-H39B	0.99
O3B-C3B	1.160(8)	C40-H40A	0.99
O2B-C2B	1.152(8)	C40-H40B	0.99
O11B-C11B	1.171(8)	C40-C41	1.500(10)
O9B-C9B	1.182(8)	C41-H41A	0.99
O7B-C7B	1.169(8)	C41-H41B	0.99
O1B-C1B	1.164(8)	C42-H42A	0.99
O12B-C12B	1.194(8)	C42-H42B	0.99
O13-C33	1.404(9)	C42-C43	1.496(10)
O13-C34	1.462(9)	C43-H43A	0.99
O14-C35	1.428(9)	C43-H43B	0.99
O14-C36	1.424(8)	C44-C45	1.397(10)
O15-C37	1.409(9)	C45-H45	0.95
O15-C38	1.415(8)	C45-C46	1.394(11)
O16-C39	1.430(8)	C46-H46	0.95
O16-C40	1.426(8)	C46-C47	1.354(12)
O17-C41	1.423(8)	C47-H47	0.95
O17-C42	1.412(8)	C47-C48	1.392(12)
O18-C43	1.428(8)	C48-H48	0.95
O18-C44	1.393(9)	O10B-C10B	1.162(8)
C33-C44	1.378(11)	O8B-C8B	1.191(8)
C33-C48	1.380(11)	O5B-C5B	1.159(9)
C34-H34A	0.99	O6B-C6B	1.179(9)
C34-H34B	0.99	O4B-C4B	1.202(9)
C34-C35	1.469(10)	Fe1A-Fe3A	2.617(3)
C35-H35A	0.99	Fe1A-Fe4A	2.663(3)
C35-H35B	0.99	Fe1A-C1A	1.77(2)
C36-H36A	0.99	Fe1A-C2A	1.85(4)
C36-H36B	0.99	Fe1A-C3A	1.81(2)

Fe1A-C0A	1.733(11)	C4D-C5D	1.39
Fe3A-Fe2A	2.657(3)	C5D-H5D	0.95
Fe3A-Fe4A	2.567(3)	C5D-C6D	1.39
Fe3A-C0A	1.987(12)	C6D-H6D	0.95
Fe3A-C8A	1.762(16)	F1DA-C1DA	1.34(2)
Fe3A-C7A	1.74(2)	C1DA-C6DA	1.39
Fe3A-C9A	1.725(14)	C1DA-C2DA	1.39
Fe2A-Fe4A	2.611(3)	C6DA-H6DA	0.95
Fe2A-C0A	1.771(12)	C6DA-C5DA	1.39
Fe2A-C5A	1.760(8)	C5DA-H5DA	0.95
Fe2A-C4A	1.811(19)	C5DA-C4DA	1.39
Fe2A-C6A	1.758(8)	C4DA-H4DA	0.95
Fe4A-C0A	1.969(12)	C4DA-C3DA	1.39
Fe4A-C12A	1.728(17)	C3DA-H3DA	0.95
Fe4A-C11A	1.758(15)	C3DA-C2DA	1.39
Fe4A-C10A	1.74(3)	C2DA-H2DA	0.95
O1A-C1A	1.17(3)	F1E-C1E	1.312(6)
O2A-C2A	1.11(5)	C1E-C2E	1.39
O12A-C12A	1.23(2)	C1E-C6E	1.39
O9A-C9A	1.18(3)	C2E-H2E	0.95
O8A-C8A	1.27(3)	C2E-C3E	1.39
O3A-C3A	1.06(3)	C3E-H3E	0.95
O11A-C11A	1.17(2)	C3E-C4E	1.39
O10A-C10A	1.21(3)	C4E-H4E	0.95
O7A-C7A	1.16(2)	C4E-C5E	1.39
O5A-C5A	1.160(8)	C5E-H5E	0.95
O4A-C4A	1.09(3)	C5E-C6E	1.39
C6A-O6A	1.150(8)	C6E-H6E	0.95
F1D-C1D	1.324(6)	F1EA-C1EA	1.38(3)
C1D-C2D	1.39	C1EA-C6EA	1.39
C1D-C6D	1.39	C1EA-C2EA	1.39
C2D-H2D	0.95	C6EA-H6EA	0.95
C2D-C3D	1.39	C6EA-C5EA	1.39
C3D-H3D	0.95	C5EA-H5EA	0.95
C3D-C4D	1.39	C5EA-C4EA	1.39
C4D-H4D	0.95	C4EA-H4EA	0.95

C4EA-C3EA	1.39	C5F-C6F	1.39
C3EA-H3EA	0.95	C6F-H6F	0.95
C3EA-C2EA	1.39	F1FA-C1FA	1.34(2)
C2EA-H2EA	0.95	C1FA-C2FA	1.39
F1F-C1F	1.307(6)	C1FA-C6FA	1.39
C1F-C2F	1.39	C2FA-H2FA	0.95
C1F-C6F	1.39	C2FA-C3FA	1.39
C2F-H2F	0.95	C3FA-H3FA	0.95
C2F-C3F	1.39	C3FA-C4FA	1.39
C3F-H3F	0.95	C4FA-H4FA	0.95
C3F-C4F	1.39	C4FA-C5FA	1.39
C4F-H4F	0.95	C5FA-H5FA	0.95
C4F-C5F	1.39	C5FA-C6FA	1.39
C5F-H5F	0.95	C6FA-H6FA	0.95

Fe3B-Fe1B-Fe4B	57.71(4)
C3B-Fe1B-Fe3B	93.5(2)
C3B-Fe1B-Fe4B	147.9(2)
C3B-Fe1B-C2B	100.7(3)
C3B-Fe1B-C0B	102.8(3)
C2B-Fe1B-Fe3B	108.6(2)
C2B-Fe1B-Fe4B	101.9(2)
C1B-Fe1B-Fe3B	145.5(2)
C1B-Fe1B-Fe4B	97.4(2)
C1B-Fe1B-C3B	101.1(3)
C1B-Fe1B-C2B	99.3(3)
C1B-Fe1B-C0B	97.6(3)
C0B-Fe1B-Fe3B	48.3(2)
C0B-Fe1B-Fe4B	48.5(2)
C0B-Fe1B-C2B	147.7(3)
Fe1B-Fe3B-Fe2B	85.69(5)
Fe4B-Fe3B-Fe1B	61.42(4)
Fe4B-Fe3B-Fe2B	61.43(5)
C0B-Fe3B-Fe1B	42.9(2)
C0B-Fe3B-Fe2B	42.8(2)
C0B-Fe3B-Fe4B	50.1(2)
C7B-Fe3B-Fe1B	81.3(2)
C7B-Fe3B-Fe2B	157.0(2)
C7B-Fe3B-Fe4B	95.6(2)
C7B-Fe3B-C0B	122.0(3)
C8B-Fe3B-Fe1B	102.5(2)
C8B-Fe3B-Fe2B	103.0(2)
C8B-Fe3B-Fe4B	156.8(2)
C8B-Fe3B-C0B	106.6(3)
C8B-Fe3B-C7B	98.4(3)
C9B-Fe3B-Fe1B	156.8(3)
C9B-Fe3B-Fe2B	83.0(3)
C9B-Fe3B-Fe4B	95.4(3)
C9B-Fe3B-C0B	123.2(3)
C9B-Fe3B-C7B	102.0(3)
C9B-Fe3B-C8B	99.7(4)

Fe3B-Fe2B-Fe4B	57.27(4)
C0B-Fe2B-Fe3B	47.7(2)
C0B-Fe2B-Fe4B	48.2(2)
C5B-Fe2B-Fe3B	98.2(3)
C5B-Fe2B-Fe4B	153.6(3)
C5B-Fe2B-C0B	109.3(3)
C5B-Fe2B-C6B	98.0(4)
C6B-Fe2B-Fe3B	104.9(3)
C6B-Fe2B-Fe4B	97.9(3)
C6B-Fe2B-C0B	142.8(4)
C4B-Fe2B-Fe3B	144.4(3)
C4B-Fe2B-Fe4B	99.6(3)
C4B-Fe2B-C0B	96.8(4)
C4B-Fe2B-C5B	96.6(4)
C4B-Fe2B-C6B	104.9(4)
Fe1B-Fe4B-Fe2B	85.35(5)
Fe3B-Fe4B-Fe1B	60.87(4)
Fe3B-Fe4B-Fe2B	61.31(5)
C0B-Fe4B-Fe1B	42.6(2)
C0B-Fe4B-Fe3B	49.5(2)
C0B-Fe4B-Fe2B	42.7(2)
C11B-Fe4B-Fe1B	84.8(2)
C11B-Fe4B-Fe3B	101.9(2)
C11B-Fe4B-Fe2B	163.2(2)
C11B-Fe4B-C0B	126.2(3)
C11B-Fe4B-C10B	99.9(4)
C12B-Fe4B-Fe1B	155.6(3)
C12B-Fe4B-Fe3B	95.4(3)
C12B-Fe4B-Fe2B	88.0(3)
C12B-Fe4B-C0B	126.9(3)
C12B-Fe4B-C11B	95.4(3)
C12B-Fe4B-C10B	103.1(4)
C10B-Fe4B-Fe1B	100.9(2)
C10B-Fe4B-Fe3B	149.7(3)
C10B-Fe4B-Fe2B	95.3(3)
C10B-Fe4B-C0B	100.4(3)

O7-K2-O8	60.96(13)
O7-K2-O9	122.06(13)
O7-K2-O11	115.82(14)
O7-K2-O12	55.78(12)
O7-K2-C19	43.04(13)
O7-K2-C20	82.64(14)
O7-K2-C26	94.85(15)
O7-K2-O4	91.27(13)
O7-K2-C8	103.47(15)
O7-K2-O3B	89.54(14)
O8-K2-O9	62.03(13)
O8-K2-O11	165.93(14)
O8-K2-O12	116.47(13)
O8-K2-C19	23.34(14)
O8-K2-C20	23.52(13)
O8-K2-C26	147.66(15)
O8-K2-O4	102.43(13)
O8-K2-C8	125.58(15)
O9-K2-C19	83.66(14)
O9-K2-C20	44.19(13)
O9-K2-C26	141.54(15)
O9-K2-C8	100.81(14)
O10-K2-O7	164.90(14)
O10-K2-O8	117.08(14)
O10-K2-O9	61.17(13)
O10-K2-O11	62.01(14)
O10-K2-O12	122.17(14)
O10-K2-C19	129.58(15)
O10-K2-C20	93.74(15)
O10-K2-C26	80.38(15)
O10-K2-O4	103.59(13)
O10-K2-C8	89.68(15)
O10-K2-O3B	75.43(14)
O11-K2-O9	121.99(13)
O11-K2-C19	145.44(15)
O11-K2-C20	149.80(15)

O11-K2-C26	22.08(13)
O11-K2-O4	91.16(13)
O11-K2-C8	68.15(15)
O12-K2-O9	175.23(13)
O12-K2-O11	60.67(13)
O12-K2-C19	95.66(14)
O12-K2-C20	135.79(14)
O12-K2-C26	42.04(14)
O12-K2-O4	84.66(13)
O12-K2-C8	76.27(15)
C19-K2-C26	124.61(16)
C19-K2-C8	134.28(16)
C20-K2-C19	40.44(15)
C20-K2-C26	147.77(17)
C20-K2-C8	133.56(16)
O4-K2-O9	91.24(13)
O4-K2-C19	112.68(15)
O4-K2-C20	113.16(15)
O4-K2-C26	98.99(16)
O4-K2-C8	23.19(14)
C8-K2-C26	78.39(17)
O3B-K2-O8	82.34(14)
O3B-K2-O9	92.60(14)
O3B-K2-O11	83.97(14)
O3B-K2-O12	91.64(14)
O3B-K2-C19	71.12(15)
O3B-K2-C20	71.92(15)
O3B-K2-C26	75.94(16)
O3B-K2-O4	174.91(15)
O3B-K2-C8	152.08(16)
O9-K1-O4	90.50(13)
O9-K1-C4	101.25(16)
O9-K1-O5	106.94(14)
O9-K1-C9	115.82(15)
O9-K1-C10	118.12(15)
O9-K1-C3A	166.0(4)

O1-K1-O9	85.67(14)
O1-K1-O2	61.40(15)
O1-K1-O4	174.99(14)
O1-K1-C4	81.00(17)
O1-K1-O5	117.23(14)
O1-K1-O6	55.94(13)
O1-K1-C9	136.21(15)
O1-K1-C10	96.43(16)
O1-K1-C3A	89.1(4)
O2-K1-O9	88.85(14)
O2-K1-O4	121.82(14)
O2-K1-C4	22.19(17)
O2-K1-O5	164.15(14)
O2-K1-O6	116.05(15)
O2-K1-C9	147.76(16)
O2-K1-C10	144.83(16)
O2-K1-C3A	77.2(4)
O3-K1-O9	101.47(14)
O3-K1-O1	123.19(16)
O3-K1-O2	62.49(16)
O3-K1-O4	60.75(14)
O3-K1-C4	42.21(17)
O3-K1-O5	114.09(16)
O3-K1-O6	160.62(15)
O3-K1-C9	91.06(16)
O3-K1-C10	125.97(17)
O3-K1-C3A	70.7(4)
O4-K1-C4	102.95(16)
O4-K1-C9	43.44(14)
O4-K1-C10	82.53(15)
O4-K1-C3A	95.3(4)
O5-K1-O4	60.89(13)
O5-K1-C4	147.14(17)
O5-K1-C9	23.12(14)
O5-K1-C10	23.28(14)
O5-K1-C3A	87.0(4)

O6-K1-O9	97.78(14)
O6-K1-O4	121.62(14)
O6-K1-C4	131.05(16)
O6-K1-O5	61.44(14)
O6-K1-C9	82.50(15)
O6-K1-C10	43.05(15)
O6-K1-C3A	90.0(4)
C9-K1-C4	126.21(18)
C10-K1-C4	140.33(17)
C10-K1-C9	40.08(16)
O3A-K1-O9	164.4(4)
O3A-K1-O1	79.5(4)
O3A-K1-O2	79.7(5)
O3A-K1-O3	82.8(5)
O3A-K1-O4	104.6(4)
O3A-K1-C4	71.7(5)
O3A-K1-O5	84.5(5)
O3A-K1-O6	78.1(5)
O3A-K1-C9	78.8(4)
O3A-K1-C10	69.0(5)
O3A-K1-C3A	12.5(6)
C3A-K1-C4	65.0(4)
C3A-K1-C9	76.6(4)
C3A-K1-C10	75.4(4)
O9B-K3-O12B	61.59(14)
O9B-K3-O18	91.01(15)
O9B-K3-O6B	64.99(16)
O13-K3-O9B	63.92(15)
O13-K3-O12B	122.58(15)
O13-K3-O18	52.16(15)
O13-K3-O6B	109.85(18)
O14-K3-O9B	74.97(15)
O14-K3-O12B	89.53(15)
O14-K3-O13	59.78(15)
O14-K3-O18	109.14(15)
O14-K3-O6B	137.84(17)

O15-K3-O9B	118.09(16)
O15-K3-O12B	76.55(14)
O15-K3-O13	116.16(16)
O15-K3-O14	60.49(15)
O15-K3-O18	141.30(15)
O15-K3-O6B	129.05(18)
O16-K3-O9B	135.37(16)
O16-K3-O12B	76.05(15)
O16-K3-O13	160.67(17)
O16-K3-O14	120.25(16)
O16-K3-O15	59.77(16)
O16-K3-O17	60.12(16)
O16-K3-O18	117.44(16)
O16-K3-O6B	83.00(17)
O17-K3-O9B	126.02(15)
O17-K3-O12B	115.49(15)
O17-K3-O13	110.05(16)
O17-K3-O14	152.43(16)
O17-K3-O15	112.08(16)
O17-K3-O18	58.30(15)
O17-K3-O6B	68.77(15)
O18-K3-O12B	142.13(14)
O6B-K3-O12B	60.58(16)
O6B-K3-O18	84.97(16)
C17-O7-K2	115.7(3)
C17-O7-C18	117.5(5)
C18-O7-K2	118.0(3)
C19-O8-K2	107.1(4)
C19-O8-C20	112.5(5)
C20-O8-K2	106.8(4)
K1-O9-K2	89.62(13)
C21-O9-K2	110.5(3)
C21-O9-K1	110.8(3)
C22-O9-K2	108.3(4)
C22-O9-K1	121.6(4)
C22-O9-C21	113.2(5)

C23-O10-K2	118.3(4)
C23-O10-C24	113.3(5)
C24-O10-K2	115.2(4)
C25-O11-K2	111.9(4)
C26-O11-K2	110.8(3)
C26-O11-C25	112.9(5)
C27-O12-K2	117.9(4)
C28-O12-K2	114.0(4)
C28-O12-C27	117.5(5)
O7-C17-C28	114.2(6)
O7-C17-C32	125.1(6)
C32-C17-C28	120.6(6)
O7-C18-H18A	110.4
O7-C18-H18B	110.4
O7-C18-C19	106.6(5)
H18A-C18-H18B	108.6
C19-C18-H18A	110.4
C19-C18-H18B	110.4
K2-C19-H19A	78.0
K2-C19-H19B	158.8
O8-C19-K2	49.6(3)
O8-C19-C18	107.2(5)
O8-C19-H19A	110.3
O8-C19-H19B	110.3
C18-C19-K2	85.0(4)
C18-C19-H19A	110.3
C18-C19-H19B	110.3
H19A-C19-H19B	108.5
K2-C20-H20A	158.4
K2-C20-H20B	77.5
O8-C20-K2	49.7(3)
O8-C20-H20A	109.9
O8-C20-H20B	109.9
O8-C20-C21	108.9(5)
H20A-C20-H20B	108.3
C21-C20-K2	86.5(4)

C21-C20-H20A	109.9
C21-C20-H20B	109.9
O9-C21-C20	112.6(5)
O9-C21-H21A	109.1
O9-C21-H21B	109.1
C20-C21-H21A	109.1
C20-C21-H21B	109.1
H21A-C21-H21B	107.8
O9-C22-H22A	110.1
O9-C22-H22B	110.1
O9-C22-C23	108.1(6)
H22A-C22-H22B	108.4
C23-C22-H22A	110.1
C23-C22-H22B	110.1
O10-C23-C22	109.7(6)
O10-C23-H23A	109.7
O10-C23-H23B	109.7
C22-C23-H23A	109.7
C22-C23-H23B	109.7
H23A-C23-H23B	108.2
O10-C24-H24A	110.2
O10-C24-H24B	110.2
O10-C24-C25	107.4(5)
H24A-C24-H24B	108.5
C25-C24-H24A	110.2
C25-C24-H24B	110.2
O11-C25-C24	109.3(5)
O11-C25-H25A	109.8
O11-C25-H25B	109.8
C24-C25-H25A	109.8
C24-C25-H25B	109.8
H25A-C25-H25B	108.3
K2-C26-H26A	157.1
K2-C26-H26B	83.4
O11-C26-K2	47.2(3)
O11-C26-H26A	110.0

