Supporting Information for

Isolation, Characterization, and Reactivity of $Fe_8Me_{12}^-$: Kochi's *S* = 1/2 Species in Iron-Catalyzed Cross-Couplings with MeMgBr and Ferric Salts

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1. Experimental

1.1 General Considerations. All reagents were purchased from commercial sources. All air and moisture sensitive manipulations were carried out in an MBraun inert-atmosphere (N_2) dry box equipped with a direct liquid nitrogen inlet line, or using standard Schlenk techniques. All anhydrous solvents were freshly dried using activated alumina/4Å molecular sieves and stored under inert-atmosphere.

1.2 Preparation of $[MgCl(THF)_5][Fe_8Me_{12}]$ (1). A 20 mL scintillation vial was charged with $FeCl_3$ (65 mg, 0.4 mmol) and dissolved in THF (1 mL) with stirring. The solution was then cooled to -80 °C. To the green slurry was added a room temperature solution of MeMgBr in THF (1.0 M, 2 mL, 2.0 mmol) dropwise over the course of twenty minutes while stirring. The resulting brown mixture was stirred for an additional thirty minutes at -80 °C, after which the vial was placed on a room temperature stir plate for five minutes bringing the internal temperature of the solution to ca. 0 °C. The reaction mixture was then chilled once again to -80 °C for 30 minutes while stirring. Cold pentane (-80 °C, 2 mL) was added to the scintillation vial and the resulting solution filtered through Celite (precooled to -80 °C). The filtrate was then stored at -80 °C for one week rendering dark yellow brown crystalline shards of **1**.

*****Handling of temperature sensitive crystals of 1 for X-ray diffraction*.** Manipulations were carried out inside a nitrogen purged glovebag. Scintillation vials with crystalline material of **1** were stored in an aluminum Pie-Block containing dry ice. A specialized aluminum block with a hollow internal chamber, equipped with and inlet and outlet nozzle, was cooled by the passage of liquid nitrogen through the block. Microscope slides containing SilOil were precooled on the cold aluminum block, upon which an aliquot of cold solution from the scintillation vial was pipetted. Crystalline specimens for X-ray diffraction were examined microscopically. Appropriate single crystals were removed from the glass slide with a goniometer pin and transported to the diffractometer while being held over a hand dewar containing liquid nitrogen.

1.3 Reactions of Ferric Salts with Grignards. As an example of the general procedure employed to generate Kochi's $S = 1/2$ species in-situ, the reaction of $FeCl_3$ with 20 equiv of MeMgBr is described. A 0.25 mL aliquot of 10 mM $FeCl_3$ in THF was diluted with 1 mL of THF and 0.75 mL of 2-methyl-THF at room temperature. After drop-wise addition of 0.5 mL of MeMgBr (0.1 M in 2-methyl-THF) at room temperature, the reaction was stirred for 5 minutes before loading and freeze-trapping an EPR sample.

1.4 Preparation of solution MCD samples of 1. Scintillation vials containing **1** were transported quickly into a glove box in a liquid nitrogen precooled Pie-Block. The vials were then placed in a cold well at -80 °C and the mother liquor was decanted and discarded. The residual crystalline material was washed with cold pentane (-80 °C, 2mL) and decanted. The washing and decanting process was repeated five times. A small portion of the crystalline material of **1** was dissolved in a 20 mL scintillation vial containing a cold 1:1 mixture of 2-MeTHF and THF (-80 °C, 3 mL). The MCD cell was preassembled and cooled in the cold well. A precooled syringe was used to draw out the amber solution containing **1** and deliver an

appropriate aliquot to the cold MCD cell. The cell was promptly frozen and stored in liquid nitrogen.

1.5 Preparation of solution EPR samples of 1. The washing and decanting of the crystalline material was performed as described above. A portion of the crystalline material of **1** was dissolved in a 20 mL scintillation vial containing cold THF (-80 °C, 2 mL). An EPR tube was cooled to -80 °C and a cold syringe was used to deliver 0.25 mL of the cold amber solution to the tube. The EPR tube was then frozen and stored in liquid nitrogen.

1.6 Preparation of SilOil mull MCD sample of 1. The washing and decanting of the crystalline material was performed as described above. A mortar and pestle were placed on top of an aluminum block submerged in liquid nitrogen for cooling. A liquid nitrogen chilled metal spatula was used to collect crystalline material from the vial and the frozen crystalline solids were chipped off onto the mortar. A few drops of cold SilOil (-80 °C) were added to the mortar. The mortar was lifted from the aluminum block long enough to allow the SilOil to thaw and the solids were promptly ground with the cold pestle and refrozen. The process was repeated until a fine mull was obtained. A quartz disc was placed on the cold aluminum pie block surface and a cold spatula was used to transfer the frozen mull material onto the disc. The quartz disc was lifted from the aluminum block long enough to allow for the material to thaw and spread thinly over the disc. A second precooled quartz disc was quickly set on top of the first disc and the material refrozen. All components of the MCD cell were precooled in liquid nitrogen then assembled on top of the cold aluminum block.

1.7 Preparation of solid EPR sample of 1. The washing and decanting of the crystalline material, **1**, was performed as described above. A liquid nitrogen cooled spatula was used to transfer the crystalline material to an EPR tube submerged in liquid nitrogen. The spatula was cooled once again in liquid nitrogen and used to repeat the transfer process until a sufficient amount of the crystalline material was transferred to the EPR tube. The EPR tube was then stored in liquid nitrogen.

1.8 Reaction of 1 with electrophile. Crystalline **1** was dissolved in cold THF (-80 °C, 0.75 mL) and the resulting yellow brown solution was transferred to a scintillation vial equipped with a stir bar and THF (4.25 mL) at room temperature. Soon thereafter an aliquot was collected (0.5 mL) of which a portion was delivered to an EPR tube (0.25 mL). A premeasured solution of THF (0.5 mL) containing dodecane (3.4 mg, 0.02 mmol) and β-bromostyrene (7.3 mg, 0.04 mmol) was delivered to the scintillation vial, containing **1**, while simultaneously freeze quenching the aforementioned EPR tube in liquid nitrogen. Promptly, an aliquot of the resulting reaction mixture (0.5 mL) was collected and a portion (0.25 mL) delivered to an EPR tube with the remainder of the aliquot (0.25 mL) delivered to a GC vial containing a THF/HCl quenching solution (0.75 mL) while simultaneously freeze quenching the EPR sample. The reaction was monitored for five minutes by collection of aliquots for GC analysis and EPR. The initial concentration of **1** in solution was determined by EPR spin integration of the aliquot collected. The yield of the cross-coupling product, β-methylstyrene, was found to be on the order of 6 % (ca. 0.1 min^{-1}). Analogous results were obtained across multiple reaction runs.

1.9 Reaction of 1 with electrophile and MeMgBr. Crystalline **1** was dissolved in cold THF (-80 °C, 0.75 mL) and the resulting yellow brown solution was transferred to a scintillation vial equipped with a stir bar and THF (4.25 mL) at room temperature. Soon thereafter an aliquot was collected (0.5 mL) of which a portion was delivered to an EPR tube (0.4 mL). A premeasured solution of THF (0.5 mL) containing dodecane (3.4 mg, 0.02 mmol) and β-bromostyrene (7.3 mg, 0.04 mmol) was delivered to the scintillation vial, containing **1**, while simultaneously freeze quenching the EPR tube in liquid nitrogen. An aliquot of the resulting reaction mixture (0.65 mL) was collected and a portion (0.4 mL) delivered to an EPR tube with the remainder of the aliquot (0.25 mL) delivered to a GC vial containing a THF/HCl quenching solution (0.75 mL) while simultaneously freeze quenching the subsequent EPR sample. To the mixture of **1** and β-bromostyrene was quickly added a premeasured aliquot of dilute MeMgBr (0.65mL, 0.05 mmol) in THF. The reaction was further monitored by collection of GC and EPR samples over the course of five minutes. The initial concentration of **1** in solution was determined by EPR spin integration of the aliquot collected. The conversion of β-bromostyrene to β-methylstyrene was complete within the first 40 seconds of reaction after addition of MeMgBr, yield 99% (ca. 1 min^{-1}). Analogous results were obtained across multiple reaction runs.

1.10 Thermal stability assessment of 1 in solution. Crystalline material, **1**, was dissolved in cold THF (-80 °C, 0.75 mL). The yellow brown solution was transferred to a scintillation vial containing a stir bar and THF (4.25 mL) at room temperature. Over the course of 5 minutes solution aliquots for EPR were taken at regular time intervals and freeze quenched in liquid nitrogen. The decay of **1** was found to be ca. 25 ± 10 % over five minutes by EPR spin integration.