O11-C26-H26B	110.0
O11-C26-C27	108.5(5)
H26A-C26-H26B	108.4
C27-C26-K2	82.8(4)
C27-C26-H26A	110.0
C27-C26-H26B	110.0
O12-C27-C26	106.7(5)
O12-C27-H27A	110.4
O12-C27-H27B	110.4
C26-C27-H27A	110.4
C26-C27-H27B	110.4
H27A-C27-H27B	108.6
O12-C28-C17	115.4(6)
O12-C28-C29	124.2(6)
C29-C28-C17	120.3(6)
C28-C29-H29	120.7
C30-C29-C28	118.5(7)
C30-C29-H29	120.7
C29-C30-H30	119.4
C31-C30-C29	121.1(7)
C31-C30-H30	119.4
C30-C31-H31	119.9
C30-C31-C32	120.1(6)
C32-C31-H31	119.9
C17-C32-C31	119.2(6)
C17-C32-H32	120.4
C31-C32-H32	120.4
C1-O1-K1	118.2(4)
C1-O1-C2	116.5(6)
C2-O1-K1	117.8(4)
O1-C1-C12	113.6(6)
C16-C1-O1	125.4(7)
C16-C1-C12	120.9(7)
C3-O2-K1	112.4(4)
C4-O2-K1	111.6(4)
C4-O2-C3	111.4(5)

O1-C2-H2A	110.3
O1-C2-H2B	110.3
O1-C2-C3	107.1(6)
H2A-C2-H2B	108.6
C3-C2-H2A	110.3
C3-C2-H2B	110.3
C5-O3-K1	116.5(4)
C6-O3-K1	119.7(4)
C6-O3-C5	112.8(5)
O2-C3-C2	109.5(6)
O2-C3-H3A	109.8
O2-C3-H3B	109.8
C2-C3-H3A	109.8
C2-C3-H3B	109.8
H3A-C3-H3B	108.2
K2-O4-K1	88.28(13)
C7-O4-K2	127.9(4)
C7-O4-K1	106.9(4)
C8-O4-K2	106.9(4)
C8-O4-K1	110.4(4)
C8-O4-C7	113.1(5)
K1-C4-H4A	155.3
K1-C4-H4B	89.4
O2-C4-K1	46.2(3)
O2-C4-H4A	109.9
O2-C4-H4B	109.9
O2-C4-C5	108.9(5)
H4A-C4-H4B	108.3
C5-C4-K1	78.5(4)
C5-C4-H4A	109.9
C5-C4-H4B	109.9
C9-O5-K1	107.6(4)
C10-O5-K1	106.7(4)
C10-O5-C9	112.4(5)
O3-C5-C4	108.7(6)
O3-C5-H5A	109.9

O3-C5-H5B	109.9
C4-C5-H5A	109.9
C4-C5-H5B	109.9
H5A-C5-H5B	108.3
C11-O6-K1	117.0(4)
C12-O6-K1	117.5(4)
C12-O6-C11	118.5(5)
O3-C6-H6A	109.7
O3-C6-H6B	109.7
O3-C6-C7	109.9(6)
H6A-C6-H6B	108.2
C7-C6-H6A	109.7
C7-C6-H6B	109.7
O4-C7-C6	109.1(5)
O4-C7-H7A	109.9
O4-C7-H7B	109.9
C6-C7-H7A	109.9
C6-C7-H7B	109.9
H7A-C7-H7B	108.3
K2-C8-H8A	59.1
K2-C8-H8B	120.1
O4-C8-K2	49.9(3)
O4-C8-H8A	108.9
O4-C8-H8B	108.9
O4-C8-C9	113.3(6)
H8A-C8-H8B	107.7
C9-C8-K2	130.9(4)
C9-C8-H8A	108.9
C9-C8-H8B	108.9
K1-C9-H9A	77.7
K1-C9-H9B	158.4
O5-C9-K1	49.3(3)
O5-C9-C8	107.2(5)
O5-C9-H9A	110.3
O5-C9-H9B	110.3
C8-C9-K1	85.6(4)

C8-C9-H9A	110.3
C8-C9-H9B	110.3
H9A-C9-H9B	108.5
K1-C10-H10A	159.4
K1-C10-H10B	79.0
O5-C10-K1	50.0(3)
O5-C10-H10A	110.0
O5-C10-H10B	110.0
O5-C10-C11	108.5(5)
H10A-C10-H10B	108.4
C11-C10-K1	84.2(4)
C11-C10-H10A	110.0
C11-C10-H10B	110.0
O6-C11-C10	108.3(5)
O6-C11-H11A	110.0
O6-C11-H11B	110.0
C10-C11-H11A	110.0
C10-C11-H11B	110.0
H11A-C11-H11B	108.4
O6-C12-C1	116.5(6)
O6-C12-C13	123.7(6)
C13-C12-C1	119.8(7)
C12-C13-H13	120.6
C12-C13-C14	118.8(7)
C14-C13-H13	120.6
C13-C14-H14	119.5
C15-C14-C13	120.9(8)
C15-C14-H14	119.5
C14-C15-H15	120.2
C14-C15-C16	119.6(8)
C16-C15-H15	120.2
C1-C16-C15	119.9(8)
C1-C16-H16	120.0
C15-C16-H16	120.0
C3B-O3B-K2	135.4(5)
C9B-O9B-K3	142.6(5)

C12B-O12B-K3	135.2(5)
C33-O13-K3	123.1(5)
C33-O13-C34	117.9(6)
C34-O13-K3	110.5(4)
C35-O14-K3	117.2(4)
C36-O14-K3	115.5(4)
C36-O14-C35	111.4(5)
C37-O15-K3	111.5(4)
C37-O15-C38	112.7(6)
C38-O15-K3	112.0(4)
C39-O16-K3	118.1(4)
C40-O16-K3	118.0(4)
C40-O16-C39	112.1(6)
C41-O17-K3	109.7(4)
C42-O17-K3	110.0(4)
C42-O17-C41	112.3(6)
C43-O18-K3	115.1(4)
C44-O18-K3	119.1(4)
C44-O18-C43	116.6(6)
C44-C33-O13	112.5(7)
C44-C33-C48	121.3(8)
C48-C33-O13	126.2(8)
O13-C34-H34A	109.9
O13-C34-H34B	109.9
O13-C34-C35	109.0(7)
H34A-C34-H34B	108.3
C35-C34-H34A	109.9
C35-C34-H34B	109.9
O14-C35-C34	108.1(6)
O14-C35-H35A	110.1
O14-C35-H35B	110.1
C34-C35-H35A	110.1
C34-C35-H35B	110.1
H35A-C35-H35B	108.4
O14-C36-H36A	110.0
O14-C36-H36B	110.0

O14-C36-C37	108.3(6)
H36A-C36-H36B	108.4
C37-C36-H36A	110.0
C37-C36-H36B	110.0
O15-C37-C36	109.4(6)
O15-C37-H37A	109.8
O15-C37-H37B	109.8
C36-C37-H37A	109.8
C36-C37-H37B	109.8
H37A-C37-H37B	108.2
O15-C38-H38A	109.9
O15-C38-H38B	109.9
O15-C38-C39	109.0(7)
H38A-C38-H38B	108.3
C39-C38-H38A	109.9
C39-C38-H38B	109.9
O16-C39-C38	108.5(6)
O16-C39-H39A	110.0
O16-C39-H39B	110.0
C38-C39-H39A	110.0
C38-C39-H39B	110.0
H39A-C39-H39B	108.4
O16-C40-H40A	109.7
O16-C40-H40B	109.7
O16-C40-C41	109.6(6)
H40A-C40-H40B	108.2
C41-C40-H40A	109.7
C41-C40-H40B	109.7
O17-C41-C40	108.3(6)
O17-C41-H41A	110.0
O17-C41-H41B	110.0
C40-C41-H41A	110.0
C40-C41-H41B	110.0
H41A-C41-H41B	108.4
O17-C42-H42A	109.9
O17-C42-H42B	109.9

O17-C42-C43	108.9(6)
H42A-C42-H42B	108.3
C43-C42-H42A	109.9
C43-C42-H42B	109.9
O18-C43-C42	109.1(6)
O18-C43-H43A	109.9
O18-C43-H43B	109.9
C42-C43-H43A	109.9
C42-C43-H43B	109.9
H43A-C43-H43B	108.3
O18-C44-C45	123.1(8)
C33-C44-O18	117.7(7)
C33-C44-C45	119.3(8)
C44-C45-H45	120.7
C46-C45-C44	118.7(9)
C46-C45-H45	120.7
C45-C46-H46	119.2
C47-C46-C45	121.5(9)
C47-C46-H46	119.2
C46-C47-H47	120.0
C46-C47-C48	120.0(9)
C48-C47-H47	120.0
C33-C48-C47	119.2(9)
C33-C48-H48	120.4
C47-C48-H48	120.4
C6B-O6B-K3	130.0(6)
O3B-C3B-Fe1B	178.2(7)
O2B-C2B-Fe1B	178.2(6)
O1B-C1B-Fe1B	178.7(7)
Fe1B-C0B-Fe3B	88.8(3)
Fe1B-C0B-Fe2B	177.5(4)
Fe1B-C0B-Fe4B	88.8(3)
Fe3B-C0B-Fe4B	80.3(3)
Fe2B-C0B-Fe3B	89.5(3)
Fe2B-C0B-Fe4B	89.1(3)
O7B-C7B-Fe3B	175.7(7)

O8B-C8B-Fe3B	176.9(6)
O9B-C9B-Fe3B	176.6(7)
O11B-C11B-Fe4B	174.1(7)
O5B-C5B-Fe2B	177.0(8)
O12B-C12B-Fe4B	175.8(7)
O10B-C10B-Fe4B	176.6(8)
O6B-C6B-Fe2B	177.5(8)
O4B-C4B-Fe2B	174.9(8)
Fe3A-Fe1A-Fe4A	58.17(9)
C1A-Fe1A-Fe3A	95.4(10)
C1A-Fe1A-Fe4A	147.8(10)
C1A-Fe1A-C2A	103.7(17)
C1A-Fe1A-C3A	99.0(12)
C2A-Fe1A-Fe3A	106.5(9)
C2A-Fe1A-Fe4A	101.7(14)
C3A-Fe1A-Fe3A	146.4(7)
C3A-Fe1A-Fe4A	96.1(7)
C3A-Fe1A-C2A	99.3(12)
C0A-Fe1A-Fe3A	49.4(4)
C0A-Fe1A-Fe4A	47.6(4)
C0A-Fe1A-C1A	102.0(10)
C0A-Fe1A-C2A	146.4(12)
C0A-Fe1A-C3A	97.8(8)
Fe1A-Fe3A-Fe2A	83.25(10)
Fe4A-Fe3A-Fe1A	61.80(9)
Fe4A-Fe3A-Fe2A	59.93(9)
C0A-Fe3A-Fe1A	41.5(3)
C0A-Fe3A-Fe2A	41.8(3)
C0A-Fe3A-Fe4A	49.2(3)
C8A-Fe3A-Fe1A	80.5(5)
C8A-Fe3A-Fe2A	159.4(5)
C8A-Fe3A-Fe4A	100.9(5)
C8A-Fe3A-C0A	120.8(6)
C7A-Fe3A-Fe1A	103.0(8)
C7A-Fe3A-Fe2A	99.6(8)
C7A-Fe3A-Fe4A	154.3(9)

C7A-Fe3A-C0A	105.3(10)
C7A-Fe3A-C8A	96.3(10)
C9A-Fe3A-Fe1A	153.6(6)
C9A-Fe3A-Fe2A	87.1(5)
C9A-Fe3A-Fe4A	92.2(5)
C9A-Fe3A-C0A	124.5(6)
C9A-Fe3A-C8A	102.1(7)
C9A-Fe3A-C7A	102.8(10)
Fe4A-Fe2A-Fe3A	58.32(9)
C0A-Fe2A-Fe3A	48.4(4)
C0A-Fe2A-Fe4A	48.9(4)
C0A-Fe2A-C4A	104.2(8)
C5A-Fe2A-Fe3A	101.3(13)
C5A-Fe2A-Fe4A	108.9(17)
C5A-Fe2A-C0A	147.4(15)
C5A-Fe2A-C4A	98.8(15)
C4A-Fe2A-Fe3A	147.1(7)
C4A-Fe2A-Fe4A	90.5(7)
C6A-Fe2A-Fe3A	95.3(10)
C6A-Fe2A-Fe4A	139.9(11)
C6A-Fe2A-C0A	91.0(11)
C6A-Fe2A-C5A	105(2)
C6A-Fe2A-C4A	104.2(12)
Fe3A-Fe4A-Fe1A	60.02(9)
Fe3A-Fe4A-Fe2A	61.75(9)
Fe2A-Fe4A-Fe1A	83.27(10)
C0A-Fe4A-Fe1A	40.6(3)
C0A-Fe4A-Fe3A	49.8(3)
C0A-Fe4A-Fe2A	42.7(3)
C12A-Fe4A-Fe1A	89.9(5)
C12A-Fe4A-Fe3A	92.2(6)
C12A-Fe4A-Fe2A	153.0(6)
C12A-Fe4A-C0A	125.9(6)
C12A-Fe4A-C11A	95.6(7)
C12A-Fe4A-C10A	102.9(10)
C11A-Fe4A-Fe1A	162.2(6)

C11A-Fe4A-Fe3A	102.7(5)
C11A-Fe4A-Fe2A	84.2(5)
C11A-Fe4A-C0A	125.8(6)
C10A-Fe4A-Fe1A	94.4(8)
C10A-Fe4A-Fe3A	150.5(7)
C10A-Fe4A-Fe2A	103.7(9)
C10A-Fe4A-C0A	101.5(8)
C10A-Fe4A-C11A	100.8(9)
C3A-O3A-K1	135(2)
O1A-C1A-Fe1A	175(3)
O2A-C2A-Fe1A	176(4)
Fe1A-C3A-K1	146.4(10)
O3A-C3A-K1	32.5(17)
O3A-C3A-Fe1A	179(2)
Fe1A-C0A-Fe3A	89.2(5)
Fe1A-C0A-Fe2A	179.0(8)
Fe1A-C0A-Fe4A	91.8(5)
Fe2A-C0A-Fe3A	89.8(5)
Fe2A-C0A-Fe4A	88.4(5)
Fe4A-C0A-Fe3A	80.9(5)
O8A-C8A-Fe3A	172.4(17)
O7A-C7A-Fe3A	178(2)
O9A-C9A-Fe3A	170(2)
O12A-C12A-Fe4A	177.3(16)
O11A-C11A-Fe4A	175.5(17)
O10A-C10A-Fe4A	174.8(19)
O5A-C5A-Fe2A	177(4)
O4A-C4A-Fe2A	170(3)
O6A-C6A-Fe2A	174(3)
F1D-C1D-C2D	119.6(6)
F1D-C1D-C6D	120.3(6)
C2D-C1D-C6D	120.0
C1D-C2D-H2D	120.0
C3D-C2D-C1D	120.0
C3D-C2D-H2D	120.0
C2D-C3D-H3D	120.0

C2D-C3D-C4D	120.0
C4D-C3D-H3D	120.0
C3D-C4D-H4D	120.0
C5D-C4D-C3D	120.0
C5D-C4D-H4D	120.0
C4D-C5D-H5D	120.0
C4D-C5D-C6D	120.0
C6D-C5D-H5D	120.0
C1D-C6D-H6D	120.0
C5D-C6D-C1D	120.0
C5D-C6D-H6D	120.0
F1DA-C1DA-C6DA	111(2)
F1DA-C1DA-C2DA	129(2)
C6DA-C1DA-C2DA	120.0
C1DA-C6DA-H6DA	120.0
C5DA-C6DA-C1DA	120.0
C5DA-C6DA-H6DA	120.0
C6DA-C5DA-H5DA	120.0
C6DA-C5DA-C4DA	120.0
C4DA-C5DA-H5DA	120.0
C5DA-C4DA-H4DA	120.0
C3DA-C4DA-C5DA	120.0
C3DA-C4DA-H4DA	120.0
C4DA-C3DA-H3DA	120.0
C4DA-C3DA-C2DA	120.0
C2DA-C3DA-H3DA	120.0
C1DA-C2DA-H2DA	120.0
C3DA-C2DA-C1DA	120.0
C3DA-C2DA-H2DA	120.0
F1E-C1E-C2E	119.9(6)
F1E-C1E-C6E	120.1(6)
C2E-C1E-C6E	120.0
C1E-C2E-H2E	120.0
C1E-C2E-C3E	120.0
C3E-C2E-H2E	120.0
C2E-C3E-H3E	120.0

C2E-C3E-C4E	120.0
C4E-C3E-H3E	120.0
C3E-C4E-H4E	120.0
C5E-C4E-C3E	120.0
C5E-C4E-H4E	120.0
C4E-C5E-H5E	120.0
C4E-C5E-C6E	120.0
C6E-C5E-H5E	120.0
C1E-C6E-H6E	120.0
C5E-C6E-C1E	120.0
C5E-C6E-H6E	120.0
F1EA-C1EA-C6EA	118(2)
F1EA-C1EA-C2EA	122(2)
C6EA-C1EA-C2EA	120.0
C1EA-C6EA-H6EA	120.0
C5EA-C6EA-C1EA	120.0
C5EA-C6EA-H6EA	120.0
C6EA-C5EA-H5EA	120.0
C6EA-C5EA-C4EA	120.0
C4EA-C5EA-H5EA	120.0
C5EA-C4EA-H4EA	120.0
C3EA-C4EA-C5EA	120.0
C3EA-C4EA-H4EA	120.0
C4EA-C3EA-H3EA	120.0
C2EA-C3EA-C4EA	120.0
C2EA-C3EA-H3EA	120.0
C1EA-C2EA-H2EA	120.0
C3EA-C2EA-C1EA	120.0
C3EA-C2EA-H2EA	120.0
F1F-C1F-C2F	120.3(6)
F1F-C1F-C6F	119.5(6)
C2F-C1F-C6F	120.0
C1F-C2F-H2F	120.0
C3F-C2F-C1F	120.0
C3F-C2F-H2F	120.0
C2F-C3F-H3F	120.0