1.11 Electron Paramagnetic Resonance (EPR) Spectroscopy. All samples for EPR spectroscopy were prepared in an inert atmosphere glove box equipped with a liquid nitrogen fill port to enable sample freezing to 77 K within the glove box. EPR samples were prepared in 4 mm OD suprasil quartz EPR tubes from Wilmad Labglass. Samples for spin integration utilized high precision suprasil quartz tubes to allow for direct comparison of intensities between different samples. X-band EPR spectra were recorded on a Bruker EMXplus spectrometer equipped with a 4119HS cavity and an Oxford ESR-900 helium flow cryostat. The instrumental parameters employed for all samples were as follows: 1 mW power; time constant 41 ms; modulation amplitude 8 G; 9.38 GHz; modulation frequency 100 kHz. Samples exhibiting S = 1/2 EPR spectra were spin integrated using a 3 mM $CuSO_4$ standard under non-saturating conditions. Identical instrumentation parameters were used for both the iron and standard samples.

1.12 Magnetic Circular Dichroism (MCD) Spectroscopy. All samples for MCD spectroscopy were prepared in an inert atmosphere glove box equipped with a liquid nitrogen fill port to enable sample freezing to 77 K within the glove box. MCD samples were prepared in 1:1 (v:v) THF:2-MeTHF (to form low temperature optical glasses) in copper cells fitted with quartz disks and a 3 mm gasket. Low temperature near-infrared (NIR) MCD experiments were conducted using a Jasco J-730 spectropolarimeter and a liquid nitrogen cooled InSb detector. The instrument utilizes a modified sample compartment incorporating focusing optics and an Oxford Instruments SM4000-7T superconducting magnet/cryostat. This set-up permits measurements

from 1.6 K to 290 K with magnetic fields up to 7 T. A calibrated Cernox sensor directly inserted in the copper sample holder is used to measure the temperature at the sample to 0.001 K. All MCD spectra were baseline-corrected against zero-field scans.

1.13 Mössbauer Spectroscopy. Solution samples for ^{57}Fe Mössbauer spectroscopy were prepared from $^{57}Fe(acac)_3$ to enable data collection from dilute, freeze-trapped solution samples. All samples were prepared in an inert atmosphere glove box equipped with a liquid nitrogen fill port to enable sample freezing to 77 K within the glove box. Each sample was loaded into a Delrin Mössbauer sample cup for measurements and loaded under liquid nitrogen. Low temperature ^{57}Fe Mössbauer measurements were performed using a See Co. MS4 Mössbauer spectrometer integrated with a Janis SVT-400T He/N_2 cryostat for measurements at 80 K with a 0.07 T applied magnetic field. Isomer shifts were determined relative to α-Fe at 298 K. All Mössbauer spectra were fit using the program WMoss (SeeCo). Errors of the fit analyses were the following: $\delta \pm 0.02$ mm/s and $\Delta E_Q \pm 3\%$.

1.14 NMR Spectroscopy. A scintillation vial containing crystalline **1** was decanted and washed with cold pentane five times (-80 °C, 7 mL). The residual pentane was removed under reduced pressure by momentarily allowing the sample to warm outside of the cold well (less than 30 seconds) followed by quickly cooling the vial in liquid nitrogen and returning to the cold well. The drying process was repeated five times. The integrity of the material as genuine **1**, after the warm vacuum process, was verified by preparation of an EPR sample from the same dry solid material. A THF-d_8 solution from dry crystalline **1** was prepared at -80 °C in a J-Young NMR tube and frozen in liquid nitrogen. The cold NMR tube was loaded into a precooled sample compartment (-80 °C) of a 500 MHz Bruker spectrometer for spectrum collection.

2. Supplementary Data

2.1 EPR Spectra

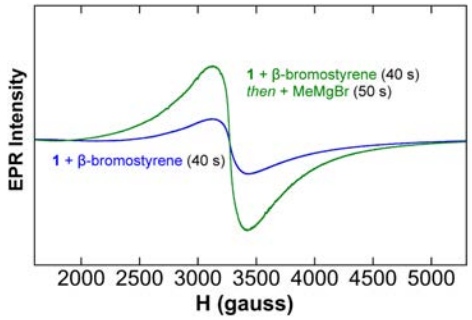


Figure S1. 5 K EPR spectrum of increase in **1** upon reaction of the initial **1** + β-bromostryrene solution with MeMgBr (1.25 equiv with respect to β-bromostyrene). The addition of MeMgBr results in near-quantitative re-generation of the initial $S = 1/2$ signal that was present prior to β-bromostryrene addition.

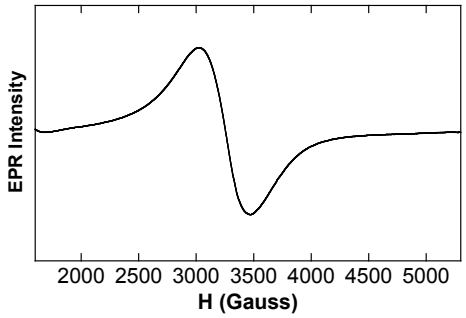


Figure S2. 5 K EPR spectrum of solid **1**.

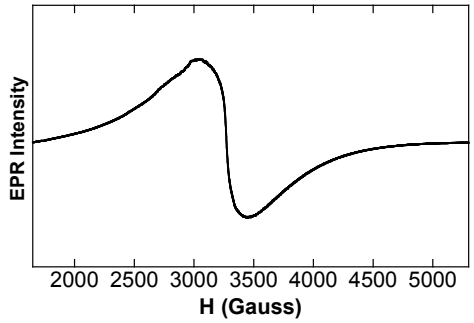


Figure S3. 5 K EPR spectrum of the in-situ formed $S = 1/2$ species from reaction of $FeCl_3$ with 20 equiv CD_3MgBr in THF.

2.2 MCD Spectra

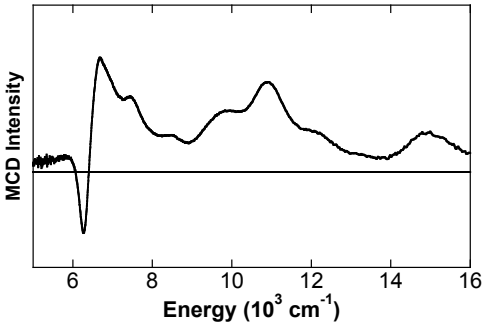


Figure S4. 5 K, 7 T NIR MCD Spectrum of Solid Mull of **1**. The solid state spectrum contains the same transitions as observed in solution, but with reduced intensities for the higher energy transitions relative to the lower energy transitions. Such differences in MCD can arise due to changes in bond distances, angles and/or close contact interactions between solution and solid state.

2.3 Mössbauer Spectra

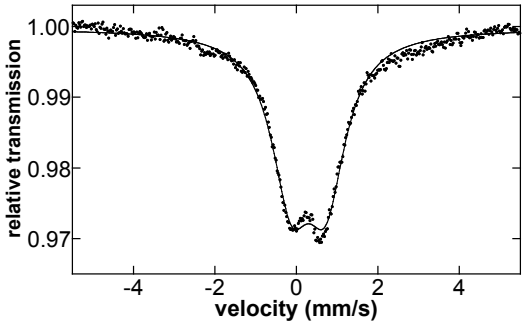


Figure S5. 80 K Mössbauer Spectrum of the In-Situ Formed $S = 1/2$ Iron Species from Reaction of $^{57}Fe(acac)_3$ with 20 equiv MeMgBr in 1:1 THF:2-MeTHF. The best fit to the broad doublet yielded Mössbauer parameters of $\delta = 0.30$ mm/s and $\Delta E_Q = 0.85$ mm/s.

2.4 ^{1}H NMR spectrum of 1 in THF-d_8

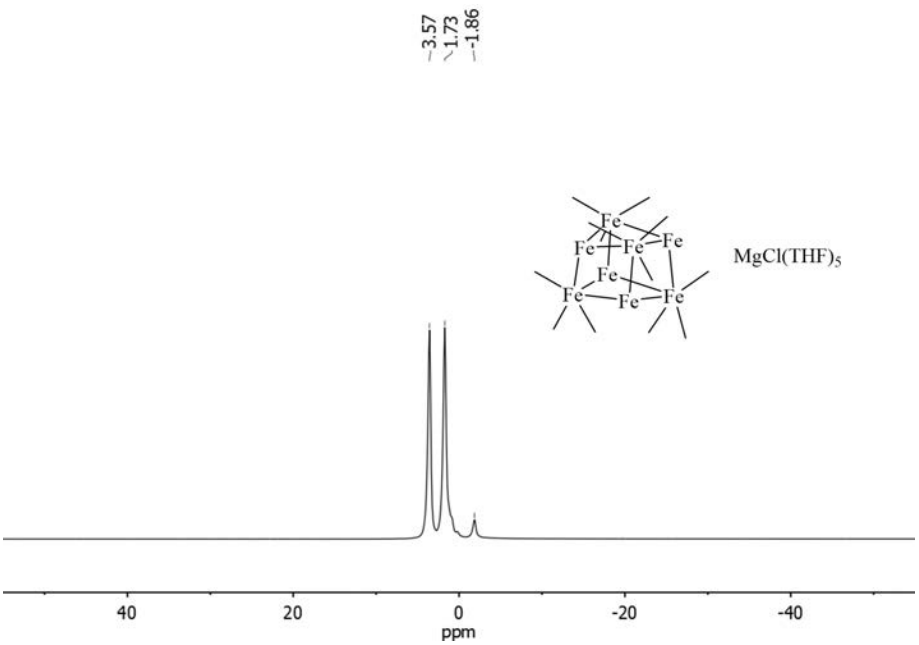
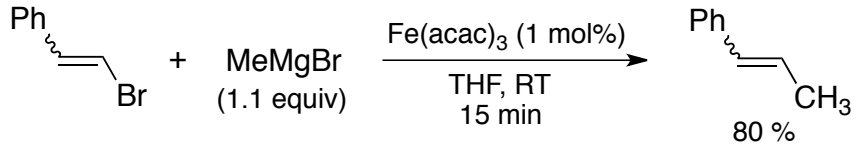


Figure S6. ^{1}H NMR spectrum of **1** in THF-d_8 at -80 ^{o}C. The ^{1}H NMR spectrum of **1** is unremarkable featuring a single broad resonance at -1.86 ppm tentatively assigned as a Fe-CH_3 resonance. No additional resonances were observed between 220 to -220 ppm.

2.5 Catalytic Reaction with β-Bromostyrene

Cross-coupling reactions were run with 3 mM $Fe(acac)_3$ (1 mol % Fe), 0.3 M β-bromostyrene, and 0.33 M methylmagnesium bromide based off of the previously reported catalytic protocol by Cahiez et al.[1] As an example of a general procedure employed, β-bromostyrene (50 μL, 6 M in THF), dodecane (50 μL, 3 M in THF - used as an internal standard), 320 μL of THF, and $Fe(acac)_3$ (0.25 mL, 12 mM in THF) were added together at room temperature. Methylmagnesium bromide (330 μL, 1 M in THF) was added dropwise and then stirred for 15 min. Upon completion, an aliquot of the reaction mixture was added to dilute HCl (10^{-5} M in diethyl ether), diluted with diethyl ether, and filtered through a pad of silica gel. Product yields were determined by quantitative GC analysis with dodecane as an internal standard



3. X-ray Crystal Structure Details of $[MgCl(THF)_5][Fe_8Me_{12}]$ (1)

CRYSTAL STRUCTURE REPORT

$C_{52}\ H_{116}\ Br_{0.25}\ Cl_{1.75}\ Fe_8\ Mg_{1.5}\ O_{10}$

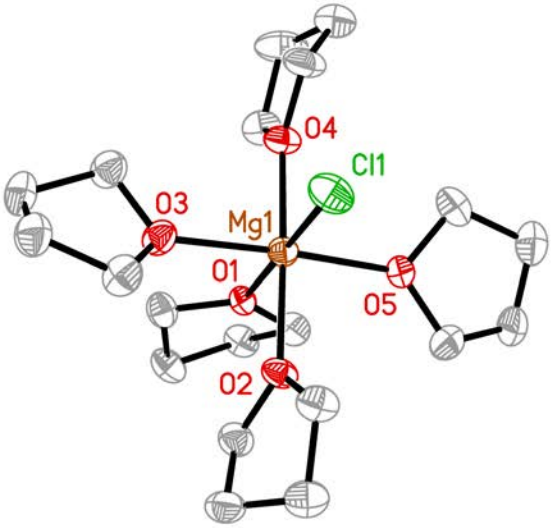
or

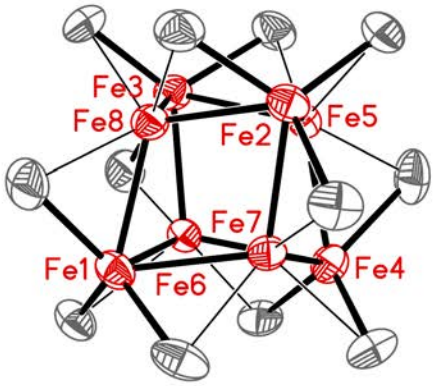
$[MgCl_{0.918}Br_{0.082}(THF)_5][Fe_8(CH_3)_{12}] \cdot \frac{1}{2}MgCl_{1.666}Br_{0.334}(THF)_4 \cdot 3THF$

Report prepared for:

Dr. S. Muñoz, Prof. M. Neidig

September 29, 2015





William W. Brennessel

X-ray Crystallographic Facility

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Data collection

A crystal (0.26 x 0.24 x 0.12 mm^3) was placed onto the tip of a thin glass optical fiber and mounted on a Bruker SMART APEX II CCD platform diffractometer for a data collection at 100.0(5) K.[2] A preliminary set of cell constants and an orientation matrix were calculated from reflections harvested from three orthogonal wedges of reciprocal space. The full data collection was carried out using MoKα radiation (graphite monochromator) with a frame time of 60 seconds and a detector distance of 4.02 cm. A randomly oriented region of reciprocal space was surveyed: four major sections of frames were collected with 0.50º steps in ω at four different ϕ settings and a detector position of -38º in 2θ. The intensity data were corrected for absorption.[3] Final cell constants were calculated from the xyz centroids of 4072 strong reflections from the actual data collection after integration.[4] See Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using SHELXT-2014/5[5] and refined using SHELXL-2014/7.[6] The space group $P2_12_12$ was determined based on systematic absences. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. Because the hydrogen atoms on the methyl ligands were unable to be located unambiguously in the difference Fourier map, they were not modeled; they were included in the molecular formula, but not in the atom list. All other hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

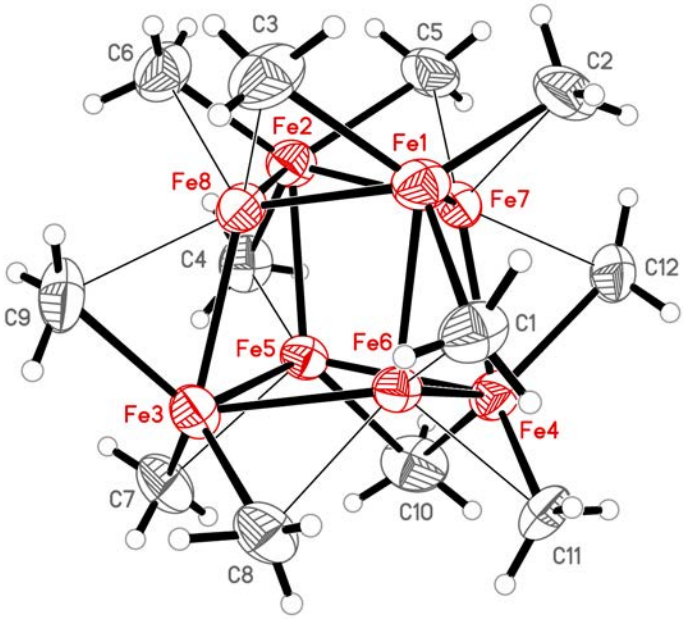
The crystal was an inversion twin (0.51:0.49). Although the current space group was uniquely defined by systematic absence statistics, a refinement in centrosymmetric space group *Pbam* was examined and found to produce a significantly worse result.

The final full matrix least squares refinement converged to $R1 = 0.0551$ (F^2, $I > 2\sigma(I)$) and $wR2 = 0.1560$ (F^2, all data).