C2F-C3F-C4F	120.0
C4F-C3F-H3F	120.0
C3F-C4F-H4F	120.0
C3F-C4F-C5F	120.0
C5F-C4F-H4F	120.0
C4F-C5F-H5F	120.0
C4F-C5F-C6F	120.0
C6F-C5F-H5F	120.0
C1F-C6F-H6F	120.0
C5F-C6F-C1F	120.0
C5F-C6F-H6F	120.0
F1FA-C1FA-C2FA	122.3(14)
F1FA-C1FA-C6FA	116.7(14)
C2FA-C1FA-C6FA	120.0
C1FA-C2FA-H2FA	120.0
C3FA-C2FA-C1FA	120.0
C3FA-C2FA-H2FA	120.0
C2FA-C3FA-H3FA	120.0
C2FA-C3FA-C4FA	120.0
C4FA-C3FA-H3FA	120.0
C3FA-C4FA-H4FA	120.0
C5FA-C4FA-C3FA	120.0
C5FA-C4FA-H4FA	120.0
C4FA-C5FA-H5FA	120.0
C6FA-C5FA-C4FA	120.0
C6FA-C5FA-H5FA	120.0
C1FA-C6FA-H6FA	120.0
C5FA-C6FA-C1FA	120.0
C5FA-C6FA-H6FA	120.0

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe1B	37(1)	40(1)	38(1)	18(1)	12(1)	9(1)
Fe3B	44(1)	36(1)	41(1)	18(1)	13(1)	7(1)
Fe2B	60(1)	39(1)	42(1)	15(1)	13(1)	10(1)
Fe4B	52(1)	38(1)	45(1)	18(1)	21(1)	11(1)
K2	28(1)	40(1)	32(1)	15(1)	7(1)	6(1)
K1	30(1)	54(1)	34(1)	23(1)	7(1)	-1(1)
K3	48(1)	42(1)	34(1)	13(1)	6(1)	8(1)
O7	27(2)	30(2)	39(3)	12(2)	14(2)	5(2)
O8	39(3)	35(2)	43(3)	18(2)	16(2)	14(2)
O9	34(2)	43(3)	35(3)	18(2)	10(2)	7(2)
O10	35(2)	49(3)	33(3)	20(2)	12(2)	8(2)
O11	33(2)	43(3)	35(3)	17(2)	9(2)	5(2)
O12	28(2)	35(2)	40(3)	16(2)	9(2)	2(2)
C17	40(4)	33(3)	21(3)	12(3)	4(3)	3(3)
C18	36(3)	33(3)	38(4)	16(3)	14(3)	5(3)
C19	43(4)	41(4)	36(4)	19(3)	15(3)	10(3)
C20	43(4)	35(3)	35(4)	15(3)	13(3)	10(3)
C21	36(3)	36(3)	33(4)	9(3)	6(3)	5(3)
C22	39(4)	47(4)	39(4)	10(3)	11(3)	12(3)
C23	37(4)	59(4)	33(4)	15(3)	11(3)	9(3)
C24	43(4)	51(4)	49(5)	26(4)	15(3)	4(3)
C25	34(4)	51(4)	49(5)	21(3)	10(3)	2(3)
C26	36(4)	53(4)	36(4)	17(3)	3(3)	-5(3)
C27	35(4)	42(4)	36(4)	13(3)	7(3)	-2(3)
C28	31(3)	37(3)	33(4)	14(3)	9(3)	8(3)
C29	46(4)	41(4)	40(4)	18(3)	8(3)	7(3)
C30	43(4)	40(4)	51(5)	16(3)	10(3)	14(3)
C31	40(4)	49(4)	36(4)	15(3)	14(3)	13(3)
C32	30(3)	40(4)	44(4)	19(3)	13(3)	9(3)
O1	40(3)	47(3)	37(3)	18(2)	8(2)	-6(2)
C1	42(4)	58(4)	31(4)	19(3)	7(3)	3(3)

O2	28(2)	63(3)	51(3)	33(3)	5(2)	-3(2)
C2	50(4)	45(4)	46(5)	15(3)	7(3)	-11(3)
O3	31(2)	66(3)	50(3)	33(3)	13(2)	6(2)
C3	51(4)	55(4)	56(5)	31(4)	4(4)	-3(3)
O4	34(2)	46(3)	41(3)	25(2)	11(2)	10(2)
C4	28(4)	71(5)	57(5)	34(4)	0(3)	-9(3)
O5	42(3)	48(3)	43(3)	28(2)	12(2)	5(2)
C5	35(4)	63(5)	61(5)	40(4)	12(3)	4(3)
O6	36(2)	44(3)	35(3)	17(2)	10(2)	-5(2)
C6	37(4)	70(5)	52(5)	35(4)	16(3)	20(3)
C7	43(4)	59(4)	46(4)	30(4)	18(3)	24(3)
C8	53(4)	43(4)	34(4)	17(3)	12(3)	10(3)
C9	50(4)	46(4)	46(4)	25(3)	15(3)	11(3)
C10	43(4)	49(4)	49(5)	27(4)	11(3)	-2(3)
C11	45(4)	48(4)	38(4)	21(3)	10(3)	-11(3)
C12	32(3)	54(4)	22(4)	12(3)	1(3)	-2(3)
C13	44(4)	57(4)	32(4)	9(3)	2(3)	1(3)
C14	37(4)	71(5)	49(5)	11(4)	6(3)	9(4)
C15	72(5)	68(5)	54(5)	9(4)	12(4)	19(4)
C16	53(5)	53(5)	55(5)	11(4)	8(4)	1(4)
O3B	41(3)	54(3)	50(3)	30(3)	13(2)	14(2)
O2B	43(3)	46(3)	48(3)	15(3)	12(2)	8(2)
O11B	52(3)	58(3)	58(4)	33(3)	17(3)	17(3)
O9B	67(3)	46(3)	66(4)	33(3)	17(3)	10(3)
O7B	54(3)	53(3)	44(3)	17(3)	10(3)	9(3)
O1B	43(3)	75(4)	75(4)	48(3)	25(3)	18(3)
O12B	65(3)	46(3)	62(4)	22(3)	20(3)	18(3)
O13	69(4)	63(4)	43(3)	16(3)	16(3)	-11(3)
O14	57(3)	63(3)	38(3)	25(3)	5(2)	10(3)
O15	55(3)	49(3)	54(3)	24(3)	10(3)	6(2)
O16	61(3)	50(3)	49(3)	20(3)	17(3)	10(3)
O17	61(3)	48(3)	42(3)	20(2)	13(3)	14(2)
O18	52(3)	43(3)	42(3)	15(2)	10(2)	-2(2)
C33	53(4)	61(5)	56(5)	25(4)	18(4)	2(4)
C34	75(5)	61(5)	53(5)	19(4)	23(4)	-1(4)
C35	62(5)	69(5)	54(5)	31(4)	12(4)	15(4)

C36	57(5)	58(5)	46(5)	27(4)	0(4)	3(4)
C37	57(5)	57(5)	54(5)	27(4)	1(4)	-1(4)
C38	56(5)	57(5)	63(5)	30(4)	22(4)	12(4)
C39	54(5)	69(5)	65(5)	30(4)	20(4)	17(4)
C40	79(5)	51(4)	42(5)	12(4)	20(4)	18(4)
C41	76(5)	52(4)	38(4)	14(3)	16(4)	19(4)
C42	69(5)	52(4)	41(5)	23(4)	-7(4)	-3(4)
C43	51(4)	55(5)	46(5)	19(4)	-10(4)	-6(4)
C44	46(4)	56(5)	56(5)	28(4)	12(4)	6(3)
C45	55(5)	59(5)	70(6)	27(4)	13(4)	-3(4)
C46	70(5)	64(5)	100(7)	40(5)	42(5)	7(4)
C47	90(6)	82(6)	84(6)	46(5)	44(5)	11(5)
C48	81(6)	75(6)	68(6)	31(5)	35(5)	8(4)
O10B	70(4)	83(4)	51(4)	27(3)	30(3)	14(3)
O8B	54(3)	67(4)	64(4)	38(3)	13(3)	17(3)
O5B	62(4)	49(3)	76(4)	16(3)	8(3)	9(3)
O6B	97(4)	45(3)	72(4)	21(3)	0(3)	15(3)
C3B	44(4)	44(4)	35(4)	18(3)	11(3)	8(3)
C2B	36(4)	40(4)	42(4)	19(3)	19(3)	14(3)
O4B	124(6)	129(7)	71(5)	58(5)	47(4)	46(5)
C1B	41(4)	44(4)	45(4)	21(3)	23(3)	12(3)
C0B	44(4)	36(3)	32(4)	12(3)	2(3)	3(3)
C7B	48(4)	38(4)	43(4)	17(3)	18(3)	11(3)
C8B	40(4)	53(4)	38(4)	26(3)	7(3)	9(3)
C9B	55(4)	45(4)	49(5)	25(4)	11(4)	6(3)
C11B	54(4)	38(4)	48(5)	25(3)	24(4)	12(3)
C5B	62(5)	40(4)	52(5)	14(3)	16(4)	15(4)
C12B	54(4)	41(4)	54(5)	20(3)	13(4)	11(3)
C10B	56(4)	49(4)	50(5)	21(4)	23(4)	12(3)
C6B	76(5)	45(4)	47(5)	11(4)	4(4)	16(4)
C4B	86(6)	73(6)	64(6)	36(5)	27(5)	24(5)
Fe1A	28(1)	54(1)	39(1)	25(1)	7(1)	9(1)
Fe3A	43(1)	32(1)	37(1)	14(1)	6(1)	2(1)
Fe2A	40(1)	54(2)	43(2)	22(1)	14(1)	14(1)
Fe4A	38(1)	35(1)	41(2)	13(1)	2(1)	0(1)
O1A	38(6)	76(9)	30(8)	33(8)	8(7)	17(6)

O2A	55(6)	40(6)	54(7)	14(5)	15(5)	18(5)
O12A	51(9)	59(8)	50(10)	23(9)	-2(9)	-15(6)
O9A	89(15)	60(14)	71(14)	36(11)	21(11)	29(11)
O8A	60(12)	17(7)	19(7)	0(5)	-14(8)	14(8)
O3A	41(7)	34(7)	39(7)	19(6)	6(5)	12(6)
O11A	35(10)	61(9)	30(11)	19(9)	-3(9)	-1(6)
O10A	56(6)	41(6)	46(6)	21(5)	17(5)	-2(5)
O7A	55(6)	50(6)	57(7)	15(5)	16(6)	1(5)
O5A	45(6)	66(7)	54(7)	21(6)	0(5)	8(5)
C1A	24(8)	46(9)	35(10)	13(7)	9(6)	6(7)
C2A	42(10)	46(9)	48(10)	14(6)	13(8)	13(6)
O4A	67(11)	37(11)	55(10)	20(8)	23(8)	25(7)
C3A	44(8)	45(8)	38(8)	20(6)	10(7)	4(7)
C0A	24(5)	23(5)	32(6)	6(4)	15(5)	4(4)
C8A	48(7)	30(6)	35(7)	23(5)	5(6)	5(6)
C7A	39(8)	38(8)	37(9)	11(7)	20(8)	0(6)
C9A	34(6)	40(7)	36(7)	19(6)	-16(5)	-2(5)
C12A	47(8)	41(7)	45(8)	24(6)	11(6)	3(6)
C11A	36(7)	38(7)	35(7)	22(6)	0(5)	5(6)
C10A	59(10)	46(9)	49(11)	28(8)	10(8)	4(7)
C5A	42(11)	55(10)	38(9)	24(7)	3(8)	7(7)
C4A	41(9)	52(9)	47(9)	28(7)	3(7)	7(7)
C6A	59(11)	72(11)	48(12)	26(8)	20(9)	15(8)
O6A	52(8)	89(9)	58(10)	47(8)	13(6)	5(6)
F1D	93(7)	114(8)	96(7)	26(6)	-24(6)	3(6)
C1D	72(5)	76(5)	84(6)	27(5)	27(5)	9(5)
C2D	78(7)	82(7)	85(7)	30(5)	30(6)	8(6)
C3D	79(6)	83(5)	84(5)	35(4)	28(4)	11(5)
C4D	74(5)	76(5)	77(5)	32(4)	25(4)	14(4)
C5D	74(5)	71(5)	73(5)	28(4)	22(4)	11(4)
C6D	67(6)	70(5)	76(6)	36(5)	21(5)	5(5)
F1DA	118(9)	136(10)	83(8)	39(8)	28(7)	1(8)
C1DA	74(5)	77(5)	78(5)	32(4)	23(5)	14(5)
C6DA	72(5)	70(5)	72(5)	32(4)	22(5)	9(5)
C5DA	55(10)	61(11)	74(12)	25(8)	22(8)	14(8)
C4DA	72(8)	77(8)	89(8)	24(6)	23(7)	13(7)

C3DA	65(11)	61(11)	62(11)	18(8)	30(8)	18(8)
C2DA	82(8)	88(8)	88(8)	38(6)	29(7)	5(7)
F1E	72(10)	90(10)	78(10)	39(8)	8(8)	19(8)
C1E	55(5)	53(5)	50(5)	24(4)	15(5)	6(4)
C2E	51(6)	50(5)	51(5)	22(4)	13(5)	10(5)
C3E	54(6)	51(5)	54(6)	23(4)	10(5)	10(5)
C4E	56(6)	54(6)	56(6)	24(5)	14(5)	8(5)
C5E	56(6)	51(6)	54(6)	22(5)	16(5)	6(5)
C6E	57(5)	52(5)	53(5)	22(4)	16(5)	5(4)
F1EA	73(9)	76(9)	70(9)	26(8)	9(8)	8(8)
C1EA	54(6)	52(5)	56(6)	24(5)	13(5)	10(5)
C6EA	56(5)	53(5)	55(5)	23(4)	14(5)	8(4)
C5EA	56(6)	52(5)	51(6)	21(5)	18(5)	6(5)
C4EA	55(6)	52(6)	49(6)	23(5)	15(5)	4(5)
C3EA	55(6)	52(5)	51(6)	23(5)	14(5)	6(5)
C2EA	52(6)	51(5)	52(6)	23(5)	13(5)	9(5)
F1F	125(9)	139(9)	150(9)	77(8)	40(7)	44(7)
C1F	92(5)	84(5)	87(5)	52(4)	19(4)	16(4)
C2F	87(5)	84(5)	85(5)	45(4)	16(5)	13(4)
C3F	85(5)	86(5)	86(5)	43(4)	16(4)	10(4)
C4F	90(5)	85(5)	86(5)	41(4)	20(4)	8(4)
C5F	93(4)	81(4)	85(4)	41(4)	20(4)	11(4)
C6F	95(5)	80(5)	80(5)	46(4)	17(4)	7(4)
F1FA	158(11)	132(11)	183(12)	33(10)	23(10)	8(10)
C1FA	85(5)	79(5)	83(5)	40(4)	26(5)	11(5)
C2FA	90(5)	78(5)	82(5)	43(4)	17(5)	11(5)
C3FA	92(5)	83(5)	81(5)	43(4)	19(4)	8(4)
C4FA	89(4)	83(4)	82(4)	44(4)	19(4)	12(4)
C5FA	87(5)	89(5)	85(5)	41(4)	17(4)	12(4)
C6FA	85(5)	83(5)	81(5)	41(4)	22(4)	13(4)

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

	x	y	z	U(eq)
H18A	1470	8154	8345	42
H18B	2039	8231	9088	42
H19A	3674	7661	8688	46
H19B	2348	7134	8320	46
H20A	2996	6479	7351	44
H20B	4354	6970	7653	44
H21A	3749	6418	6458	45
H21B	2676	6872	6491	45
H22A	5499	6906	6254	53
H22B	5925	7159	7052	53
H23A	7170	7853	6678	53
H23B	5972	8141	6457	53
H24A	7022	9405	7335	55
H24B	8173	9023	7422	55
H25A	8079	9323	8550	54
H25B	8410	10020	8426	54
H26A	7628	10630	9390	53
H26B	7061	9917	9438	53
H27A	5929	10856	9850	48
H27B	5569	10829	9112	48
H29	3997	11188	9623	51
H30	1979	11317	9702	55
H31	459	10319	9402	50
H32	913	9160	8978	45
H2A	2560	6081	4946	61
H2B	2271	6051	4206	61
H3A	942	6886	4529	65
H3B	467	6167	4591	65
H4A	-561	6805	5430	63
H4B	-140	7515	5340	63

H5A	-521	7804	6415	59
H5B	560	7406	6580	59
H6A	1617	8622	7512	59
H6B	436	8902	7255	59
H7A	1770	9675	7005	54
H7B	2054	9877	7794	54
H8A	4970	10017	7667	52
H8B	3864	10448	7706	52
H9A	3337	9951	6500	54
H9B	4656	10486	6852	54
H10A	5468	9908	5915	55
H10B	4175	9361	5500	55
H11A	5875	8871	5124	53
H11B	6404	8904	5854	53
H13	6977	7971	5038	59
H14	7540	6846	4509	70
H15	6139	5786	4148	85
H16	4180	5828	4371	72
H34A	6009	4294	9967	78
H34B	6820	4752	9706	78
H35A	8042	4364	10436	73
H35B	7511	3550	9880	73
H36A	9547	3429	9768	66
H36B	10081	4249	10308	66
H37A	10688	4490	9441	69
H37B	11411	3934	9613	69
H38A	11772	3432	8554	67
H38B	11052	3948	8313	67
H39A	11035	2857	7385	73
H39B	10314	2421	7700	73
H40A	8680	1967	6730	70
H40B	9256	2436	6399	70
H41A	7536	3018	6448	68
H41B	7103	2167	5994	68
H42A	5194	2202	6180	69
H42B	5458	3030	6715	69

H43A	3870	2322	6882	67
H43B	4847	1862	7036	67
H45	3252	1866	7549	76
H46	2501	1681	8380	89
H47	3413	2382	9500	95
H48	5025	3360	9830	88
H2D	1122	5062	7358	99
H3D	2541	5757	8396	99
H4D	4212	5301	8752	90
H5D	4465	4150	8068	88
H6D	3046	3456	7030	84
H6DA	4516	4203	8040	85
H5DA	3375	3577	6918	77
H4DA	1625	3955	6531	100
H3DA	1015	4960	7265	76
H2DA	2155	5586	8387	103
H2E	-725	5640	5887	60
H3E	1298	5492	6192	64
H4E	2223	4802	5364	67
H5E	1125	4261	4232	65
H6E	-898	4409	3927	65
H6EA	1665	4697	4831	66
H5EA	66	4361	3865	63
H4EA	-1826	4712	3961	62
H3EA	-2118	5398	5023	63
H2EA	-519	5735	5989	62
H2F	8347	557	6937	100
H3F	6810	1241	7128	102
H4F	6819	2023	8227	104
H5F	8365	2121	9135	103
H6F	9902	1438	8944	100
H2FA	9014	2035	9474	98
H3FA	10000	1517	8618	101
H4FA	8898	1048	7490	99
H5FA	6808	1098	7219	104
H6FA	5822	1616	8075	97

Table S6. Torsion angles (°) for **1**.