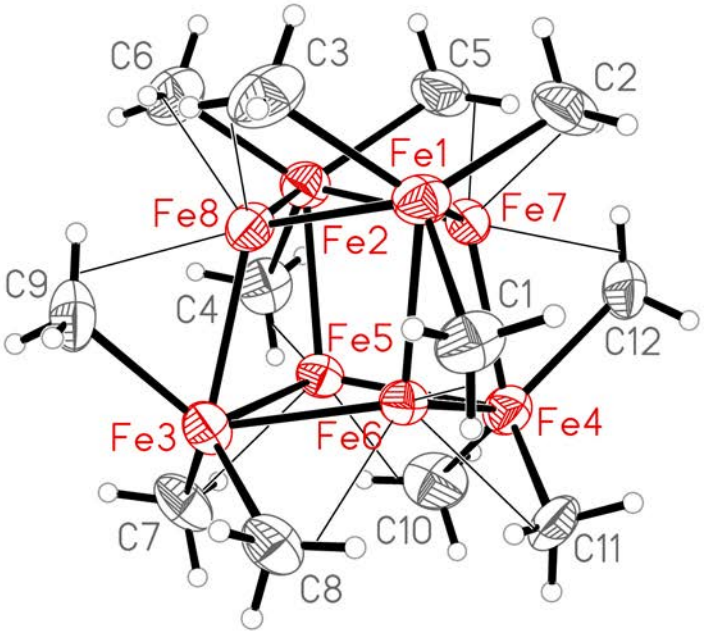
Structure description

The structure is the one suggested. The asymmetric unit contains one $MgX(THF)_5$ cation in a general position, one $Fe_8(CH_3)_{12}$ monoanionic cluster in a general position, one half of a cocrystallized $MgX_2(THF)_4$ molecule on a crystallographic two-fold axis that includes the Mg atom, and three uncoordinated cocrystallized THF solvent molecules in general positions. All species are well separated. The halido sites on both Mg species are modeled as site disorders of Cl and Br (0.918:0.082 for Cl1:Br1 and 0.833:0.167 for Cl2:Br2) and THF solvent molecules O9/C45-C48 and O10/C49-C52 are modeled as disordered over two positions each (0.60:0.40 and 0.67:0.33, respectively).

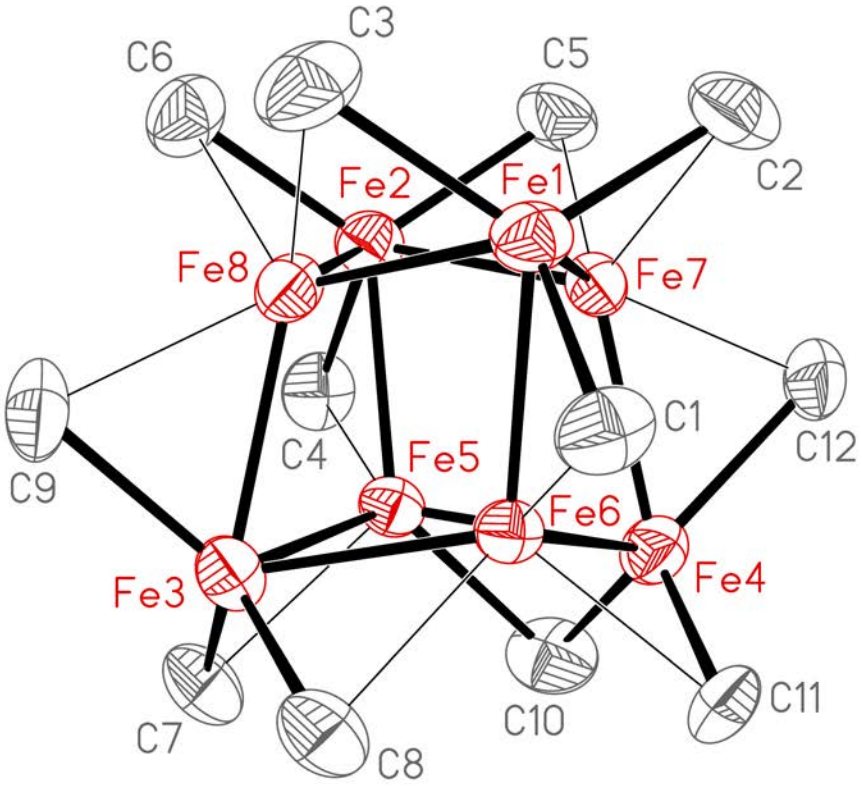
Because the methyl group hydrogen atoms on the ferrate cluster could not be located unambiguously in the difference Fourier map, two possible approaches to placing them were examined initially. The goal in the first model was to angle and rotate each hydrogen trio to minimize H…H close contacts among the twelve methyl groups.



The goal of the second model was to angle and rotate each hydrogen trio such that one C—H bond was within its Fe-C-Fe plane to geometrically favor an agostic interaction. This scenario was consistent with reported structural precedents in which an asymmetric bridging methyl group participates in one Fe—C σ bond and one C—H…Fe η^2 agostic interaction.[7]



Without independent support (e.g., spectroscopy) for either model, however, it was decided that the hydrogen atoms should be left out of the structure, but still included in the molecular formula to allow for the correct calculation of the various items in Table 1 (e.g., molecular weight, density, etc.).



Unless noted otherwise all structural diagrams containing thermal displacement ellipsoids are drawn at the 50 % probability level.

Data collection, structure solution, and structure refinement were conducted at the X-ray Crystallographic Facility, B04 Hutchison Hall, Department of Chemistry, University of Rochester. All publications arising from this report MUST either 1) include William W. Brennessel as a coauthor or 2) acknowledge William W. Brennessel and the X-ray Crystallographic Facility of the Department of Chemistry at the University of Rochester.

Some equations of interest:

$$R_{int} = \Sigma\, |F_o^2 - < F_o^2 >| \,/\, \Sigma |F_o^2|$$

$$R1 = \Sigma ||F_o| - |F_c|| \,/\, \Sigma |F_o|$$

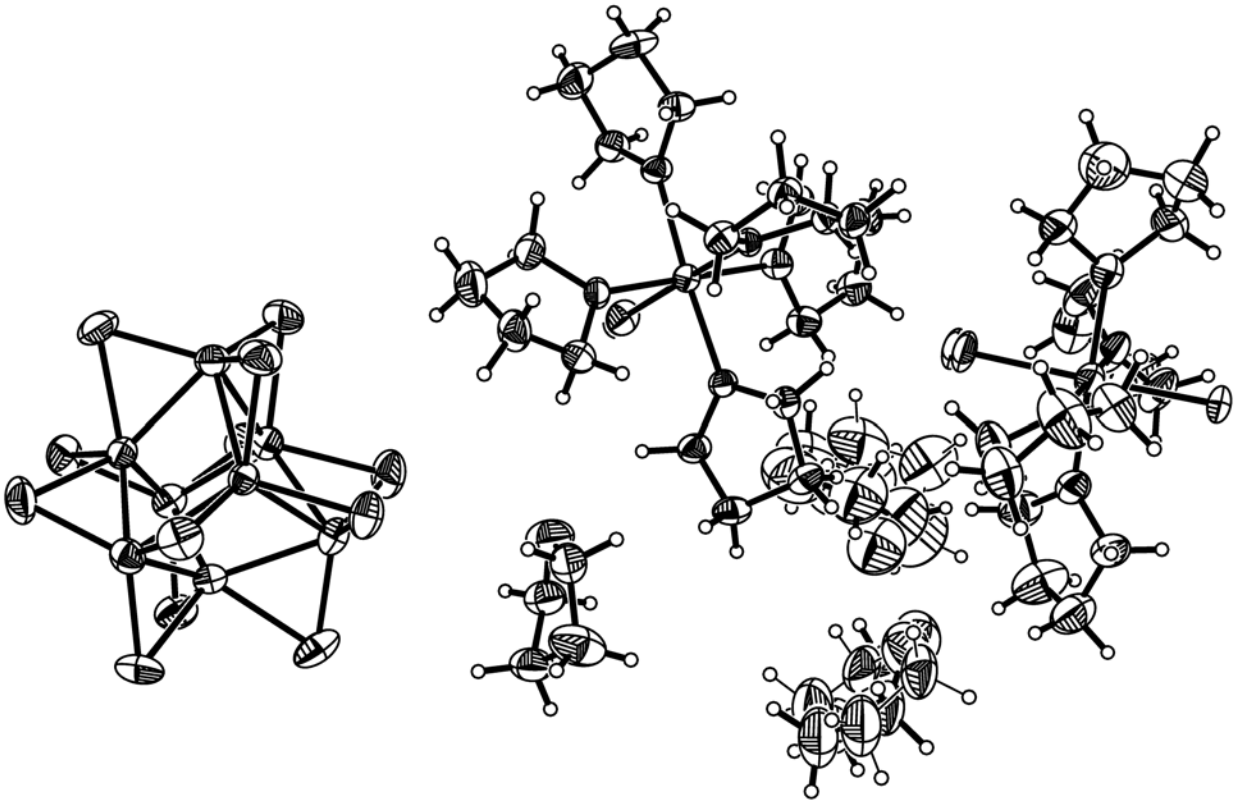
$$wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] \,/\, \Sigma\, [w(F_o^2)^2]]^{1/2}$$

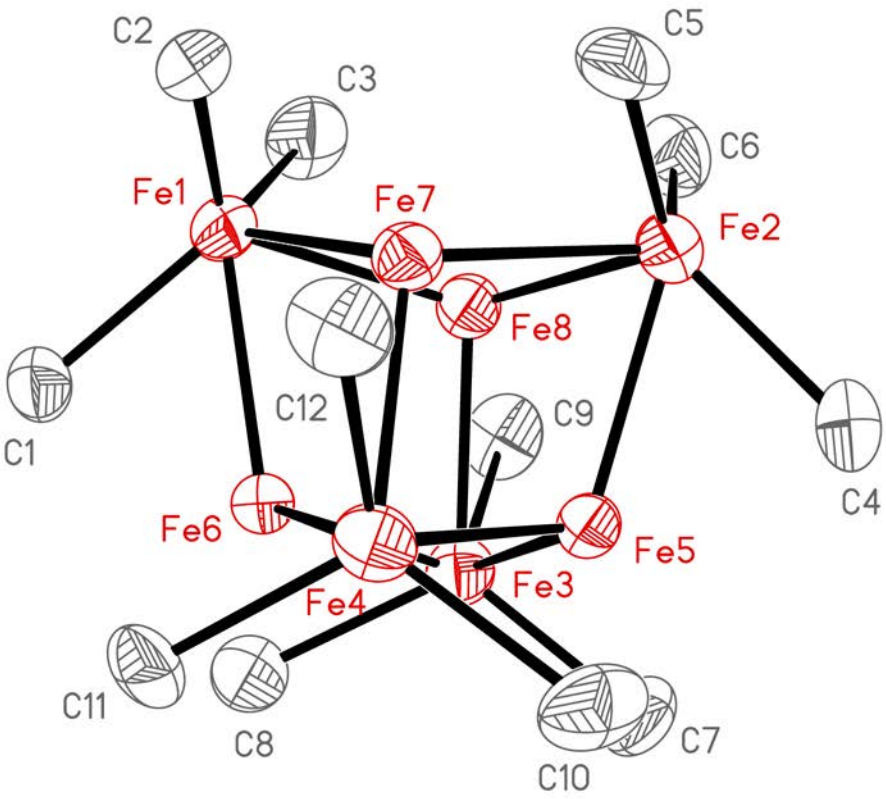
where $w = 1 \,/\, [\sigma^2 (F_o^2) + (aP)^2 + bP]$ and

$$P = 1/3 \text{ max } (0, F_o^2) + 2/3\, F_c^2$$

$$\text{GOF} = S = [\Sigma [w(F_o^2 - F_c^2)^2] \,/\, (m-n)]^{1/2}$$

where m = number of reflections and n = number of parameters




C2
C3
C5
C6
Fe1
Fe7
Fe2
Fe8
C1
C12
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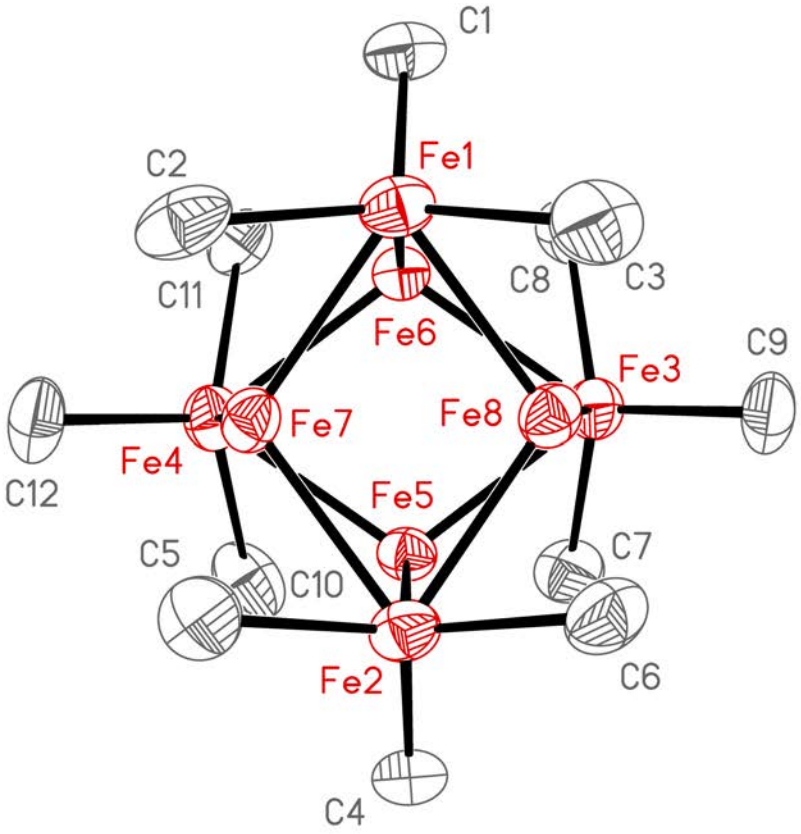
Fe3
C11
C8
C10
C7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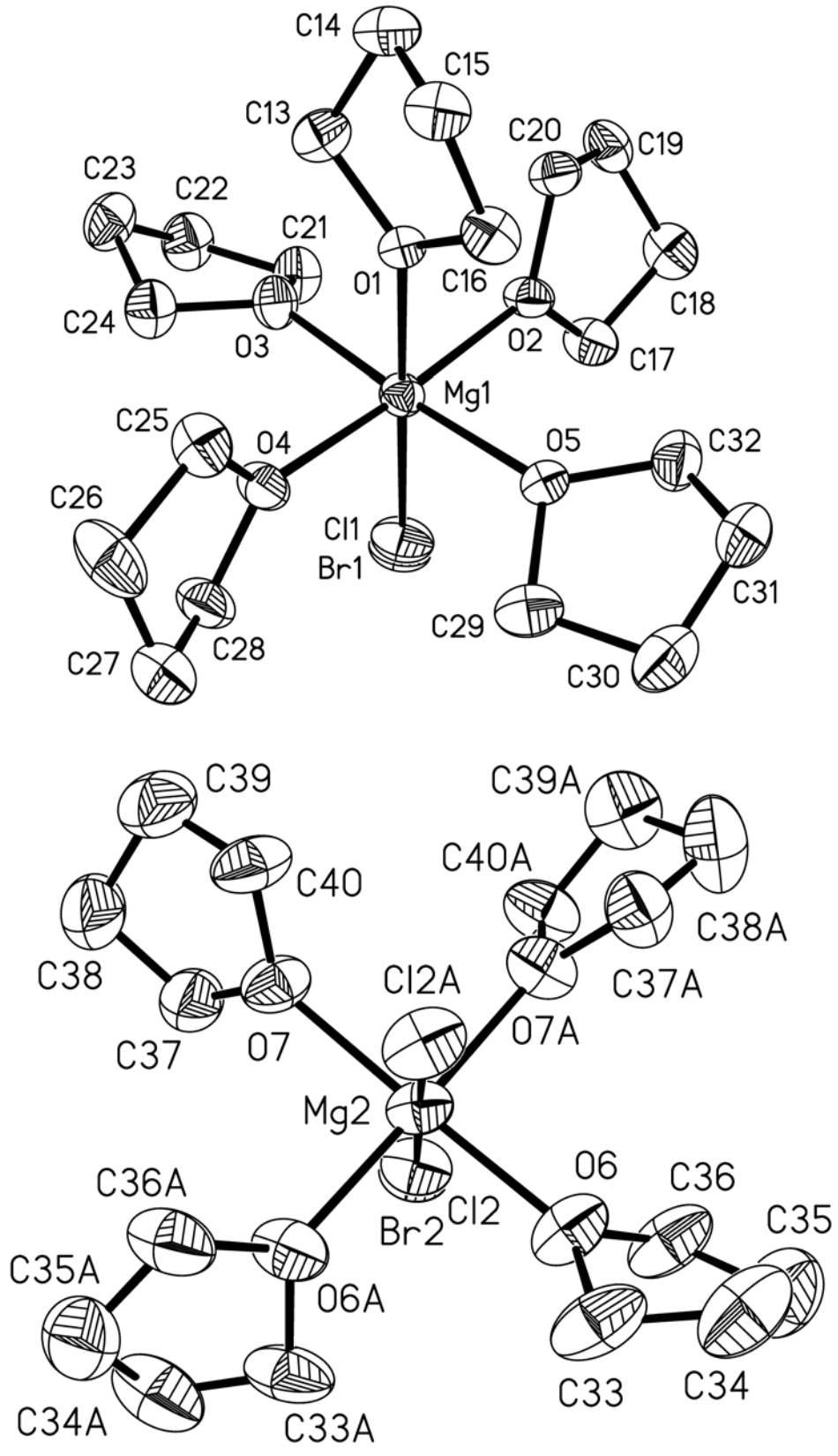
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O4
O5
C32
C26
Cl1
Br1
C31
C29
C28
C27
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C39
C39A
C40A
C40
C38A
C38
Cl2A
C37A
C37
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O7A
Mg2
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O6
C36
C35
Br2
Cl2
C35A
O6A
C33
C34
C34A
C33A

Table S1. Crystal data and structure refinement for neism18h.