Fe3B-Fe1B-C0B-Fe4B	-80.4(2)
Fe3B-Fe2B-C0B-Fe4B	80.3(2)
Fe4B-Fe1B-C0B-Fe3B	80.4(2)
Fe4B-Fe2B-C0B-Fe3B	-80.3(2)
K2-O7-C17-C28	-39.1(6)
K2-O7-C17-C32	139.6(5)
K2-O7-C18-C19	31.1(6)
K2-O8-C19-C18	67.4(5)
K2-O8-C20-C21	-67.9(5)
K2-O9-C21-C20	-27.8(6)
K2-O9-C22-C23	-54.1(6)
K2-O10-C23-C22	-44.1(7)
K2-O10-C24-C25	50.0(6)
K2-O11-C25-C24	49.4(6)
K2-O11-C26-C27	-60.7(6)
K2-O12-C27-C26	-37.4(6)
K2-O12-C28-C17	38.1(7)
K2-O12-C28-C29	-141.0(6)
K2-C20-C21-O9	21.6(5)
K2-C26-C27-O12	25.0(4)
K2-O4-C7-C6	-49.0(7)
K2-O4-C8-C9	124.7(5)
K2-C8-C9-K1	32.9(5)
K2-C8-C9-O5	-12.0(8)
K1-O9-C21-C20	-125.6(4)
K1-O9-C22-C23	47.2(7)
K1-O1-C1-C12	-33.8(7)
K1-O1-C1-C16	145.8(7)
K1-O1-C2-C3	40.0(7)
K1-O2-C3-C2	55.4(6)
K1-O2-C4-C5	-51.8(6)
K1-O3-C5-C4	-44.0(6)
K1-O3-C6-C7	45.1(7)
K1-O4-C7-C6	52.4(6)

K1-O4-C8-K2	-94.5(3)
K1-O4-C8-C9	30.2(6)
K1-C4-C5-O3	28.7(4)
K1-O5-C9-C8	68.1(6)
K1-O5-C10-C11	-65.2(5)
K1-O6-C11-C10	-31.2(7)
K1-O6-C12-C1	33.5(7)
K1-O6-C12-C13	-148.8(6)
K1-C10-C11-O6	21.6(5)
K3-O13-C33-C44	-37.3(9)
K3-O13-C33-C48	145.2(7)
K3-O13-C34-C35	-56.2(7)
K3-O14-C35-C34	-44.5(8)
K3-O14-C36-C37	41.9(7)
K3-O15-C37-C36	57.1(7)
K3-O15-C38-C39	-58.3(7)
K3-O16-C39-C38	-36.8(8)
K3-O16-C40-C41	30.8(8)
K3-O17-C41-C40	62.1(6)
K3-O17-C42-C43	-69.0(6)
K3-O18-C43-C42	-27.6(7)
K3-O18-C44-C33	25.8(9)
K3-O18-C44-C45	-153.9(6)
O7-C17-C28-O12	0.0(8)
O7-C17-C28-C29	179.2(6)
O7-C17-C32-C31	-179.1(6)
O7-C18-C19-K2	-21.2(4)
O7-C18-C19-O8	-66.1(6)
O8-C20-C21-O9	66.7(7)
O9-C22-C23-O10	67.1(7)
O10-C24-C25-O11	-66.6(7)
O11-C26-C27-O12	65.1(7)
O12-C28-C29-C30	178.5(6)
C17-O7-C18-C19	177.1(5)
C17-C28-C29-C30	-0.6(10)
C18-O7-C17-C28	174.1(5)

C18-O7-C17-C32	-7.2(9)
C19-O8-C20-K2	-117.2(5)
C19-O8-C20-C21	174.8(5)
C20-O8-C19-K2	117.0(5)
C20-O8-C19-C18	-175.6(5)
C21-O9-C22-C23	-177.0(5)
C22-O9-C21-C20	93.9(6)
C23-O10-C24-C25	-169.3(5)
C24-O10-C23-C22	176.5(5)
C25-O11-C26-K2	-126.4(5)
C25-O11-C26-C27	172.9(5)
C26-O11-C25-C24	175.2(6)
C27-O12-C28-C17	-177.8(5)
C27-O12-C28-C29	3.0(9)
C28-O12-C27-C26	180.0(5)
C28-C17-C32-C31	-0.6(10)
C28-C29-C30-C31	0.9(11)
C29-C30-C31-C32	-1.0(11)
C30-C31-C32-C17	0.9(10)
C32-C17-C28-O12	-178.7(6)
C32-C17-C28-C29	0.5(10)
O1-C1-C12-O6	0.0(9)
O1-C1-C12-C13	-177.8(6)
O1-C1-C16-C15	177.6(7)
O1-C2-C3-O2	-62.7(7)
C1-O1-C2-C3	-170.7(6)
C1-C12-C13-C14	-1.8(11)
O2-C4-C5-O3	64.1(7)
C2-O1-C1-C12	176.9(6)
C2-O1-C1-C16	-3.4(10)
O3-C6-C7-O4	-67.1(7)
C3-O2-C4-K1	-126.6(6)
C3-O2-C4-C5	-178.3(6)
O4-C8-C9-K1	-23.5(5)
O4-C8-C9-O5	-68.3(7)
C4-O2-C3-C2	-178.5(6)

O5-C10-C11-O6	65.9(7)
C5-O3-C6-C7	-172.2(5)
O6-C12-C13-C14	-179.4(6)
C6-O3-C5-C4	171.9(6)
C7-O4-C8-K2	145.8(6)
C7-O4-C8-C9	-89.5(7)
C8-O4-C7-C6	174.0(5)
C9-O5-C10-K1	-117.7(5)
C9-O5-C10-C11	177.1(6)
C10-O5-C9-K1	117.2(5)
C10-O5-C9-C8	-174.6(5)
C11-O6-C12-C1	-176.7(6)
C11-O6-C12-C13	1.0(10)
C12-C1-C16-C15	-2.8(12)
C12-O6-C11-C10	178.8(6)
C12-C13-C14-C15	1.4(12)
C13-C14-C15-C16	-1.7(13)
C14-C15-C16-C1	2.4(13)
C16-C1-C12-O6	-179.7(7)
C16-C1-C12-C13	2.5(11)
O13-C33-C44-O18	5.3(11)
O13-C33-C44-C45	-175.0(7)
O13-C33-C48-C47	176.7(8)
O13-C34-C35-O14	67.6(8)
O14-C36-C37-O15	-67.0(8)
O15-C38-C39-O16	63.2(8)
O16-C40-C41-O17	-62.5(8)
O17-C42-C43-O18	64.6(8)
O18-C44-C45-C46	177.6(7)
C33-O13-C34-C35	92.9(8)
C33-C44-C45-C46	-2.1(13)
C34-O13-C33-C44	177.8(7)
C34-O13-C33-C48	0.2(13)
C35-O14-C36-C37	178.8(6)
C36-O14-C35-C34	179.5(6)
C37-O15-C38-C39	174.9(6)

C38-O15-C37-C36	-176.0(6)
C39-O16-C40-C41	173.1(6)
C40-O16-C39-C38	-179.1(7)
C41-O17-C42-C43	168.5(6)
C42-O17-C41-C40	-175.2(6)
C43-O18-C44-C33	170.9(7)
C43-O18-C44-C45	-8.8(11)
C44-O18-C43-C42	-174.2(6)
C44-C33-C48-C47	-0.6(14)
C44-C45-C46-C47	-0.6(14)
C45-C46-C47-C48	2.7(16)
C46-C47-C48-C33	-2.0(15)
C48-C33-C44-O18	-177.0(7)
C48-C33-C44-C45	2.7(13)
C3B-Fe1B-C0B-Fe3B	-83.2(3)
C3B-Fe1B-C0B-Fe4B	-163.5(3)
C2B-Fe1B-C0B-Fe3B	52.4(6)
C2B-Fe1B-C0B-Fe4B	-27.9(7)
C1B-Fe1B-C0B-Fe3B	173.5(3)
C1B-Fe1B-C0B-Fe4B	93.2(3)
C5B-Fe2B-C0B-Fe3B	83.4(4)
C5B-Fe2B-C0B-Fe4B	163.8(3)
C6B-Fe2B-C0B-Fe3B	-51.4(7)
C6B-Fe2B-C0B-Fe4B	29.0(7)
C4B-Fe2B-C0B-Fe3B	-177.1(4)
C4B-Fe2B-C0B-Fe4B	-96.8(4)
Fe3A-Fe1A-C3A-K1	102.4(19)
Fe3A-Fe1A-C0A-Fe4A	-80.9(5)
Fe3A-Fe2A-C0A-Fe4A	80.9(5)
Fe4A-Fe1A-C3A-K1	139.5(17)
Fe4A-Fe1A-C0A-Fe3A	80.9(5)
Fe4A-Fe2A-C0A-Fe3A	-80.9(5)
C1A-Fe1A-C3A-K1	-12(2)
C1A-Fe1A-C0A-Fe3A	-86.9(10)
C1A-Fe1A-C0A-Fe4A	-167.8(10)
C2A-Fe1A-C3A-K1	-118(2)

C2A-Fe1A-C0A-Fe3A	52(3)
C2A-Fe1A-C0A-Fe4A	-29(3)
C3A-Fe1A-C0A-Fe3A	172.1(8)
C3A-Fe1A-C0A-Fe4A	91.2(8)
C0A-Fe1A-C3A-K1	91.5(18)
C5A-Fe2A-C0A-Fe3A	-25(3)
C5A-Fe2A-C0A-Fe4A	56(3)
C4A-Fe2A-C0A-Fe3A	-158.9(8)
C4A-Fe2A-C0A-Fe4A	-78.0(8)
C6A-Fe2A-C0A-Fe3A	96.2(10)
C6A-Fe2A-C0A-Fe4A	177.1(10)
F1D-C1D-C2D-C3D	-176.0(18)
F1D-C1D-C6D-C5D	176.0(18)
C1D-C2D-C3D-C4D	0.0
C2D-C1D-C6D-C5D	0.0
C2D-C3D-C4D-C5D	0.0
C3D-C4D-C5D-C6D	0.0
C4D-C5D-C6D-C1D	0.0
C6D-C1D-C2D-C3D	0.0
F1DA-C1DA-C6DA-C5DA	-178(3)
F1DA-C1DA-C2DA-C3DA	177(3)
C1DA-C6DA-C5DA-C4DA	0.0
C6DA-C1DA-C2DA-C3DA	0.0
C6DA-C5DA-C4DA-C3DA	0.0
C5DA-C4DA-C3DA-C2DA	0.0
C4DA-C3DA-C2DA-C1DA	0.0
C2DA-C1DA-C6DA-C5DA	0.0
F1E-C1E-C2E-C3E	180(2)
F1E-C1E-C6E-C5E	-180(2)
C1E-C2E-C3E-C4E	0.0
C2E-C1E-C6E-C5E	0.0
C2E-C3E-C4E-C5E	0.0
C3E-C4E-C5E-C6E	0.0
C4E-C5E-C6E-C1E	0.0
C6E-C1E-C2E-C3E	0.0
F1EA-C1EA-C6EA-C5EA	175(3)

F1EA-C1EA-C2EA-C3EA	-175(3)
C1EA-C6EA-C5EA-C4EA	0.0
C6EA-C1EA-C2EA-C3EA	0.0
C6EA-C5EA-C4EA-C3EA	0.0
C5EA-C4EA-C3EA-C2EA	0.0
C4EA-C3EA-C2EA-C1EA	0.0
C2EA-C1EA-C6EA-C5EA	0.0
F1F-C1F-C2F-C3F	174.7(13)
F1F-C1F-C6F-C5F	-174.7(13)
C1F-C2F-C3F-C4F	0.0
C2F-C1F-C6F-C5F	0.0
C2F-C3F-C4F-C5F	0.0
C3F-C4F-C5F-C6F	0.0
C4F-C5F-C6F-C1F	0.0
C6F-C1F-C2F-C3F	0.0
F1FA-C1FA-C2FA-C3FA	168.4(17)
F1FA-C1FA-C6FA-C5FA	-169.0(16)
C1FA-C2FA-C3FA-C4FA	0.0
C2FA-C1FA-C6FA-C5FA	0.0
C2FA-C3FA-C4FA-C5FA	0.0
C3FA-C4FA-C5FA-C6FA	0.0
C4FA-C5FA-C6FA-C1FA	0.0
C6FA-C1FA-C2FA-C3FA	0.0

Table S7. Crystal data and structure refinement for **2**.

Identification code	$[Fe_4Mo_2]^{2-}$	
Empirical formula	C51 H48 Fe4 K2 Mo2 O30	
Formula weight	1634.37	
Temperature	100.15 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 n 1	
Unit cell dimensions	a = 16.9288(3) Å	a= 90°.
	b = 8.76190(10) Å	b= 92.4690(10)°.
	c = 19.7002(3) Å	g = 90°.
Volume	2919.39(8) $Å^3$	
Z	2	
Density (calculated)	1.859 Mg/m^3	
Absorption coefficient	1.620 mm^{-1}	
F(000)	1640	
Crystal size	0.29 x 0.22 x 0.18 mm^3	
Theta range for data collection	2.069 to 27.484°.	
Index ranges	-21<=h<=21, -11<=k<=10, -25<=l<=25	
Reflections collected	46356	
Independent reflections	13347 [R(int) = 0.0250]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	1.0000 and 0.7843	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13347 / 1157 / 1164	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0249, wR2 = 0.0613	
R indices (all data)	R1 = 0.0261, wR2 = 0.0619	
Absolute structure parameter	0.514(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.673 and -0.484 e.$Å^{-3}$	

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo1	2812(1)	6564(1)	14087(1)	15(1)
Mo2	4117(1)	8790(2)	14617(1)	14(1)
Fe1	4991(1)	7739(1)	13493(1)	9(1)
Fe2	4396(1)	5586(2)	14249(1)	16(1)
Fe3	3514(1)	8906(2)	13238(1)	13(1)
Fe4	3885(2)	6073(4)	12971(1)	18(1)
O1A	1231(4)	8282(9)	13813(3)	32(1)
O2A	1792(4)	3705(8)	13774(3)	36(1)
O3A	2135(9)	6340(13)	15506(6)	27(2)
O4A	2705(12)	9660(20)	15487(11)	29(3)
O5A	4887(13)	11888(16)	15108(11)	20(2)
O6A	4738(9)	7700(20)	16039(8)	29(3)
O7A	3438(4)	3845(7)	15169(4)	29(1)
O8A	3200(5)	11738(10)	13958(4)	28(2)
O9A	5971(4)	10042(8)	14243(3)	32(1)
O10A	5776(5)	5316(10)	15181(5)	38(2)
O11A	4894(5)	2813(8)	13571(3)	24(1)
O12A	6331(4)	5695(7)	13758(3)	25(1)
O13A	5824(7)	9026(15)	12326(7)	31(3)
O14A	1972(5)	9624(13)	12618(5)	26(2)
O15A	4247(4)	10767(9)	12217(4)	29(2)
O16A	3088(8)	7342(18)	11734(8)	26(2)
O17A	5189(9)	5140(20)	12143(7)	25(2)
O18A	2952(9)	3379(16)	12615(8)	28(3)
C1A	1845(5)	7706(11)	13893(4)	28(2)
C2A	2188(4)	4743(9)	13871(4)	21(1)
C3A	2426(14)	6460(30)	14992(10)	20(4)
C4A	3190(11)	9270(20)	15125(9)	22(3)
C5A	4566(11)	10776(17)	14935(9)	12(2)
C6A	4530(7)	8045(14)	15495(6)	16(2)
C7A	3632(5)	4674(9)	14759(5)	24(2)

C8A	3439(5)	10537(9)	13878(4)	17(2)
C9A	5466(5)	9231(9)	14054(4)	24(2)
C10A	5210(6)	5549(11)	14849(5)	21(1)
C11A	4668(6)	3904(13)	13806(5)	19(2)
C12A	5775(4)	6451(8)	13688(3)	16(1)
C13A	5462(10)	8546(19)	12757(7)	14(3)
C14A	2560(9)	9294(19)	12881(10)	21(3)
C15A	3993(4)	10060(9)	12642(4)	18(1)
C16A	3308(10)	6947(19)	12268(10)	30(3)
C17A	4700(9)	5511(16)	12501(7)	17(2)
C18A	3277(17)	4440(20)	12802(15)	18(4)
C19A	3920(5)	7287(11)	13791(5)	11(2)
Mo3	4991(1)	8341(2)	3649(1)	27(1)
Mo4	3696(1)	6164(3)	3118(1)	24(1)
Fe5	2809(1)	7191(2)	4245(1)	19(1)
Fe6	3420(1)	9325(3)	3474(1)	31(1)
Fe7	4298(1)	6018(2)	4495(1)	24(1)
Fe8	3917(2)	8852(5)	4758(2)	22(1)
O1B	6012(6)	11201(14)	4018(6)	52(3)
O2B	5652(11)	8670(20)	2283(10)	34(4)
O3B	6529(8)	6504(18)	3908(6)	58(3)
O4B	2933(14)	3080(20)	2624(12)	23(4)
O5B	5096(15)	5250(40)	2285(11)	40(5)
O6B	3262(13)	7540(30)	1743(12)	39(5)
O7B	4358(7)	11092(12)	2537(6)	40(2)
O8B	4638(8)	3180(15)	3779(7)	36(3)
O9B	1820(6)	4881(14)	3525(5)	46(2)
O10B	2137(9)	9820(20)	2461(8)	37(4)
O11B	2960(8)	12126(13)	4162(6)	40(3)
O12B	1457(6)	9201(13)	3970(5)	40(2)
O13B	2024(15)	5930(20)	5423(11)	45(5)
O14B	5610(6)	5128(12)	5332(5)	23(2)
O15B	3557(6)	4162(12)	5515(6)	38(2)
O16B	4583(14)	7480(30)	6024(12)	31(4)
O17B	2607(17)	9950(30)	5555(17)	34(5)
O18B	4830(20)	11550(30)	5140(17)	31(5)