Identification code	neism18h	
Empirical formula	C52 H116 Br0.25 Cl1.75 Fe8 Mg1.50 O10	
Formula weight	1466.72	
Temperature	100.0(5) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12$	
Unit cell dimensions	a = 38.445(4) Å	α = 90°
	b = 13.0221(14) Å	β = 90°
	c = 13.6580(15) Å	γ = 90°
Volume	6837.6(13) Å^3	
Z	4	
Density (calculated)	1.425 Mg/m^3	
Absorption coefficient	1.922 mm^{-1}	
F(000)	3090	
Crystal color, morphology	yellow-black, block	
Crystal size	0.26 x 0.24 x 0.12 mm^3	
Theta range for data collection	1.651 to 27.492°	
Index ranges	$-49 \le h \le 49$, $-16 \le k \le 16$, $-17 \le l \le 17$	
Reflections collected	92013	
Independent reflections	15680 [R(int) = 0.0665]	
Observed reflections	12489	
Completeness to theta = 27.485°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7456 and 0.6836	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15680 / 126 / 704	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	$R1$ = 0.0551, $wR2$ = 0.1451	
R indices (all data)	$R1$ = 0.0715, $wR2$ = 0.1560	
Absolute structure parameter	0.49(3)	
Largest diff. peak and hole	1.111 and -0.453 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for neism18h. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Fe1	8160(1)	6562(1)	4943(1)	40(1)
Fe2	9053(1)	7964(1)	4771(1)	40(1)
Fe3	8943(1)	5245(1)	3635(1)	40(1)
Fe4	8957(1)	5587(1)	6471(1)	41(1)
Fe5	9227(1)	6167(1)	4958(1)	33(1)
Fe6	8578(1)	5162(1)	5084(1)	31(1)
Fe7	8658(1)	7115(1)	5910(1)	35(1)
Fe8	8652(1)	6886(1)	3873(1)	36(1)
C1	7980(2)	5010(6)	5051(7)	49(2)
C2	8072(2)	7467(7)	6225(8)	57(2)
C3	8065(2)	7291(8)	3561(8)	64(3)
C4	9595(2)	7572(7)	4786(7)	51(2)
C5	8854(2)	8814(6)	6002(7)	53(2)
C6	8857(3)	8509(7)	3400(7)	55(2)
C7	9493(2)	5077(8)	3802(7)	54(2)
C8	8649(2)	3865(7)	3922(7)	51(2)
C9	8776(2)	6075(8)	2362(6)	57(2)
C10	9506(2)	5426(8)	6293(8)	63(3)
C11	8670(2)	4173(6)	6465(6)	49(2)
C12	8767(3)	6697(7)	7535(6)	55(2)
Mg1	6994(1)	5502(2)	63(2)	26(1)
Cl1	7260(3)	7149(5)	194(10)	42(1)
Br1	7273(15)	7310(20)	190(50)	42(1)
O1	6747(1)	4046(3)	-44(3)	25(1)
C13	6440(2)	3800(5)	-638(5)	34(2)
C14	6309(2)	2786(5)	-204(6)	38(2)
C15	6645(2)	2252(5)	31(6)	35(1)
C16	6860(2)	3131(5)	488(5)	34(2)
O2	6655(1)	5786(3)	1263(3)	30(1)
C17	6689(2)	6643(6)	1949(6)	38(2)
C18	6413(2)	6444(6)	2725(6)	41(2)

C19	6128(2)	5909(6)	2141(6)	39(2)
C20	6337(2)	5212(6)	1485(5)	34(1)
O3	6611(1)	6064(4)	-880(4)	34(1)
C21	6391(2)	6947(6)	-590(5)	39(2)
C22	6209(2)	7303(6)	-1532(6)	46(2)
C23	6271(2)	6434(6)	-2246(6)	43(2)
C24	6624(2)	6044(6)	-1937(6)	40(2)
O4	7310(1)	5051(4)	-1152(3)	32(1)
C25	7301(2)	4084(5)	-1667(6)	38(2)
C26	7606(2)	4068(7)	-2372(7)	54(2)
C27	7842(2)	4919(8)	-1993(6)	53(2)
C28	7577(2)	5693(6)	-1613(6)	43(2)
O5	7356(1)	4828(4)	1039(3)	30(1)
C29	7727(2)	4775(7)	801(6)	43(2)
C30	7911(2)	4389(10)	1724(7)	66(3)
C31	7621(2)	3972(7)	2340(6)	48(2)
C32	7322(2)	4682(7)	2079(5)	44(2)
Mg2	5000	5000	-235(3)	41(1)
Cl2	5601(3)	5502(18)	-259(17)	48(1)
Br2	5651(6)	5570(40)	-280(40)	48(1)
O6	5105(1)	3895(5)	-1306(4)	56(2)
C33	4895(2)	3630(10)	-2165(7)	70(3)
C34	4925(3)	2498(10)	-2204(10)	85(4)
C35	5306(3)	2291(10)	-1903(10)	87(4)
C36	5404(2)	3201(9)	-1321(7)	68(3)
O7	4891(1)	6082(5)	872(4)	50(1)
C37	5075(3)	7025(7)	1040(7)	61(2)
C38	4856(4)	7653(9)	1717(10)	85(4)
C39	4689(3)	6840(9)	2342(8)	72(3)
C40	4635(2)	5996(8)	1625(7)	59(2)
O8	7180(2)	6060(6)	4111(5)	66(2)
C41	7037(2)	5268(8)	4659(7)	57(2)
C42	6872(3)	5665(9)	5549(8)	79(3)
C43	7062(3)	6702(7)	5671(7)	56(2)
C44	7121(3)	6969(7)	4624(6)	52(2)
O9	5420(11)	6120(20)	3918(18)	100(5)

C45	5431(4)	5787(15)	4906(16)	71(5)
C46	5678(6)	6460(20)	5375(17)	103(6)
C47	5604(5)	7458(17)	4806(16)	90(5)
C48	5475(7)	7160(19)	3869(19)	89(6)
O9'	5384(18)	6280(30)	3650(20)	100(5)
C45'	5343(7)	5530(20)	4370(20)	71(5)
C46'	5517(10)	5820(30)	5240(20)	103(6)
C47'	5746(9)	6730(30)	4900(20)	90(5)
C48'	5574(11)	7070(30)	4040(30)	89(6)
O10	6187(5)	8920(16)	882(16)	156(7)
C49	6159(6)	9674(14)	183(17)	113(6)
C50	5801(5)	10177(16)	81(18)	114(6)
C51	5597(6)	9514(18)	750(20)	131(7)
C52	5840(6)	8642(16)	960(20)	126(6)
O10'	5662(9)	9130(30)	1420(20)	126(6)
C49'	5471(13)	9770(40)	780(30)	131(7)
C50'	5534(11)	9600(40)	-320(30)	114(6)
C51'	5921(11)	9510(30)	-230(30)	113(6)
C52'	5957(11)	9120(60)	810(30)	156(7)

Table S3. Bond lengths [Å] and angles [°] for neism18h.

Fe(1)-C(2)	2.139(10)	Fe(6)-Fe(8)	2.8026(14)
Fe(1)-C(1)	2.142(8)	Fe(7)-C(12)	2.323(8)
Fe(1)-C(3)	2.144(10)	Fe(7)-C(2)	2.337(9)
Fe(1)-Fe(8)	2.4257(15)	Fe(7)-C(5)	2.342(8)
Fe(1)-Fe(7)	2.4326(15)	Fe(7)-Fe(8)	2.7990(15)
Fe(1)-Fe(6)	2.4376(13)	Fe(8)-C(6)	2.347(9)
Fe(2)-C(6)	2.139(9)	Fe(8)-C(3)	2.355(9)
Fe(2)-C(4)	2.145(8)	Fe(8)-C(9)	2.366(9)
Fe(2)-C(5)	2.153(9)	Mg(1)-O(3)	2.090(5)
Fe(2)-Fe(8)	2.4188(15)	Mg(1)-O(5)	2.116(5)
Fe(2)-Fe(7)	2.4401(15)	Mg(1)-O(1)	2.125(4)
Fe(2)-Fe(5)	2.4469(14)	Mg(1)-O(2)	2.127(5)
Fe(3)-C(7)	2.135(9)	Mg(1)-O(4)	2.138(5)
Fe(3)-C(9)	2.145(9)	Mg(1)-Cl(1)	2.382(5)
Fe(3)-C(8)	2.160(9)	Mg(1)-Br(1)	2.59(2)
Fe(3)-Fe(5)	2.4274(15)	O(1)-C(16)	1.461(8)
Fe(3)-Fe(6)	2.4285(14)	O(1)-C(13)	1.467(8)
Fe(3)-Fe(8)	2.4343(15)	C(13)-C(14)	1.533(10)
Fe(4)-C(10)	2.137(10)	C(13)-H(13A)	0.9900
Fe(4)-C(11)	2.146(8)	C(13)-H(13B)	0.9900
Fe(4)-C(12)	2.175(8)	C(14)-C(15)	1.502(9)
Fe(4)-Fe(7)	2.4219(15)	C(14)-H(14A)	0.9900
Fe(4)-Fe(5)	2.4335(16)	C(14)-H(14B)	0.9900
Fe(4)-Fe(6)	2.4514(15)	C(15)-C(16)	1.541(10)
Fe(5)-C(4)	2.325(8)	C(15)-H(15A)	0.9900
Fe(5)-C(10)	2.326(9)	C(15)-H(15B)	0.9900
Fe(5)-C(7)	2.356(8)	C(16)-H(16A)	0.9900
Fe(5)-Fe(6)	2.8203(13)	C(16)-H(16B)	0.9900
Fe(5)-Fe(8)	2.8204(15)	O(2)-C(17)	1.463(8)
Fe(5)-Fe(7)	2.8295(14)	O(2)-C(20)	1.467(8)
Fe(6)-C(11)	2.311(8)	C(17)-C(18)	1.523(10)
Fe(6)-C(1)	2.312(7)	C(17)-H(17A)	0.9900
Fe(6)-C(8)	2.332(8)	C(17)-H(17B)	0.9900
Fe(6)-Fe(7)	2.7988(14)	C(18)-C(19)	1.525(11)

C(18)-H(18A)	0.9900	C(29)-H(29A)	0.9900
C(18)-H(18B)	0.9900	C(29)-H(29B)	0.9900
C(19)-C(20)	1.506(10)	C(30)-C(31)	1.498(13)
C(19)-H(19A)	0.9900	C(30)-H(30A)	0.9900
C(19)-H(19B)	0.9900	C(30)-H(30B)	0.9900
C(20)-H(20A)	0.9900	C(31)-C(32)	1.519(11)
C(20)-H(20B)	0.9900	C(31)-H(31A)	0.9900
O(3)-C(24)	1.445(9)	C(31)-H(31B)	0.9900
O(3)-C(21)	1.481(8)	C(32)-H(32A)	0.9900
C(21)-C(22)	1.536(11)	C(32)-H(32B)	0.9900
C(21)-H(21A)	0.9900	Mg(2)-O(6)	2.092(6)
C(21)-H(21B)	0.9900	Mg(2)-O(6)#1	2.092(6)
C(22)-C(23)	1.512(12)	Mg(2)-O(7)#1	2.109(6)
C(22)-H(22A)	0.9900	Mg(2)-O(7)	2.109(6)
C(22)-H(22B)	0.9900	Mg(2)-Cl(2)	2.402(8)
C(23)-C(24)	1.512(10)	Mg(2)-Cl(2)#1	2.402(8)
C(23)-H(23A)	0.9900	Mg(2)-Br(2)	2.611(19)
C(23)-H(23B)	0.9900	Mg(2)-Br(2)#1	2.611(19)
C(24)-H(24A)	0.9900	O(6)-C(36)	1.462(11)
C(24)-H(24B)	0.9900	O(6)-C(33)	1.465(10)
O(4)-C(25)	1.442(8)	C(33)-C(34)	1.479(17)
O(4)-C(28)	1.467(8)	C(33)-H(33A)	0.9900
C(25)-C(26)	1.517(11)	C(33)-H(33B)	0.9900
C(25)-H(25A)	0.9900	C(34)-C(35)	1.544(16)
C(25)-H(25B)	0.9900	C(34)-H(34A)	0.9900
C(26)-C(27)	1.523(13)	C(34)-H(34B)	0.9900
C(26)-H(26A)	0.9900	C(35)-C(36)	1.477(16)
C(26)-H(26B)	0.9900	C(35)-H(35A)	0.9900
C(27)-C(28)	1.524(12)	C(35)-H(35B)	0.9900
C(27)-H(27A)	0.9900	C(36)-H(36A)	0.9900
C(27)-H(27B)	0.9900	C(36)-H(36B)	0.9900
C(28)-H(28A)	0.9900	O(7)-C(40)	1.427(10)
C(28)-H(28B)	0.9900	O(7)-C(37)	1.438(11)
O(5)-C(32)	1.440(8)	C(37)-C(38)	1.494(14)
O(5)-C(29)	1.467(8)	C(37)-H(37A)	0.9900
C(29)-C(30)	1.531(12)	C(37)-H(37B)	0.9900

C(38)-C(39)	1.503(15)	C(45')-C(46')	1.41(2)
C(38)-H(38A)	0.9900	C(45')-H(45C)	0.9900
C(38)-H(38B)	0.9900	C(45')-H(45D)	0.9900
C(39)-C(40)	1.487(14)	C(46')-C(47')	1.55(4)
C(39)-H(39A)	0.9900	C(46')-H(46C)	0.9900
C(39)-H(39B)	0.9900	C(46')-H(46D)	0.9900
C(40)-H(40A)	0.9900	C(47')-C(48')	1.41(2)
C(40)-H(40B)	0.9900	C(47')-H(47C)	0.9900
O(8)-C(41)	1.387(12)	C(47')-H(47D)	0.9900
O(8)-C(44)	1.394(11)	C(48')-H(48C)	0.9900
C(41)-C(42)	1.465(14)	C(48')-H(48D)	0.9900
C(41)-H(41A)	0.9900	O(10)-C(49)	1.374(16)
C(41)-H(41B)	0.9900	O(10)-C(52)	1.387(16)
C(42)-C(43)	1.544(15)	C(49)-C(50)	1.533(16)
C(42)-H(42A)	0.9900	C(49)-H(49A)	0.9900
C(42)-H(42B)	0.9900	C(49)-H(49B)	0.9900
C(43)-C(44)	1.490(13)	C(50)-C(51)	1.479(18)
C(43)-H(43A)	0.9900	C(50)-H(50A)	0.9900
C(43)-H(43B)	0.9900	C(50)-H(50B)	0.9900
C(44)-H(44A)	0.9900	C(51)-C(52)	1.500(16)
C(44)-H(44B)	0.9900	C(51)-H(51A)	0.9900
O(9)-C(48)	1.37(2)	C(51)-H(51B)	0.9900
O(9)-C(45)	1.42(2)	C(52)-H(52A)	0.9900
C(45)-C(46)	1.44(2)	C(52)-H(52B)	0.9900
C(45)-H(45A)	0.9900	O(10')-C(52')	1.413(18)
C(45)-H(45B)	0.9900	O(10')-C(49')	1.420(18)
C(46)-C(47)	1.54(3)	C(49')-C(50')	1.530(19)
C(46)-H(46A)	0.9900	C(49')-H(49C)	0.9900
C(46)-H(46B)	0.9900	C(49')-H(49D)	0.9900
C(47)-C(48)	1.43(2)	C(50')-C(51')	1.50(2)
C(47)-H(47A)	0.9900	C(50')-H(50C)	0.9900
C(47)-H(47B)	0.9900	C(50')-H(50D)	0.9900
C(48)-H(48A)	0.9900	C(51')-C(52')	1.508(18)
C(48)-H(48B)	0.9900	C(51')-H(51C)	0.9900
O(9')-C(48')	1.37(2)	C(51')-H(51D)	0.9900
O(9')-C(45')	1.40(2)	C(52')-H(52C)	0.9900