C1B	5638(9)	10127(18)	3934(8)	43(3)
C2B	5391(18)	8480(40)	2831(12)	36(6)
C3B	5973(8)	7277(17)	3855(7)	36(3)
C4B	3240(20)	4180(30)	2800(20)	16(5)
C5B	4612(16)	5760(30)	2619(12)	33(6)
C6B	3459(12)	7210(20)	2296(12)	22(4)
C7B	4134(9)	10281(16)	2964(9)	40(3)
C8B	4402(10)	4354(16)	3892(7)	31(3)
C9B	2330(7)	5695(16)	3702(7)	36(3)
C10B	2657(13)	9570(30)	2846(13)	20(4)
C11B	3165(11)	11010(20)	3924(9)	33(4)
C12B	2031(7)	8510(15)	4059(6)	30(2)
C13B	2321(19)	6400(50)	4957(15)	22(6)
C14B	5124(8)	5326(15)	4933(6)	21(1)
C15B	3806(8)	4883(14)	5098(7)	30(2)
C16B	4333(12)	7840(30)	5488(12)	34(5)
C17B	3097(16)	9480(30)	5236(13)	21(4)
C18B	4512(19)	10460(30)	4928(17)	29(6)
C19B	3846(10)	7694(17)	3955(9)	23(3)
K1	3730(1)	9368(1)	10731(1)	22(1)
O1	3186(2)	6770(3)	10003(2)	20(1)
O2	2180(2)	9127(3)	10359(2)	20(1)
O3	2754(2)	11825(3)	10920(2)	21(1)
O4	4346(2)	12328(3)	10677(2)	23(1)
O5	5314(2)	9752(4)	10623(2)	27(1)
O6	4653(2)	6872(3)	10381(2)	24(1)
C1	3688(3)	6022(5)	9587(2)	19(1)
C2	3444(3)	5184(5)	9021(2)	24(1)
C3	4008(3)	4433(5)	8644(2)	31(1)
C4	4798(3)	4540(6)	8831(2)	34(1)
C5	5041(3)	5377(6)	9399(2)	30(1)
C6	4492(3)	6093(5)	9788(2)	23(1)
C7	2362(3)	6777(5)	9791(2)	22(1)
C8	1922(3)	7588(5)	10325(2)	23(1)
C9	1703(3)	10051(5)	10772(2)	24(1)
C10	1948(3)	11670(5)	10682(2)	23(1)

C11	3051(3)	13304(5)	10785(2)	23(1)
C12	3895(3)	13394(5)	11046(2)	23(1)
C13	5159(3)	12383(5)	10881(3)	30(1)
C14	5589(3)	11233(5)	10469(3)	30(1)
C15	5771(3)	8569(6)	10356(3)	30(1)
C16	5455(3)	7102(6)	10623(3)	29(1)
K2	4072(1)	5674(1)	7024(1)	23(1)
O7	3139(2)	8163(3)	7355(2)	24(1)
O8	2492(2)	5262(4)	7113(2)	27(1)
O9	3455(2)	2705(3)	7057(2)	22(1)
O10	5051(2)	3219(3)	6842(2)	20(1)
O11	5619(2)	5915(3)	7417(2)	21(1)
O12	4602(2)	8292(3)	7750(2)	20(1)
C17	3291(3)	8940(5)	7955(2)	20(1)
C18	2730(3)	9650(5)	8341(2)	27(1)
C19	2973(3)	10480(5)	8912(2)	32(1)
C20	3753(3)	10609(5)	9102(2)	29(1)
C21	4320(3)	9872(5)	8729(2)	24(1)
C22	4093(3)	9037(5)	8159(2)	19(1)
C23	2335(3)	7927(5)	7112(3)	26(1)
C24	2015(3)	6478(6)	7371(3)	29(1)
C25	2199(3)	3791(5)	7250(3)	31(1)
C26	2640(3)	2671(5)	6844(3)	27(1)
C27	3913(3)	1659(5)	6687(2)	25(1)
C28	4749(3)	1732(5)	6955(2)	24(1)
C29	5845(3)	3377(5)	7085(2)	23(1)
C30	6094(3)	5006(5)	7003(2)	24(1)
C31	5871(3)	7468(5)	7444(2)	22(1)
C32	5420(3)	8276(5)	7969(2)	21(1)

Table S9. Bond lengths [Å] and angles [°] for **2**.

Mo1-Mo2	3.0944(16)	Fe3-C19A	1.899(8)
Mo1-Fe2	2.8199(15)	Fe4-C16A	1.828(18)
Mo1-Fe3	2.9299(15)	Fe4-C17A	1.764(16)
Mo1-Fe4	2.9432(19)	Fe4-C18A	1.783(18)
Mo1-C1A	1.942(8)	Fe4-C19A	1.933(11)
Mo1-C2A	1.950(8)	O1A-C1A	1.160(9)
Mo1-C3A	1.927(19)	O2A-C2A	1.142(9)
Mo1-C7A	2.503(9)	O3A-C3A	1.149(14)
Mo1-C19A	2.087(8)	O4A-C4A	1.160(14)
Mo2-Fe1	2.8668(16)	O5A-C5A	1.160(13)
Mo2-Fe2	2.942(2)	O6A-C6A	1.152(13)
Mo2-Fe3	2.8614(18)	O7A-C7A	1.146(9)
Mo2-C4A	1.945(17)	O8A-C8A	1.141(10)
Mo2-C5A	1.989(16)	O9A-C9A	1.160(10)
Mo2-C6A	1.951(12)	O10A-C10A	1.155(12)
Mo2-C8A	2.374(9)	O11A-C11A	1.136(12)
Mo2-C9A	2.610(8)	O12A-C12A	1.154(8)
Mo2-C19A	2.108(11)	O13A-C13A	1.148(14)
Fe1-Fe2	2.6310(17)	O14A-C14A	1.141(13)
Fe1-Fe3	2.7282(18)	O15A-C15A	1.141(9)
Fe1-Fe4	2.555(3)	O15A-K1	3.259(8)
Fe1-C9A	1.872(7)	O16A-C16A	1.155(14)
Fe1-C12A	1.773(7)	O16A-K1	2.901(16)
Fe1-C13A	1.827(14)	O17A-C17A	1.157(13)
Fe1-C19A	1.970(8)	O18A-C18A	1.136(15)
Fe2-Fe4	2.661(3)	Mo3-Mo4	3.055(3)
Fe2-C7A	1.852(7)	Mo3-Fe6	2.802(3)
Fe2-C10A	1.777(10)	Mo3-Fe7	2.910(2)
Fe2-C11A	1.784(12)	Mo3-Fe8	2.936(3)
Fe2-C19A	1.903(8)	Mo3-C1B	1.978(15)
Fe3-Fe4	2.620(3)	Mo3-C2B	1.78(2)
Fe3-C8A	1.914(8)	Mo3-C3B	1.934(12)
Fe3-C14A	1.765(14)	Mo3-C7B	2.579(15)
Fe3-C15A	1.773(8)	Mo3-C19B	2.131(17)

Mo4-Fe5	2.879(3)	O8B-C8B	1.130(15)
Mo4-Fe6	2.900(4)	O9B-C9B	1.162(14)
Mo4-Fe7	2.860(3)	O10B-C10B	1.159(17)
Mo4-C4B	1.99(3)	O11B-C11B	1.147(16)
Mo4-C5B	1.90(2)	O12B-C12B	1.151(13)
Mo4-C6B	1.89(2)	O13B-C13B	1.144(19)
Mo4-C8B	2.473(16)	O14B-C14B	1.127(14)
Mo4-C19B	2.132(17)	O15B-C15B	1.132(13)
Fe5-Fe6	2.648(3)	O15B-K2	3.337(13)
Fe5-Fe7	2.746(3)	O16B-C16B	1.164(18)
Fe5-Fe8	2.547(4)	O16B-K2	2.70(2)
Fe5-C9B	1.856(12)	O17B-C17B	1.136(18)
Fe5-C12B	1.779(12)	O18B-C18B	1.168(17)
Fe5-C13B	1.80(3)	K1-O1	2.823(3)
Fe5-C19B	1.921(17)	K1-O2	2.702(3)
Fe6-Fe8	2.663(4)	K1-O3	2.749(3)
Fe6-C7B	1.810(13)	K1-O4	2.800(3)
Fe6-C10B	1.76(2)	K1-O5	2.721(3)
Fe6-C11B	1.783(19)	K1-O6	2.791(3)
Fe6-C19B	1.845(15)	O1-C1	1.373(5)
Fe7-Fe8	2.623(4)	O1-C7	1.439(5)
Fe7-C8B	1.893(15)	O2-C8	1.419(5)
Fe7-C14B	1.721(13)	O2-C9	1.423(5)
Fe7-C15B	1.783(11)	O3-C10	1.430(6)
Fe7-C19B	1.950(15)	O3-C11	1.419(5)
Fe8-C16B	1.81(2)	O4-C12	1.426(5)
Fe8-C17B	1.80(3)	O4-C13	1.418(6)
Fe8-C18B	1.75(3)	O5-C14	1.416(6)
Fe8-C19B	1.878(18)	O5-C15	1.408(6)
O1B-C1B	1.143(15)	O6-C6	1.371(5)
O2B-C2B	1.195(18)	O6-C16	1.434(6)
O3B-C3B	1.161(13)	C1-C2	1.384(6)
O4B-C4B	1.141(18)	C1-C6	1.401(6)
O5B-C5B	1.163(17)	C2-H2	0.95
O6B-C6B	1.162(17)	C2-C3	1.400(7)
O7B-C7B	1.176(15)	C3-H3	0.95

C3-C4	1.375(8)	O7-C17	1.378(5)
C4-H4	0.95	O7-C23	1.438(6)
C4-C5	1.385(7)	O8-C24	1.441(6)
C5-H5	0.95	O8-C25	1.411(6)
C5-C6	1.380(6)	O9-C26	1.426(6)
C7-H7A	0.99	O9-C27	1.421(5)
C7-H7B	0.99	O10-C28	1.420(5)
C7-C8	1.495(6)	O10-C29	1.414(6)
C8-H8A	0.99	O11-C30	1.416(5)
C8-H8B	0.99	O11-C31	1.427(5)
C9-H9A	0.99	O12-C22	1.370(5)
C9-H9B	0.99	O12-C32	1.434(5)
C9-C10	1.491(6)	C17-C18	1.389(6)
C10-H10A	0.99	C17-C22	1.402(6)
C10-H10B	0.99	C18-H18	0.95
C11-H11A	0.99	C18-C19	1.387(7)
C11-H11B	0.99	C19-H19	0.95
C11-C12	1.500(7)	C19-C20	1.363(8)
C12-H12A	0.99	C20-H20	0.95
C12-H12B	0.99	C20-C21	1.392(6)
C13-H13A	0.99	C21-H21	0.95
C13-H13B	0.99	C21-C22	1.381(6)
C13-C14	1.501(7)	C23-H23A	0.99
C14-H14A	0.99	C23-H23B	0.99
C14-H14B	0.99	C23-C24	1.479(7)
C15-H15A	0.99	C24-H24A	0.99
C15-H15B	0.99	C24-H24B	0.99
C15-C16	1.497(7)	C25-H25A	0.99
C16-H16A	0.99	C25-H25B	0.99
C16-H16B	0.99	C25-C26	1.487(7)
K2-O7	2.787(3)	C26-H26A	0.99
K2-O8	2.713(3)	C26-H26B	0.99
K2-O9	2.805(3)	C27-H27A	0.99
K2-O10	2.748(3)	C27-H27B	0.99
K2-O11	2.706(3)	C27-C28	1.490(7)
K2-O12	2.829(3)	C28-H28A	0.99

C28-H28B	0.99	C31-H31A	0.99
C29-H29A	0.99	C31-H31B	0.99
C29-H29B	0.99	C31-C32	1.490(6)
C29-C30	1.499(6)	C32-H32A	0.99
C30-H30A	0.99	C32-H32B	0.99
C30-H30B	0.99		

Fe2-Mo1-Mo2	59.45(4)	C7A-Mo1-Fe3	122.39(17)
Fe2-Mo1-Fe3	82.56(4)	C7A-Mo1-Fe4	87.24(18)
Fe2-Mo1-Fe4	54.94(7)	C19A-Mo1-Mo2	42.7(3)
Fe3-Mo1-Mo2	56.64(4)	C19A-Mo1-Fe2	42.4(2)
Fe3-Mo1-Fe4	52.98(7)	C19A-Mo1-Fe3	40.2(2)
Fe4-Mo1-Mo2	83.64(7)	C19A-Mo1-Fe4	40.9(3)
C1A-Mo1-Mo2	109.0(3)	C19A-Mo1-C7A	82.2(3)
C1A-Mo1-Fe2	165.5(3)	Fe1-Mo2-Mo1	85.52(5)
C1A-Mo1-Fe3	83.5(3)	Fe1-Mo2-Fe2	53.84(4)
C1A-Mo1-Fe4	118.1(2)	Fe2-Mo2-Mo1	55.63(4)
C1A-Mo1-C2A	86.3(4)	Fe3-Mo2-Mo1	58.78(4)
C1A-Mo1-C7A	152.7(3)	Fe3-Mo2-Fe1	56.88(4)
C1A-Mo1-C19A	123.3(4)	Fe3-Mo2-Fe2	81.65(5)
C2A-Mo1-Mo2	164.0(2)	C4A-Mo2-Mo1	74.4(6)
C2A-Mo1-Fe2	106.2(2)	C4A-Mo2-Fe1	157.3(6)
C2A-Mo1-Fe3	132.7(2)	C4A-Mo2-Fe2	118.4(6)
C2A-Mo1-Fe4	93.6(2)	C4A-Mo2-Fe3	102.6(6)
C2A-Mo1-C7A	81.7(3)	C4A-Mo2-C5A	87.3(8)
C2A-Mo1-C19A	132.2(4)	C4A-Mo2-C6A	83.2(7)
C3A-Mo1-Mo2	89.0(8)	C4A-Mo2-C8A	78.2(6)
C3A-Mo1-Fe2	103.9(7)	C4A-Mo2-C9A	158.0(6)
C3A-Mo1-Fe3	136.2(8)	C4A-Mo2-C19A	115.4(6)
C3A-Mo1-Fe4	158.3(7)	C5A-Mo2-Mo1	156.2(5)
C3A-Mo1-C1A	83.7(8)	C5A-Mo2-Fe1	108.8(6)
C3A-Mo1-C2A	87.8(9)	C5A-Mo2-Fe2	148.1(5)
C3A-Mo1-C7A	71.5(8)	C5A-Mo2-Fe3	112.6(5)
C3A-Mo1-C19A	128.1(8)	C5A-Mo2-C8A	78.3(5)
C7A-Mo1-Mo2	82.3(2)	C5A-Mo2-C9A	71.0(6)
C7A-Mo1-Fe2	40.17(17)	C5A-Mo2-C19A	146.7(6)

C6A-Mo2-Mo1	108.2(4)	C12A-Fe1-Fe3	162.0(3)
C6A-Mo2-Fe1	113.6(4)	C12A-Fe1-Fe4	104.6(3)
C6A-Mo2-Fe2	81.0(4)	C12A-Fe1-C9A	91.0(4)
C6A-Mo2-Fe3	162.4(4)	C12A-Fe1-C13A	94.0(6)
C6A-Mo2-C5A	84.0(6)	C12A-Fe1-C19A	119.9(3)
C6A-Mo2-C8A	154.8(4)	C13A-Fe1-Mo2	138.2(5)
C6A-Mo2-C9A	98.0(4)	C13A-Fe1-Fe2	156.6(5)
C6A-Mo2-C19A	120.9(4)	C13A-Fe1-Fe3	97.9(5)
C8A-Mo2-Mo1	83.1(2)	C13A-Fe1-Fe4	103.9(5)
C8A-Mo2-Fe1	89.2(2)	C13A-Fe1-C9A	90.4(6)
C8A-Mo2-Fe2	122.89(19)	C13A-Fe1-C19A	138.9(6)
C8A-Mo2-Fe3	41.59(19)	C19A-Fe1-Mo2	47.3(3)
C8A-Mo2-C9A	93.1(3)	C19A-Fe1-Fe2	46.1(2)
C9A-Mo2-Mo1	125.14(17)	C19A-Fe1-Fe3	44.1(2)
C9A-Mo2-Fe1	39.63(16)	C19A-Fe1-Fe4	48.5(3)
C9A-Mo2-Fe2	83.37(18)	Mo1-Fe2-Mo2	64.92(4)
C9A-Mo2-Fe3	82.84(17)	Fe1-Fe2-Mo1	95.93(5)
C19A-Mo2-Mo1	42.2(2)	Fe1-Fe2-Mo2	61.62(4)
C19A-Mo2-Fe1	43.4(2)	Fe1-Fe2-Fe4	57.73(8)
C19A-Mo2-Fe2	40.2(2)	Fe4-Fe2-Mo1	64.89(5)
C19A-Mo2-Fe3	41.6(2)	Fe4-Fe2-Mo2	91.78(8)
C19A-Mo2-C8A	82.7(3)	C7A-Fe2-Mo1	60.7(3)
C19A-Mo2-C9A	83.0(3)	C7A-Fe2-Mo2	98.9(3)
Fe2-Fe1-Mo2	64.54(5)	C7A-Fe2-Fe1	155.5(3)
Fe2-Fe1-Fe3	90.13(6)	C7A-Fe2-Fe4	112.1(3)
Fe3-Fe1-Mo2	61.46(5)	C7A-Fe2-C19A	107.7(4)
Fe4-Fe1-Mo2	95.78(7)	C10A-Fe2-Mo1	142.0(3)
Fe4-Fe1-Fe2	61.72(8)	C10A-Fe2-Mo2	89.0(3)
Fe4-Fe1-Fe3	59.35(7)	C10A-Fe2-Fe1	94.8(3)
C9A-Fe1-Mo2	62.8(3)	C10A-Fe2-Fe4	147.5(3)
C9A-Fe1-Fe2	109.4(3)	C10A-Fe2-C7A	99.9(4)
C9A-Fe1-Fe3	102.4(2)	C10A-Fe2-C11A	95.8(5)
C9A-Fe1-Fe4	157.8(3)	C10A-Fe2-C19A	129.1(4)
C9A-Fe1-C19A	110.0(4)	C11A-Fe2-Mo1	117.4(3)
C12A-Fe1-Mo2	116.3(2)	C11A-Fe2-Mo2	163.0(3)
C12A-Fe1-Fe2	73.9(2)	C11A-Fe2-Fe1	101.6(3)

C11A-Fe2-Fe4	75.5(3)	Fe1-Fe4-Fe2	60.55(8)
C11A-Fe2-C7A	96.3(4)	Fe1-Fe4-Fe3	63.63(8)
C11A-Fe2-C19A	121.9(4)	Fe2-Fe4-Mo1	60.17(6)
C19A-Fe2-Mo1	47.7(2)	Fe3-Fe4-Mo1	63.25(6)
C19A-Fe2-Mo2	45.6(3)	Fe3-Fe4-Fe2	91.88(9)
C19A-Fe2-Fe1	48.3(2)	C16A-Fe4-Mo1	100.2(6)
C19A-Fe2-Fe4	46.5(3)	C16A-Fe4-Fe1	115.1(5)
Mo2-Fe3-Mo1	64.58(4)	C16A-Fe4-Fe2	157.7(6)
Fe1-Fe3-Mo1	91.36(5)	C16A-Fe4-Fe3	68.3(6)
Fe1-Fe3-Mo2	61.66(4)	C16A-Fe4-C19A	113.5(6)
Fe4-Fe3-Mo1	63.77(6)	C17A-Fe4-Mo1	162.7(5)
Fe4-Fe3-Mo2	94.48(8)	C17A-Fe4-Fe1	78.1(5)
Fe4-Fe3-Fe1	57.02(7)	C17A-Fe4-Fe2	102.9(5)
C8A-Fe3-Mo1	96.2(3)	C17A-Fe4-Fe3	124.7(5)
C8A-Fe3-Mo2	55.4(3)	C17A-Fe4-C16A	97.1(7)
C8A-Fe3-Fe1	104.2(3)	C17A-Fe4-C18A	97.9(11)
C8A-Fe3-Fe4	149.7(3)	C17A-Fe4-C19A	126.6(5)
C14A-Fe3-Mo1	88.6(6)	C18A-Fe4-Mo1	83.5(10)
C14A-Fe3-Mo2	131.9(7)	C18A-Fe4-Fe1	160.0(9)
C14A-Fe3-Fe1	163.8(7)	C18A-Fe4-Fe2	102.1(10)
C14A-Fe3-Fe4	109.0(6)	C18A-Fe4-Fe3	130.9(9)
C14A-Fe3-C8A	91.9(7)	C18A-Fe4-C16A	84.8(11)
C14A-Fe3-C15A	93.6(7)	C18A-Fe4-C19A	126.4(11)
C14A-Fe3-C19A	132.4(6)	C19A-Fe4-Mo1	45.0(2)
C15A-Fe3-Mo1	170.3(3)	C19A-Fe4-Fe1	49.7(3)
C15A-Fe3-Mo2	119.6(3)	C19A-Fe4-Fe2	45.6(2)
C15A-Fe3-Fe1	83.9(2)	C19A-Fe4-Fe3	46.3(3)
C15A-Fe3-Fe4	106.7(3)	C15A-O15A-K1	111.0(6)
C15A-Fe3-C8A	93.2(4)	C16A-O16A-K1	133.5(12)
C15A-Fe3-C19A	129.9(3)	O1A-C1A-Mo1	173.4(8)
C19A-Fe3-Mo1	45.2(2)	O2A-C2A-Mo1	175.8(6)
C19A-Fe3-Mo2	47.5(3)	O3A-C3A-Mo1	174(2)
C19A-Fe3-Fe1	46.2(2)	O4A-C4A-Mo2	171.2(19)
C19A-Fe3-Fe4	47.4(3)	O5A-C5A-Mo2	174.5(18)
C19A-Fe3-C8A	102.3(4)	O6A-C6A-Mo2	174.1(13)
Fe1-Fe4-Mo1	94.65(9)	Fe2-C7A-Mo1	79.2(3)

O7A-C7A-Mo1	128.5(6)	Fe7-Mo3-Fe8	53.32(10)
O7A-C7A-Fe2	152.2(8)	Fe8-Mo3-Mo4	83.80(9)
Fe3-C8A-Mo2	83.0(3)	C1B-Mo3-Mo4	166.2(5)
O8A-C8A-Mo2	132.5(7)	C1B-Mo3-Fe6	107.6(5)
O8A-C8A-Fe3	144.4(8)	C1B-Mo3-Fe7	128.6(5)
Fe1-C9A-Mo2	77.6(3)	C1B-Mo3-Fe8	91.2(4)
O9A-C9A-Mo2	127.0(6)	C1B-Mo3-C7B	85.3(7)
O9A-C9A-Fe1	155.3(7)	C1B-Mo3-C19B	129.0(6)
O10A-C10A-Fe2	168.8(9)	C2B-Mo3-Mo4	91.7(10)
O11A-C11A-Fe2	173.5(9)	C2B-Mo3-Fe6	105.2(10)
O12A-C12A-Fe1	172.2(6)	C2B-Mo3-Fe7	138.3(11)
O13A-C13A-Fe1	173.7(15)	C2B-Mo3-Fe8	159.2(10)
O14A-C14A-Fe3	174.6(16)	C2B-Mo3-C1B	88.4(11)
O15A-C15A-Fe3	173.8(8)	C2B-Mo3-C3B	82.4(11)
O16A-C16A-Fe4	163.2(16)	C2B-Mo3-C7B	72.9(11)
O17A-C17A-Fe4	173.9(13)	C2B-Mo3-C19B	131.4(11)
O18A-C18A-Fe4	170(3)	C3B-Mo3-Mo4	111.6(5)
Mo1-C19A-Mo2	95.1(4)	C3B-Mo3-Fe6	167.6(4)
Fe1-C19A-Mo1	173.9(6)	C3B-Mo3-Fe7	84.6(4)
Fe1-C19A-Mo2	89.3(4)	C3B-Mo3-Fe8	118.1(4)
Fe2-C19A-Mo1	89.8(3)	C3B-Mo3-C1B	82.0(7)
Fe2-C19A-Mo2	94.2(4)	C3B-Mo3-C7B	152.5(5)
Fe2-C19A-Fe1	85.6(3)	C3B-Mo3-C19B	126.6(6)
Fe2-C19A-Fe4	87.8(4)	C7B-Mo3-Mo4	81.5(4)
Fe3-C19A-Mo1	94.5(4)	C7B-Mo3-Fe6	39.0(3)
Fe3-C19A-Mo2	91.0(4)	C7B-Mo3-Fe7	122.0(3)
Fe3-C19A-Fe1	89.7(3)	C7B-Mo3-Fe8	86.3(3)
Fe3-C19A-Fe2	172.9(6)	C19B-Mo3-Mo4	44.2(5)
Fe3-C19A-Fe4	86.3(4)	C19B-Mo3-Fe6	41.2(4)
Fe4-C19A-Mo1	94.1(4)	C19B-Mo3-Fe7	42.1(4)
Fe4-C19A-Mo2	170.6(4)	C19B-Mo3-Fe8	39.7(5)
Fe4-C19A-Fe1	81.8(4)	C19B-Mo3-C7B	80.0(5)
Fe6-Mo3-Mo4	59.15(8)	Fe5-Mo4-Mo3	86.04(9)
Fe6-Mo3-Fe7	83.23(7)	Fe5-Mo4-Fe6	54.55(7)
Fe6-Mo3-Fe8	55.25(10)	Fe6-Mo4-Mo3	56.07(7)
Fe7-Mo3-Mo4	57.24(7)	Fe7-Mo4-Mo3	58.82(7)

Fe7-Mo4-Fe5	57.18(7)	Fe8-Fe5-Fe6	61.64(11)
Fe7-Mo4-Fe6	82.41(10)	Fe8-Fe5-Fe7	59.26(10)
C4B-Mo4-Mo3	156.1(11)	C9B-Fe5-Mo4	64.2(4)
C4B-Mo4-Fe5	108.0(12)	C9B-Fe5-Fe6	109.9(5)
C4B-Mo4-Fe6	147.8(11)	C9B-Fe5-Fe7	102.4(4)
C4B-Mo4-Fe7	112.1(12)	C9B-Fe5-Fe8	158.1(4)
C4B-Mo4-C8B	78.7(12)	C9B-Fe5-C19B	111.9(7)
C4B-Mo4-C19B	145.5(13)	C12B-Fe5-Mo4	116.8(4)
C5B-Mo4-Mo3	72.9(8)	C12B-Fe5-Fe6	74.2(4)
C5B-Mo4-Fe5	156.9(8)	C12B-Fe5-Fe7	161.1(4)
C5B-Mo4-Fe6	116.5(8)	C12B-Fe5-Fe8	103.7(5)
C5B-Mo4-Fe7	102.5(8)	C12B-Fe5-C9B	92.2(6)
C5B-Mo4-C4B	89.2(14)	C12B-Fe5-C13B	92.8(12)
C5B-Mo4-C8B	79.4(9)	C12B-Fe5-C19B	117.9(6)
C5B-Mo4-C19B	116.4(9)	C13B-Fe5-Mo4	139.0(13)
C6B-Mo4-Mo3	96.6(7)	C13B-Fe5-Fe6	157.5(13)
C6B-Mo4-Fe5	114.3(7)	C13B-Fe5-Fe7	99.5(11)
C6B-Mo4-Fe6	73.4(7)	C13B-Fe5-Fe8	105.4(13)
C6B-Mo4-Fe7	152.8(7)	C13B-Fe5-C9B	88.5(14)
C6B-Mo4-C4B	95.0(14)	C13B-Fe5-C19B	141.0(12)
C6B-Mo4-C5B	78.2(10)	C19B-Fe5-Mo4	47.8(5)
C6B-Mo4-C8B	156.9(8)	C19B-Fe5-Fe6	44.2(4)
C6B-Mo4-C19B	111.9(8)	C19B-Fe5-Fe7	45.2(4)
C8B-Mo4-Mo3	82.5(3)	C19B-Fe5-Fe8	47.2(5)
C8B-Mo4-Fe5	88.8(4)	Mo3-Fe6-Mo4	64.78(8)
C8B-Mo4-Fe6	122.8(3)	Fe5-Fe6-Mo3	95.97(8)
C8B-Mo4-Fe7	40.8(3)	Fe5-Fe6-Mo4	62.32(8)
C19B-Mo4-Mo3	44.2(5)	Fe5-Fe6-Fe8	57.32(10)
C19B-Mo4-Fe5	41.9(5)	Fe8-Fe6-Mo3	64.93(8)
C19B-Mo4-Fe6	39.4(4)	Fe8-Fe6-Mo4	91.93(11)
C19B-Mo4-Fe7	43.0(4)	C7B-Fe6-Mo3	63.8(5)
C19B-Mo4-C8B	83.5(5)	C7B-Fe6-Mo4	100.9(5)
Fe6-Fe5-Mo4	63.12(9)	C7B-Fe6-Fe5	158.8(5)
Fe6-Fe5-Fe7	89.37(8)	C7B-Fe6-Fe8	114.1(6)
Fe7-Fe5-Mo4	61.07(8)	C7B-Fe6-C19B	112.9(7)
Fe8-Fe5-Mo4	94.86(10)	C10B-Fe6-Mo3	141.9(10)

C10B-Fe6-Mo4	93.9(8)	C15B-Fe7-Fe5	82.9(4)
C10B-Fe6-Fe5	101.3(8)	C15B-Fe7-Fe8	105.7(4)
C10B-Fe6-Fe8	151.3(9)	C15B-Fe7-C8B	92.7(6)
C10B-Fe6-C7B	92.3(10)	C15B-Fe7-C19B	126.9(6)
C10B-Fe6-C11B	93.5(11)	C19B-Fe7-Mo3	47.1(5)
C10B-Fe6-C19B	135.5(9)	C19B-Fe7-Mo4	48.2(5)
C11B-Fe6-Mo3	116.3(6)	C19B-Fe7-Fe5	44.4(5)
C11B-Fe6-Mo4	162.7(6)	C19B-Fe7-Fe8	45.6(5)
C11B-Fe6-Fe5	100.9(6)	Fe5-Fe8-Mo3	94.99(13)
C11B-Fe6-Fe8	74.3(6)	Fe5-Fe8-Fe6	61.04(11)
C11B-Fe6-C7B	94.3(8)	Fe5-Fe8-Fe7	64.15(11)
C11B-Fe6-C19B	118.9(8)	Fe6-Fe8-Mo3	59.83(9)
C19B-Fe6-Mo3	49.5(5)	Fe7-Fe8-Mo3	62.83(9)
C19B-Fe6-Mo4	47.2(5)	Fe7-Fe8-Fe6	91.74(14)
C19B-Fe6-Fe5	46.5(5)	C16B-Fe8-Mo3	106.5(7)
C19B-Fe6-Fe8	44.8(5)	C16B-Fe8-Fe5	106.8(7)
Mo4-Fe7-Mo3	63.95(7)	C16B-Fe8-Fe6	158.2(8)
Fe5-Fe7-Mo3	91.43(7)	C16B-Fe8-Fe7	66.5(8)
Fe5-Fe7-Mo4	61.75(7)	C16B-Fe8-C19B	114.4(9)
Fe8-Fe7-Mo3	63.85(8)	C17B-Fe8-Mo3	162.5(8)
Fe8-Fe7-Mo4	93.67(10)	C17B-Fe8-Fe5	79.2(8)
Fe8-Fe7-Fe5	56.59(10)	C17B-Fe8-Fe6	103.4(8)
C8B-Fe7-Mo3	97.4(4)	C17B-Fe8-Fe7	126.7(9)
C8B-Fe7-Mo4	58.6(5)	C17B-Fe8-C16B	91.0(11)
C8B-Fe7-Fe5	106.6(5)	C17B-Fe8-C19B	125.9(10)
C8B-Fe7-Fe8	152.0(5)	C18B-Fe8-Mo3	84.0(11)
C8B-Fe7-C19B	106.4(7)	C18B-Fe8-Fe5	160.2(10)
C14B-Fe7-Mo3	101.2(4)	C18B-Fe8-Fe6	102.3(11)
C14B-Fe7-Mo4	137.7(5)	C18B-Fe8-Fe7	130.7(10)
C14B-Fe7-Fe5	160.2(5)	C18B-Fe8-C16B	92.3(12)
C14B-Fe7-Fe8	115.9(5)	C18B-Fe8-C17B	95.9(14)
C14B-Fe7-C8B	87.0(7)	C18B-Fe8-C19B	127.6(12)
C14B-Fe7-C15B	82.1(6)	C19B-Fe8-Mo3	46.4(5)
C14B-Fe7-C19B	146.1(7)	C19B-Fe8-Fe5	48.6(5)
C15B-Fe7-Mo3	169.5(4)	C19B-Fe8-Fe6	43.8(5)
C15B-Fe7-Mo4	120.0(5)	C19B-Fe8-Fe7	47.9(5)

C15B-O15B-K2	109.5(11)	Fe8-C19B-Mo4	172.8(9)
C16B-O16B-K2	134.8(18)	Fe8-C19B-Fe5	84.2(7)
O1B-C1B-Mo3	171.8(15)	Fe8-C19B-Fe7	86.5(7)
O2B-C2B-Mo3	176(3)	O16A-K1-O15A	73.3(3)
O3B-C3B-Mo3	170.6(15)	O1-K1-O15A	145.99(14)
O4B-C4B-Mo4	175(3)	O1-K1-O16A	74.3(3)
O5B-C5B-Mo4	167(3)	O2-K1-O15A	119.54(14)
O6B-C6B-Mo4	165(2)	O2-K1-O16A	75.4(3)
Fe6-C7B-Mo3	77.2(5)	O2-K1-O1	60.51(9)
O7B-C7B-Mo3	125.5(11)	O2-K1-O3	61.01(9)
O7B-C7B-Fe6	156.9(14)	O2-K1-O4	114.90(10)
Fe7-C8B-Mo4	80.7(5)	O2-K1-O5	159.66(10)
O8B-C8B-Mo4	128.9(12)	O2-K1-O6	114.80(10)
O8B-C8B-Fe7	150.3(14)	O3-K1-O15A	73.95(14)
O9B-C9B-Fe5	155.1(11)	O3-K1-O16A	98.2(3)
O10B-C10B-Fe6	175(2)	O3-K1-O1	121.02(10)
O11B-C11B-Fe6	173.8(16)	O3-K1-O4	60.44(9)
O12B-C12B-Fe5	170.2(11)	O3-K1-O6	173.29(10)
O13B-C13B-Fe5	178(3)	O4-K1-O15A	66.37(14)
O14B-C14B-Fe7	163.2(13)	O4-K1-O16A	138.1(3)
O15B-C15B-Fe7	173.7(13)	O4-K1-O1	147.30(10)
O16B-C16B-Fe8	165(2)	O5-K1-O15A	78.23(14)
O17B-C17B-Fe8	176(3)	O5-K1-O16A	121.9(3)
O18B-C18B-Fe8	168(3)	O5-K1-O1	111.16(10)
Mo3-C19B-Mo4	91.6(7)	O5-K1-O3	120.94(10)
Fe5-C19B-Mo3	177.7(9)	O5-K1-O4	60.81(10)
Fe5-C19B-Mo4	90.4(6)	O5-K1-O6	60.88(10)
Fe5-C19B-Fe7	90.4(6)	O6-K1-O15A	112.64(14)
Fe6-C19B-Mo3	89.3(6)	O6-K1-O16A	85.3(3)
Fe6-C19B-Mo4	93.3(7)	O6-K1-O1	54.33(9)
Fe6-C19B-Fe5	89.3(7)	O6-K1-O4	120.20(10)
Fe6-C19B-Fe7	177.8(10)	C1-O1-K1	119.4(2)
Fe6-C19B-Fe8	91.3(7)	C1-O1-C7	116.5(3)
Fe7-C19B-Mo3	90.9(7)	C7-O1-K1	115.8(2)
Fe7-C19B-Mo4	88.8(6)	C8-O2-K1	112.3(2)
Fe8-C19B-Mo3	94.0(7)	C8-O2-C9	112.8(3)

C9-O2-K1	111.7(2)	C8-C7-H7B	110.2
C10-O3-K1	116.9(2)	O2-C8-C7	108.9(3)
C11-O3-K1	118.1(2)	O2-C8-H8A	109.9
C11-O3-C10	111.4(3)	O2-C8-H8B	109.9
C12-O4-K1	112.3(2)	C7-C8-H8A	109.9
C13-O4-K1	112.3(3)	C7-C8-H8B	109.9
C13-O4-C12	111.6(3)	H8A-C8-H8B	108.3
C14-O5-K1	117.6(3)	O2-C9-H9A	110.2
C15-O5-K1	119.8(3)	O2-C9-H9B	110.2
C15-O5-C14	113.8(3)	O2-C9-C10	107.8(3)
C6-O6-K1	120.5(3)	H9A-C9-H9B	108.5
C6-O6-C16	120.3(4)	C10-C9-H9A	110.2
C16-O6-K1	109.9(3)	C10-C9-H9B	110.2
O1-C1-C2	124.2(4)	O3-C10-C9	108.6(4)
O1-C1-C6	115.4(4)	O3-C10-H10A	110.0
C2-C1-C6	120.3(4)	O3-C10-H10B	110.0
C1-C2-H2	120.3	C9-C10-H10A	110.0
C1-C2-C3	119.4(5)	C9-C10-H10B	110.0
C3-C2-H2	120.3	H10A-C10-H10B	108.4
C2-C3-H3	119.9	O3-C11-H11A	109.9
C4-C3-C2	120.2(4)	O3-C11-H11B	109.9
C4-C3-H3	119.9	O3-C11-C12	108.9(3)
C3-C4-H4	119.9	H11A-C11-H11B	108.3
C3-C4-C5	120.3(4)	C12-C11-H11A	109.9
C5-C4-H4	119.9	C12-C11-H11B	109.9
C4-C5-H5	119.8	O4-C12-C11	108.3(3)
C6-C5-C4	120.3(5)	O4-C12-H12A	110.0
C6-C5-H5	119.8	O4-C12-H12B	110.0
O6-C6-C1	114.6(4)	C11-C12-H12A	110.0
O6-C6-C5	125.9(5)	C11-C12-H12B	110.0
C5-C6-C1	119.5(4)	H12A-C12-H12B	108.4
O1-C7-H7A	110.2	O4-C13-H13A	110.1
O1-C7-H7B	110.2	O4-C13-H13B	110.1
O1-C7-C8	107.7(4)	O4-C13-C14	108.2(4)
H7A-C7-H7B	108.5	H13A-C13-H13B	108.4
C8-C7-H7A	110.2	C14-C13-H13A	110.1

C14-C13-H13B	110.1	O10-K2-O15B	73.08(19)
O5-C14-C13	109.1(4)	O10-K2-O7	173.81(10)
O5-C14-H14A	109.9	O10-K2-O9	60.28(9)
O5-C14-H14B	109.9	O10-K2-O12	121.39(10)
C13-C14-H14A	109.9	O11-K2-O15B	119.89(18)
C13-C14-H14B	109.9	O11-K2-O7	115.04(10)
H14A-C14-H14B	108.3	O11-K2-O8	159.49(10)
O5-C15-H15A	110.3	O11-K2-O9	114.99(10)
O5-C15-H15B	110.3	O11-K2-O10	61.12(9)
O5-C15-C16	106.9(4)	O11-K2-O12	60.68(9)
H15A-C15-H15B	108.6	O12-K2-O15B	146.90(17)
C16-C15-H15A	110.3	C17-O7-K2	120.0(3)
C16-C15-H15B	110.3	C17-O7-C23	119.7(3)
O6-C16-C15	110.6(4)	C23-O7-K2	110.3(2)
O6-C16-H16A	109.5	C24-O8-K2	119.5(3)
O6-C16-H16B	109.5	C25-O8-K2	119.3(3)
C15-C16-H16A	109.5	C25-O8-C24	113.7(4)
C15-C16-H16B	109.5	C26-O9-K2	111.7(3)
H16A-C16-H16B	108.1	C27-O9-K2	112.0(2)
O16B-K2-O15B	70.3(5)	C27-O9-C26	112.2(3)
O16B-K2-O7	85.1(6)	C28-O10-K2	118.3(2)
O16B-K2-O8	118.3(5)	C29-O10-K2	116.7(2)
O16B-K2-O9	133.8(6)	C29-O10-C28	112.4(3)
O16B-K2-O10	98.6(6)	C30-O11-K2	111.0(3)
O16B-K2-O11	80.0(5)	C30-O11-C31	112.4(3)
O16B-K2-O12	77.8(5)	C31-O11-K2	111.7(2)
O7-K2-O15B	112.96(19)	C22-O12-K2	119.4(2)
O7-K2-O9	120.35(10)	C22-O12-C32	116.9(3)
O7-K2-O12	54.38(9)	C32-O12-K2	115.2(2)
O8-K2-O15B	77.54(18)	O7-C17-C18	125.7(4)
O8-K2-O7	61.21(10)	O7-C17-C22	114.8(4)
O8-K2-O9	60.40(10)	C18-C17-C22	119.4(4)
O8-K2-O10	120.42(10)	C17-C18-H18	120.2
O8-K2-O12	111.54(10)	C19-C18-C17	119.6(5)
O9-K2-O15B	64.46(17)	C19-C18-H18	120.2
O9-K2-O12	148.28(9)	C18-C19-H19	119.5

C20-C19-C18	121.1(4)	O9-C27-H27B	110.0
C20-C19-H19	119.5	O9-C27-C28	108.7(4)
C19-C20-H20	120.0	H27A-C27-H27B	108.3
C19-C20-C21	119.9(4)	C28-C27-H27A	110.0
C21-C20-H20	120.0	C28-C27-H27B	110.0
C20-C21-H21	120.0	O10-C28-C27	109.1(4)
C22-C21-C20	120.0(4)	O10-C28-H28A	109.9
C22-C21-H21	120.0	O10-C28-H28B	109.9
O12-C22-C17	115.3(4)	C27-C28-H28A	109.9
O12-C22-C21	124.8(4)	C27-C28-H28B	109.9
C21-C22-C17	119.9(4)	H28A-C28-H28B	108.3
O7-C23-H23A	109.4	O10-C29-H29A	109.9
O7-C23-H23B	109.4	O10-C29-H29B	109.9
O7-C23-C24	111.4(4)	O10-C29-C30	108.9(4)
H23A-C23-H23B	108.0	H29A-C29-H29B	108.3
C24-C23-H23A	109.4	C30-C29-H29A	109.9
C24-C23-H23B	109.4	C30-C29-H29B	109.9
O8-C24-C23	107.1(4)	O11-C30-C29	107.7(3)
O8-C24-H24A	110.3	O11-C30-H30A	110.2
O8-C24-H24B	110.3	O11-C30-H30B	110.2
C23-C24-H24A	110.3	C29-C30-H30A	110.2
C23-C24-H24B	110.3	C29-C30-H30B	110.2
H24A-C24-H24B	108.5	H30A-C30-H30B	108.5
O8-C25-H25A	110.1	O11-C31-H31A	110.0
O8-C25-H25B	110.1	O11-C31-H31B	110.0
O8-C25-C26	108.2(4)	O11-C31-C32	108.5(3)
H25A-C25-H25B	108.4	H31A-C31-H31B	108.4
C26-C25-H25A	110.1	C32-C31-H31A	110.0
C26-C25-H25B	110.1	C32-C31-H31B	110.0
O9-C26-C25	109.3(4)	O12-C32-C31	108.3(3)
O9-C26-H26A	109.8	O12-C32-H32A	110.0
O9-C26-H26B	109.8	O12-C32-H32B	110.0
C25-C26-H26A	109.8	C31-C32-H32A	110.0
C25-C26-H26B	109.8	C31-C32-H32B	110.0
H26A-C26-H26B	108.3	H32A-C32-H32B	108.4
O9-C27-H27A	110.0		

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo1	13(1)	18(1)	13(1)	0(1)	2(1)	-3(1)
Mo2	13(1)	15(1)	14(1)	0(1)	0(1)	0(1)
Fe1	8(1)	10(1)	10(1)	-5(1)	0(1)	2(1)
Fe2	21(1)	13(1)	14(1)	1(1)	-3(1)	4(1)
Fe3	19(1)	12(1)	8(1)	2(1)	0(1)	3(1)
Fe4	18(1)	20(1)	15(1)	-4(1)	1(1)	4(1)
O1A	20(3)	51(4)	27(3)	6(3)	1(2)	12(3)
O2A	23(3)	39(3)	47(3)	-21(3)	8(2)	-6(2)
O3A	36(5)	32(5)	14(3)	-5(3)	5(3)	13(4)
O4A	24(6)	28(5)	37(5)	-8(4)	10(4)	1(4)
O5A	24(5)	10(4)	25(4)	0(4)	-1(3)	-8(4)
O6A	33(6)	36(6)	18(3)	3(3)	-5(3)	-4(4)
O7A	25(3)	28(3)	34(3)	5(3)	3(3)	8(2)
O8A	37(4)	25(4)	22(3)	-7(3)	-7(3)	12(3)
O9A	16(3)	47(4)	30(3)	-23(3)	-6(2)	-3(3)
O10A	34(4)	43(4)	37(4)	2(3)	2(3)	-7(3)
O11A	34(3)	19(3)	21(3)	-2(2)	3(2)	6(3)
O12A	19(3)	26(3)	29(3)	10(2)	3(2)	4(2)
O13A	16(4)	36(6)	41(5)	16(4)	13(3)	-3(3)
O14A	15(3)	33(4)	29(4)	8(3)	0(3)	-1(3)
O15A	24(3)	35(3)	28(3)	13(3)	8(3)	7(2)
O16A	28(5)	28(4)	21(4)	0(3)	-2(3)	2(4)
O17A	17(4)	41(4)	17(4)	-6(4)	5(3)	-3(3)
O18A	25(4)	27(6)	33(4)	-4(5)	-1(2)	-14(5)
C1A	30(4)	40(4)	13(3)	0(3)	0(3)	4(3)
C2A	15(3)	30(3)	17(3)	-10(3)	1(2)	2(3)
C3A	17(6)	20(5)	23(4)	0(3)	-10(4)	3(4)
C4A	20(5)	23(5)	23(6)	0(4)	0(4)	1(3)
C5A	11(4)	10(5)	14(4)	0(4)	-4(3)	-2(4)
C6A	15(4)	15(4)	19(3)	-2(3)	-1(3)	-1(3)
C7A	17(3)	20(3)	35(4)	-2(3)	13(3)	4(3)

C8A	20(3)	15(3)	17(3)	-2(3)	-4(3)	0(3)
C9A	21(3)	26(3)	24(3)	-10(3)	-7(3)	4(3)
C11A	27(4)	17(4)	13(3)	4(3)	1(3)	3(4)
C12A	20(3)	15(3)	11(2)	8(2)	-1(2)	-2(2)
C14A	21(4)	18(5)	23(4)	-1(4)	10(3)	-4(4)
C15A	12(3)	20(3)	22(3)	-3(3)	-2(2)	7(2)
C16A	32(6)	26(6)	33(4)	-3(4)	7(4)	1(4)
C17A	11(4)	21(4)	18(5)	-5(4)	-2(4)	-1(3)
C18A	16(5)	20(6)	18(5)	-5(5)	-2(4)	4(4)
C19A	10(3)	13(3)	10(3)	4(3)	4(2)	5(3)
Mo3	19(1)	37(1)	26(1)	10(1)	2(1)	-5(1)
Mo4	25(1)	22(1)	26(1)	4(1)	-2(1)	1(1)
Fe5	15(1)	19(1)	22(1)	2(1)	5(1)	2(1)
Fe6	32(1)	26(1)	34(1)	16(1)	-7(1)	4(1)
Fe7	31(1)	21(1)	21(1)	11(1)	-1(1)	4(1)
Fe8	17(2)	26(1)	24(2)	5(1)	4(1)	4(1)
O1B	33(5)	61(6)	62(6)	-32(5)	-4(4)	1(4)
O2B	29(8)	36(8)	38(6)	11(5)	12(5)	-3(5)
O3B	54(7)	76(7)	44(6)	23(6)	11(5)	34(6)
O5B	34(7)	47(8)	40(10)	-9(7)	20(6)	-15(6)
O6B	42(9)	54(9)	20(5)	11(5)	-9(6)	1(7)
O7B	37(5)	31(5)	53(6)	12(5)	9(5)	7(4)
O8B	42(6)	26(6)	39(6)	5(6)	-7(5)	5(6)
O9B	29(5)	72(7)	37(5)	-17(5)	6(4)	-5(4)
O10B	38(7)	40(6)	33(7)	4(5)	-1(5)	-13(5)
O11B	54(7)	25(5)	41(6)	10(4)	-11(5)	0(5)
O12B	27(4)	52(6)	41(5)	23(4)	0(4)	4(4)
O13B	40(7)	48(9)	46(9)	12(7)	8(6)	9(7)
O15B	39(5)	38(4)	39(4)	15(4)	13(4)	4(4)
O16B	37(7)	32(6)	25(5)	3(4)	-2(5)	1(5)
O17B	16(6)	40(10)	47(8)	-12(6)	4(5)	0(6)
O18B	28(6)	31(10)	34(6)	2(8)	6(4)	-17(8)
C1B	38(6)	50(6)	42(6)	-10(5)	16(5)	2(5)
C2B	34(8)	39(8)	36(8)	-2(5)	-5(5)	4(5)
C3B	33(5)	45(5)	30(5)	10(4)	1(4)	8(4)
C4B	12(7)	18(7)	19(7)	3(6)	2(5)	4(6)

C5B	26(7)	40(8)	32(8)	1(6)	1(5)	-1(5)
C6B	22(6)	17(6)	26(5)	8(4)	1(4)	5(5)
C7B	32(5)	34(5)	53(6)	3(5)	4(5)	1(4)
C8B	31(6)	30(6)	33(5)	-4(4)	2(5)	-4(5)
C9B	32(5)	41(5)	34(5)	-7(4)	-9(4)	8(4)
C10B	29(7)	17(7)	15(5)	3(4)	10(4)	-2(5)
C11B	38(6)	28(6)	33(6)	3(5)	-6(5)	-6(6)
C12B	27(5)	29(5)	34(5)	5(4)	-3(4)	-7(4)
C13B	10(7)	30(8)	28(8)	-5(5)	4(6)	7(5)
C15B	28(5)	32(5)	29(5)	0(4)	-1(4)	8(4)
C16B	33(7)	36(7)	35(6)	7(5)	0(5)	1(5)
C17B	19(7)	24(7)	19(7)	5(5)	-2(5)	-6(5)
C18B	27(7)	33(9)	27(7)	-3(6)	3(5)	3(6)
C19B	27(6)	19(5)	23(5)	0(4)	2(4)	5(4)
K1	18(1)	19(1)	28(1)	-1(1)	1(1)	-2(1)
O1	16(2)	22(1)	22(1)	-5(1)	0(1)	-1(1)
O2	17(1)	19(1)	24(1)	-1(1)	3(1)	-1(1)
O3	22(2)	19(1)	21(1)	3(1)	-1(1)	-1(1)
O4	22(2)	22(1)	26(1)	-4(1)	2(1)	-5(1)
O5	19(2)	22(2)	42(2)	-2(1)	3(1)	-2(1)
O6	18(2)	26(2)	28(2)	-7(1)	0(1)	-1(1)
C1	25(2)	15(2)	19(2)	2(1)	4(2)	-3(2)
C2	33(2)	21(2)	17(2)	-1(2)	2(2)	-4(2)
C3	53(3)	24(2)	16(2)	0(2)	6(2)	-1(2)
C4	45(3)	30(2)	28(2)	0(2)	16(2)	4(2)
C5	28(2)	30(2)	31(2)	3(2)	10(2)	1(2)
C6	26(2)	17(2)	25(2)	1(2)	6(2)	-1(2)
C7	18(2)	20(2)	26(2)	0(2)	-4(2)	-3(2)
C8	16(2)	23(2)	31(2)	1(2)	1(2)	-1(2)
C9	20(2)	28(2)	25(2)	-3(2)	4(2)	0(2)
C10	20(2)	26(2)	23(2)	-2(2)	5(2)	3(2)
C11	31(2)	15(2)	24(2)	0(2)	3(2)	0(2)
C12	29(2)	19(2)	22(2)	-6(2)	2(2)	-1(2)
C13	24(2)	28(2)	38(2)	-6(2)	1(2)	-7(2)
C14	19(2)	29(2)	42(3)	-3(2)	4(2)	-8(2)
C15	20(2)	27(2)	41(2)	-2(2)	4(2)	-2(2)

C16	21(2)	29(2)	36(2)	-1(2)	-3(2)	2(2)
K2	17(1)	20(1)	31(1)	-1(1)	1(1)	-1(1)
O7	18(2)	23(2)	31(2)	-5(1)	-2(1)	-2(1)
O8	24(2)	22(2)	35(2)	-1(1)	6(1)	-3(1)
O9	22(2)	22(1)	23(1)	-7(1)	4(1)	-2(1)
O10	23(2)	16(1)	21(1)	3(1)	2(1)	-1(1)
O11	17(1)	19(1)	26(1)	-1(1)	4(1)	-1(1)
O12	16(2)	22(1)	22(1)	-3(1)	-2(1)	-2(1)
C17	20(2)	18(2)	21(2)	2(2)	2(2)	-4(2)
C18	26(2)	27(2)	29(2)	-1(2)	10(2)	0(2)
C19	41(3)	29(2)	28(2)	0(2)	16(2)	4(2)
C20	45(3)	25(2)	18(2)	-2(2)	8(2)	-3(2)
C21	31(2)	23(2)	19(2)	4(2)	0(2)	-6(2)
C22	22(2)	16(2)	20(2)	1(1)	5(2)	-2(2)
C23	18(2)	28(2)	33(2)	-4(2)	-5(2)	-2(2)
C24	18(2)	33(2)	37(2)	-3(2)	1(2)	1(2)
C25	22(2)	26(2)	46(3)	-5(2)	6(2)	-6(2)
C26	24(2)	22(2)	36(2)	-6(2)	2(2)	-8(2)
C27	32(3)	15(2)	28(2)	-4(2)	8(2)	-5(2)
C28	29(2)	16(2)	28(2)	2(2)	8(2)	1(2)
C29	21(2)	25(2)	24(2)	-2(2)	3(2)	6(2)
C30	19(2)	26(2)	26(2)	-4(2)	8(2)	-2(2)
C31	19(2)	18(2)	28(2)	3(2)	-2(2)	-5(2)
C32	18(2)	22(2)	23(2)	-1(2)	-4(2)	-2(2)

Table S11. Hydrogen coordinates ($\times 10^4$ Å) and isotropic displacement parameters (Å$^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H2	2898	5120	8889	29
H3	3845	3846	8257	37
H4	5179	4038	8570	40
H5	5588	5458	9522	35
H7A	2165	5719	9737	26
H7B	2286	7310	9350	26
H8A	1347	7549	10213	28
H8B	2023	7084	10771	28
H9A	1777	9748	11255	29
H9B	1137	9925	10634	29
H10A	1893	11957	10197	28
H10B	1608	12353	10943	28
H11A	2731	14083	11012	28
H11B	3018	13504	10290	28
H12A	4102	14440	10983	28
H12B	3932	13148	11537	28
H13A	5229	12142	11371	36
H13B	5372	13418	10803	36
H14A	5494	11445	9978	36
H14B	6165	11302	10576	36
H15A	6334	8695	10502	35
H15B	5727	8580	9854	35
H16A	5786	6242	10475	35
H16B	5480	7125	11126	35
H18	2184	9569	8215	32
H19	2588	10965	9176	39
H20	3911	11201	9489	35
H21	4864	9944	8867	29
H23A	2311	7909	6609	32
H23B	2004	8787	7261	32

H24A	2042	6473	7874	35
H24B	1456	6350	7212	35
H25A	1627	3738	7125	38
H25B	2274	3558	7740	38
H26A	2424	1634	6909	33
H26B	2580	2929	6355	33
H27A	3884	1926	6198	30
H27B	3705	611	6738	30
H28A	4774	1501	7447	29
H28B	5071	966	6722	29
H29A	6190	2700	6825	35
H29B	5895	3081	7570	35
H30A	6659	5128	7144	28
H30B	6022	5322	6522	28
H31A	5773	7959	6996	26
H31B	6445	7520	7562	26
H32A	5488	7743	8411	25
H32B	5618	9334	8026	25

Table 12. Torsion angles (°) for **2**.

Mo1-Fe2-C7A-O7A	-175.9(19)	C7A-Fe2-C10A-O10A	99(4)
Mo1-Fe2-C10A-O10A	153(4)	C8A-Fe3-C19A-Mo1	86.5(4)
Mo1-Fe3-C19A-Mo2	-95.2(4)	C8A-Fe3-C19A-Mo2	-8.7(4)
Mo1-Fe3-C19A-Fe1	175.6(6)	C8A-Fe3-C19A-Fe1	-97.9(4)
Mo1-Fe3-C19A-Fe4	93.8(4)	C8A-Fe3-C19A-Fe4	-179.7(3)
Mo1-Fe4-C16A-O16A	-172(5)	C10A-Fe2-C7A-Mo1	145.0(4)
Mo2-Fe1-C9A-O9A	175.7(19)	C10A-Fe2-C7A-O7A	-30.9(18)
Mo2-Fe2-C7A-Mo1	54.5(2)	C11A-Fe2-C7A-Mo1	-118.0(4)
Mo2-Fe2-C7A-O7A	-121.4(17)	C11A-Fe2-C7A-O7A	66.1(18)
Mo2-Fe2-C10A-O10A	-162(4)	C11A-Fe2-C10A-O10A	1(4)
Mo2-Fe3-C19A-Mo1	95.2(4)	C12A-Fe1-C9A-Mo2	-119.4(2)
Mo2-Fe3-C19A-Fe1	-89.3(4)	C12A-Fe1-C9A-O9A	56.4(18)
Mo2-Fe3-C19A-Fe4	-171.0(4)	C13A-Fe1-C9A-Mo2	146.6(6)
Fe1-Fe2-C7A-Mo1	19.1(9)	C13A-Fe1-C9A-O9A	-37.6(19)
Fe1-Fe2-C7A-O7A	-156.9(13)	C14A-Fe3-C19A-Mo1	-17.7(11)
Fe1-Fe2-C10A-O10A	-101(4)	C14A-Fe3-C19A-Mo2	-112.9(10)
Fe1-Fe3-C19A-Mo1	-175.6(6)	C14A-Fe3-C19A-Fe1	157.9(9)
Fe1-Fe3-C19A-Mo2	89.3(4)	C14A-Fe3-C19A-Fe4	76.1(10)
Fe1-Fe3-C19A-Fe4	-81.8(3)	C15A-Fe3-C19A-Mo1	-168.7(4)
Fe1-Fe4-C16A-O16A	88(5)	C15A-Fe3-C19A-Mo2	96.2(5)
Fe2-Fe1-C9A-Mo2	-46.1(2)	C15A-Fe3-C19A-Fe1	6.9(7)
Fe2-Fe1-C9A-O9A	129.6(18)	C15A-Fe3-C19A-Fe4	-74.9(6)
Fe2-Fe4-C16A-O16A	161(4)	C17A-Fe4-C16A-O16A	8(5)
Fe3-Fe1-C9A-Mo2	48.47(19)	C18A-Fe4-C16A-O16A	-89(5)
Fe3-Fe1-C9A-O9A	-135.8(18)	C19A-Fe1-C9A-Mo2	3.1(3)
Fe3-Fe4-C16A-O16A	133(5)	C19A-Fe1-C9A-O9A	178.8(18)
Fe4-Fe1-C9A-Mo2	16.0(8)	C19A-Fe2-C7A-Mo1	8.4(4)
Fe4-Fe1-C9A-O9A	-168.3(13)	C19A-Fe2-C7A-O7A	-167.5(17)
Fe4-Fe2-C7A-Mo1	-41.1(3)	C19A-Fe2-C10A-O10A	-139(4)
Fe4-Fe2-C7A-O7A	143.0(17)	C19A-Fe4-C16A-O16A	143(5)
Fe4-Fe2-C10A-O10A	-71(5)	Mo3-Mo4-C6B-O6B	154(8)
Fe4-Fe3-C19A-Mo1	-93.8(4)	Mo3-Fe6-C7B-O7B	171(4)
Fe4-Fe3-C19A-Mo2	171.0(4)	Mo3-Fe6-C19B-Mo4	-91.5(7)
Fe4-Fe3-C19A-Fe1	81.8(4)	Mo3-Fe6-C19B-Fe5	178.1(10)

Mo3-Fe6-C19B-Fe8	93.9(7)	Fe6-Fe8-C19B-Fe5	-89.2(7)
Mo3-Fe7-C8B-Mo4	-53.2(3)	Fe6-Fe8-C19B-Fe7	-179.9(10)
Mo3-Fe7-C8B-O8B	122(3)	Fe7-Mo4-C6B-O6B	177(7)
Mo3-Fe7-C14B-O14B	94(4)	Fe7-Fe5-C9B-O9B	136(3)
Mo3-Fe8-C16B-O16B	128(8)	Fe7-Fe8-C16B-O16B	177(8)
Mo3-Fe8-C18B-O18B	-173(14)	Fe7-Fe8-C18B-O18B	-127(14)
Mo3-Fe8-C19B-Fe5	-178.6(8)	Fe7-Fe8-C19B-Mo3	-90.6(7)
Mo3-Fe8-C19B-Fe6	-89.4(6)	Fe7-Fe8-C19B-Fe5	90.8(6)
Mo3-Fe8-C19B-Fe7	90.6(7)	Fe7-Fe8-C19B-Fe6	179.9(10)
Mo4-Fe5-C9B-O9B	-175(3)	Fe8-Fe5-C9B-O9B	167(2)
Mo4-Fe6-C7B-Mo3	-54.7(4)	Fe8-Fe6-C7B-Mo3	42.5(5)
Mo4-Fe6-C7B-O7B	116(4)	Fe8-Fe6-C7B-O7B	-147(4)
Mo4-Fe6-C19B-Mo3	91.5(7)	Fe8-Fe6-C19B-Mo3	-93.9(7)
Mo4-Fe6-C19B-Fe5	-90.3(7)	Fe8-Fe6-C19B-Mo4	174.5(10)
Mo4-Fe6-C19B-Fe8	-174.5(10)	Fe8-Fe6-C19B-Fe5	84.2(7)
Mo4-Fe7-C8B-O8B	175(3)	Fe8-Fe7-C8B-Mo4	-7.9(12)
Mo4-Fe7-C14B-O14B	158(4)	Fe8-Fe7-C8B-O8B	166.9(19)
Fe5-Mo4-C6B-O6B	-118(8)	Fe8-Fe7-C14B-O14B	28(4)
Fe5-Fe6-C7B-Mo3	-18.8(18)	C4B-Mo4-C6B-O6B	-6(8)
Fe5-Fe6-C7B-O7B	152(3)	C5B-Mo4-C6B-O6B	83(8)
Fe5-Fe6-C19B-Mo3	-178.1(10)	C7B-Fe6-C19B-Mo3	7.9(9)
Fe5-Fe6-C19B-Mo4	90.3(7)	C7B-Fe6-C19B-Mo4	-83.7(8)
Fe5-Fe6-C19B-Fe8	-84.2(7)	C7B-Fe6-C19B-Fe5	-174.0(7)
Fe5-Fe7-C8B-Mo4	40.5(4)	C7B-Fe6-C19B-Fe8	101.8(8)
Fe5-Fe7-C8B-O8B	-145(2)	C8B-Mo4-C6B-O6B	67(9)
Fe5-Fe7-C14B-O14B	-35(5)	C8B-Fe7-C14B-O14B	-169(4)
Fe5-Fe8-C16B-O16B	-132(8)	C10B-Fe6-C7B-Mo3	-149.1(9)
Fe5-Fe8-C18B-O18B	99(14)	C10B-Fe6-C7B-O7B	22(4)
Fe5-Fe8-C19B-Mo3	178.6(8)	C10B-Fe6-C19B-Mo3	127.4(14)
Fe5-Fe8-C19B-Fe6	89.2(7)	C10B-Fe6-C19B-Mo4	35.9(17)
Fe5-Fe8-C19B-Fe7	-90.8(6)	C10B-Fe6-C19B-Fe5	-54.4(17)
Fe6-Mo4-C6B-O6B	-155(8)	C10B-Fe6-C19B-Fe8	-138.6(14)
Fe6-Fe5-C9B-O9B	-130(3)	C11B-Fe6-C7B-Mo3	117.2(6)
Fe6-Fe8-C16B-O16B	176(7)	C11B-Fe6-C7B-O7B	-72(4)
Fe6-Fe8-C18B-O18B	130(14)	C11B-Fe6-C19B-Mo3	-101.2(8)
Fe6-Fe8-C19B-Mo3	89.4(6)	C11B-Fe6-C19B-Mo4	167.3(7)

C11B-Fe6-C19B-Fe5	77.0(9)	K1-O1-C1-C6	30.0(4)
C11B-Fe6-C19B-Fe8	-7.2(11)	K1-O1-C7-C8	-34.0(4)
C12B-Fe5-C9B-O9B	-56(3)	K1-O2-C8-C7	-62.6(4)
C13B-Fe5-C9B-O9B	36(3)	K1-O2-C9-C10	61.1(4)
C14B-Fe7-C8B-Mo4	-154.2(5)	K1-O3-C10-C9	34.1(4)
C14B-Fe7-C8B-O8B	21(3)	K1-O3-C11-C12	-40.6(4)
C15B-Fe7-C8B-Mo4	123.9(5)	K1-O4-C12-C11	-54.8(4)
C15B-Fe7-C8B-O8B	-61(3)	K1-O4-C13-C14	53.0(4)
C15B-Fe7-C14B-O14B	-76(4)	K1-O5-C14-C13	42.8(5)
C16B-Fe8-C18B-O18B	-67(14)	K1-O5-C15-C16	-38.8(5)
C16B-Fe8-C19B-Mo3	-89.9(9)	K1-O6-C6-C1	-33.3(5)
C16B-Fe8-C19B-Fe5	91.4(9)	K1-O6-C6-C5	148.1(4)
C16B-Fe8-C19B-Fe6	-179.4(8)	K1-O6-C16-C15	-55.9(4)
C16B-Fe8-C19B-Fe7	0.7(10)	O1-C1-C2-C3	-178.3(4)
C17B-Fe8-C16B-O16B	-53(8)	O1-C1-C6-O6	1.6(5)
C17B-Fe8-C18B-O18B	25(14)	O1-C1-C6-C5	-179.8(4)
C17B-Fe8-C19B-Mo3	159.5(10)	O1-C7-C8-O2	63.7(4)
C17B-Fe8-C19B-Fe5	-19.1(13)	O2-C9-C10-O3	-62.8(4)
C17B-Fe8-C19B-Fe6	70.1(12)	O3-C11-C12-O4	63.3(4)
C17B-Fe8-C19B-Fe7	-109.9(11)	O4-C13-C14-O5	-63.8(5)
C18B-Fe8-C16B-O16B	43(8)	O5-C15-C16-O6	63.3(5)
C18B-Fe8-C19B-Mo3	23.9(15)	C1-O1-C7-C8	177.7(3)
C18B-Fe8-C19B-Fe5	-154.7(13)	C1-C2-C3-C4	-0.7(7)
C18B-Fe8-C19B-Fe6	-65.6(15)	C2-C1-C6-O6	-175.8(4)
C18B-Fe8-C19B-Fe7	114.5(13)	C2-C1-C6-C5	2.8(6)
C19B-Mo4-C6B-O6B	-163(8)	C2-C3-C4-C5	0.8(7)
C19B-Fe5-C9B-O9B	-178(3)	C3-C4-C5-C6	0.9(7)
C19B-Fe6-C7B-Mo3	-6.7(8)	C4-C5-C6-O6	175.8(4)
C19B-Fe6-C7B-O7B	164(4)	C4-C5-C6-C1	-2.7(7)
C19B-Fe7-C8B-Mo4	-5.9(7)	C6-O6-C16-C15	90.8(5)
C19B-Fe7-C8B-O8B	169(2)	C6-C1-C2-C3	-1.2(6)
C19B-Fe7-C14B-O14B	76(4)	C7-O1-C1-C2	-5.7(5)
C19B-Fe8-C16B-O16B	177(8)	C7-O1-C1-C6	177.1(4)
C19B-Fe8-C18B-O18B	170(14)	C8-O2-C9-C10	-171.3(4)
K1-O16A-C16A-Fe4	-64(6)	C9-O2-C8-C7	170.1(4)
K1-O1-C1-C2	-152.8(3)	C10-O3-C11-C12	180.0(3)

C11-O3-C10-C9	174.0(3)	C20-C21-C22-O12	178.8(4)
C12-O4-C13-C14	-179.9(4)	C20-C21-C22-C17	0.4(6)
C13-O4-C12-C11	178.1(4)	C22-O12-C32-C31	-177.8(3)
C14-O5-C15-C16	174.3(4)	C22-C17-C18-C19	1.8(7)
C15-O5-C14-C13	-169.5(4)	C23-O7-C17-C18	-5.4(6)
C16-O6-C6-C1	-176.5(4)	C23-O7-C17-C22	177.0(4)
C16-O6-C6-C5	4.9(6)	C24-O8-C25-C26	168.7(4)
K2-O16B-C16B-Fe8	110(7)	C25-O8-C24-C23	-172.7(4)
K2-O7-C17-C18	-147.7(4)	C26-O9-C27-C28	-178.2(4)
K2-O7-C17-C22	34.6(4)	C27-O9-C26-C25	-179.9(4)
K2-O7-C23-C24	55.2(4)	C28-O10-C29-C30	-175.0(3)
K2-O8-C24-C23	37.7(5)	C29-O10-C28-C27	180.0(3)
K2-O8-C25-C26	-41.7(5)	C30-O11-C31-C32	-171.4(4)
K2-O9-C26-C25	-53.2(4)	C31-O11-C30-C29	172.6(4)
K2-O9-C27-C28	55.3(4)	C32-O12-C22-C17	-175.8(3)
K2-O10-C28-C27	39.3(4)	C32-O12-C22-C21	5.7(6)
K2-O10-C29-C30	-33.7(4)		
K2-O11-C30-C29	-61.4(4)		
K2-O11-C31-C32	63.0(4)		
K2-O12-C22-C17	-29.5(4)		
K2-O12-C22-C21	152.1(3)		
K2-O12-C32-C31	34.4(4)		
O7-C17-C18-C19	-175.8(4)		
O7-C17-C22-O12	-2.7(5)		
O7-C17-C22-C21	175.9(4)		
O7-C23-C24-O8	-61.9(5)		
O8-C25-C26-O9	62.9(5)		
O9-C27-C28-O10	-62.9(4)		
O10-C29-C30-O11	63.3(4)		
O11-C31-C32-O12	-64.6(4)		
C17-O7-C23-C24	-90.4(5)		
C17-C18-C19-C20	-0.1(7)		
C18-C17-C22-O12	179.5(4)		
C18-C17-C22-C21	-2.0(6)		
C18-C19-C20-C21	-1.5(7)		
C19-C20-C21-C22	1.3(7)		

References

1) Beamson, G.; Pickup, B. T.; Li, W.; Mai, S.-M. XPS Studies of Chain Conformation in PEG, PTrMO, and PTMG Linear Polyethers. *J. Phys. Chem. B* **2000**, *104* (12), 2656–2672. https://doi.org/10.1021/jp9905629.

2) CrysAlisPro V1.171.41.70a. Rigaku Oxford Diffraction, The Woodlands, TX, USA .

3) SHELXT. Sheldrick, G. M. (2015) *Acta. Cryst.* A71, 3-8.

4) Sheldrick, G. M. (2015). SHELXL-2013/3. Program for the Refinement of Crystal Structures. *Acta Cryst.,* C71, 3-8.

5) Spek, A. L. (2009). PLATON, A Multipurpose Crystallographic Tool. Utrecht University, The Netherlands. *Acta Cryst.* D65, 148-155.

6) OLEX2. Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. and Puschmann, H. A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.* 42, 339-341.

7) $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection. $R(F) = \Sigma (|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma (F_o))$. $S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n-p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

8) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, A. J. C. Wilson, editor, Boston: Kluwer Academic Press.

9) Sheldrick, G. M. (1994). SHELXTL/PC (Version 5.03). Siemens Analytical X-ray Instruments, Inc., Madison, Wisconsin, USA.

10) CrystalClear 1.40 (2008). Rigaku Americas Corporation, The Woodlands, TX.