C(52')-H(52D)	0.9900	C(8)-Fe(3)-Fe(5)	120.7(2)
C(2)-Fe(1)-C(1)	114.3(4)	C(7)-Fe(3)-Fe(6)	118.7(3)
C(2)-Fe(1)-C(3)	116.7(4)	C(9)-Fe(3)-Fe(6)	120.6(2)
C(1)-Fe(1)-C(3)	115.0(4)	C(8)-Fe(3)-Fe(6)	60.8(2)
C(2)-Fe(1)-Fe(8)	121.4(2)	Fe(5)-Fe(3)-Fe(6)	71.02(4)
C(1)-Fe(1)-Fe(8)	117.3(2)	C(7)-Fe(3)-Fe(8)	122.1(3)
C(3)-Fe(1)-Fe(8)	61.7(3)	C(9)-Fe(3)-Fe(8)	61.8(3)
C(2)-Fe(1)-Fe(7)	61.1(3)	C(8)-Fe(3)-Fe(8)	117.7(2)
C(1)-Fe(1)-Fe(7)	119.8(2)	Fe(5)-Fe(3)-Fe(8)	70.92(5)
C(3)-Fe(1)-Fe(7)	118.8(3)	Fe(6)-Fe(3)-Fe(8)	70.39(4)
Fe(8)-Fe(1)-Fe(7)	70.36(4)	C(10)-Fe(4)-C(11)	115.1(4)
C(2)-Fe(1)-Fe(6)	116.9(3)	C(10)-Fe(4)-C(12)	118.2(4)
C(1)-Fe(1)-Fe(6)	60.2(2)	C(11)-Fe(4)-C(12)	113.6(3)
C(3)-Fe(1)-Fe(6)	120.9(3)	C(10)-Fe(4)-Fe(7)	120.9(3)
Fe(8)-Fe(1)-Fe(6)	70.38(4)	C(11)-Fe(4)-Fe(7)	117.4(2)
Fe(7)-Fe(1)-Fe(6)	70.16(4)	C(12)-Fe(4)-Fe(7)	60.4(2)
C(6)-Fe(2)-C(4)	115.4(4)	C(10)-Fe(4)-Fe(5)	60.8(3)
C(6)-Fe(2)-C(5)	112.8(4)	C(11)-Fe(4)-Fe(5)	118.8(2)
C(4)-Fe(2)-C(5)	117.3(4)	C(12)-Fe(4)-Fe(5)	120.3(3)
C(6)-Fe(2)-Fe(8)	61.6(3)	Fe(7)-Fe(4)-Fe(5)	71.29(4)
C(4)-Fe(2)-Fe(8)	119.1(3)	C(10)-Fe(4)-Fe(6)	118.4(3)
C(5)-Fe(2)-Fe(8)	117.9(3)	C(11)-Fe(4)-Fe(6)	59.9(2)
C(6)-Fe(2)-Fe(7)	119.3(3)	C(12)-Fe(4)-Fe(6)	117.9(3)
C(4)-Fe(2)-Fe(7)	119.4(2)	Fe(7)-Fe(4)-Fe(6)	70.10(4)
C(5)-Fe(2)-Fe(7)	60.9(2)	Fe(5)-Fe(4)-Fe(6)	70.53(4)
Fe(8)-Fe(2)-Fe(7)	70.35(5)	C(4)-Fe(5)-C(10)	97.1(4)
C(6)-Fe(2)-Fe(5)	120.3(3)	C(4)-Fe(5)-C(7)	98.2(3)
C(4)-Fe(2)-Fe(5)	60.4(2)	C(10)-Fe(5)-C(7)	94.3(4)
C(5)-Fe(2)-Fe(5)	120.5(3)	C(4)-Fe(5)-Fe(3)	126.0(2)
Fe(8)-Fe(2)-Fe(5)	70.85(4)	C(10)-Fe(5)-Fe(3)	125.9(3)
Fe(7)-Fe(2)-Fe(5)	70.76(4)	C(7)-Fe(5)-Fe(3)	53.0(2)
C(7)-Fe(3)-C(9)	115.8(4)	C(4)-Fe(5)-Fe(4)	126.1(2)
C(7)-Fe(3)-C(8)	114.5(4)	C(10)-Fe(5)-Fe(4)	53.3(3)
C(9)-Fe(3)-C(8)	114.1(4)	C(7)-Fe(5)-Fe(4)	124.6(3)
C(7)-Fe(3)-Fe(5)	61.8(2)	Fe(3)-Fe(5)-Fe(4)	106.69(5)
C(9)-Fe(3)-Fe(5)	119.3(3)	C(4)-Fe(5)-Fe(2)	53.3(2)

C(10)-Fe(5)-Fe(2)	127.2(3)	C(1)-Fe(6)-Fe(4)	128.7(2)
C(7)-Fe(5)-Fe(2)	128.7(3)	C(8)-Fe(6)-Fe(4)	128.3(2)
Fe(3)-Fe(5)-Fe(2)	105.83(5)	Fe(3)-Fe(6)-Fe(4)	106.10(5)
Fe(4)-Fe(5)-Fe(2)	105.58(5)	Fe(1)-Fe(6)-Fe(4)	106.45(5)
C(4)-Fe(5)-Fe(6)	155.4(2)	C(11)-Fe(6)-Fe(7)	99.2(2)
C(10)-Fe(5)-Fe(6)	99.7(3)	C(1)-Fe(6)-Fe(7)	101.2(2)
C(7)-Fe(5)-Fe(6)	98.3(2)	C(8)-Fe(6)-Fe(7)	156.8(2)
Fe(3)-Fe(5)-Fe(6)	54.51(4)	Fe(3)-Fe(6)-Fe(7)	103.03(5)
Fe(4)-Fe(5)-Fe(6)	55.03(4)	Fe(1)-Fe(6)-Fe(7)	54.84(4)
Fe(2)-Fe(5)-Fe(6)	102.04(4)	Fe(4)-Fe(6)-Fe(7)	54.46(4)
C(4)-Fe(5)-Fe(8)	99.4(2)	C(11)-Fe(6)-Fe(8)	155.9(2)
C(10)-Fe(5)-Fe(8)	155.7(3)	C(1)-Fe(6)-Fe(8)	99.1(2)
C(7)-Fe(5)-Fe(8)	100.8(2)	C(8)-Fe(6)-Fe(8)	99.6(2)
Fe(3)-Fe(5)-Fe(8)	54.66(4)	Fe(3)-Fe(6)-Fe(8)	54.90(4)
Fe(4)-Fe(5)-Fe(8)	102.40(5)	Fe(1)-Fe(6)-Fe(8)	54.61(4)
Fe(2)-Fe(5)-Fe(8)	54.11(4)	Fe(4)-Fe(6)-Fe(8)	102.44(5)
Fe(6)-Fe(5)-Fe(8)	59.58(4)	Fe(7)-Fe(6)-Fe(8)	59.96(4)
C(4)-Fe(5)-Fe(7)	100.0(2)	C(11)-Fe(6)-Fe(5)	100.0(2)
C(10)-Fe(5)-Fe(7)	100.2(3)	C(1)-Fe(6)-Fe(5)	156.8(2)
C(7)-Fe(5)-Fe(7)	155.0(2)	C(8)-Fe(6)-Fe(5)	101.1(2)
Fe(3)-Fe(5)-Fe(7)	102.18(5)	Fe(3)-Fe(6)-Fe(5)	54.47(4)
Fe(4)-Fe(5)-Fe(7)	54.17(4)	Fe(1)-Fe(6)-Fe(5)	103.34(5)
Fe(2)-Fe(5)-Fe(7)	54.51(4)	Fe(4)-Fe(6)-Fe(5)	54.44(4)
Fe(6)-Fe(5)-Fe(7)	59.39(3)	Fe(7)-Fe(6)-Fe(5)	60.47(3)
Fe(8)-Fe(5)-Fe(7)	59.39(4)	Fe(8)-Fe(6)-Fe(5)	60.21(4)
C(11)-Fe(6)-C(1)	96.9(3)	C(12)-Fe(7)-C(2)	92.6(4)
C(11)-Fe(6)-C(8)	97.7(3)	C(12)-Fe(7)-C(5)	96.4(3)
C(1)-Fe(6)-C(8)	92.3(3)	C(2)-Fe(7)-C(5)	96.6(3)
C(11)-Fe(6)-Fe(3)	127.0(2)	C(12)-Fe(7)-Fe(4)	54.5(2)
C(1)-Fe(6)-Fe(3)	124.3(2)	C(2)-Fe(7)-Fe(4)	124.1(2)
C(8)-Fe(6)-Fe(3)	53.9(2)	C(5)-Fe(7)-Fe(4)	127.3(2)
C(11)-Fe(6)-Fe(1)	125.6(2)	C(12)-Fe(7)-Fe(1)	126.3(3)
C(1)-Fe(6)-Fe(1)	53.6(2)	C(2)-Fe(7)-Fe(1)	53.2(3)
C(8)-Fe(6)-Fe(1)	124.3(2)	C(5)-Fe(7)-Fe(1)	124.2(3)
Fe(3)-Fe(6)-Fe(1)	106.45(5)	Fe(4)-Fe(7)-Fe(1)	107.55(5)
C(11)-Fe(6)-Fe(4)	53.5(2)	C(12)-Fe(7)-Fe(2)	127.0(3)

C(2)-Fe(7)-Fe(2)	128.9(3)	C(3)-Fe(8)-Fe(3)	127.8(3)
C(5)-Fe(7)-Fe(2)	53.5(2)	C(9)-Fe(8)-Fe(3)	53.1(2)
Fe(4)-Fe(7)-Fe(2)	106.15(5)	Fe(2)-Fe(8)-Fe(3)	106.49(6)
Fe(1)-Fe(7)-Fe(2)	106.07(6)	Fe(1)-Fe(8)-Fe(3)	106.64(5)
C(12)-Fe(7)-Fe(6)	101.1(2)	C(6)-Fe(8)-Fe(7)	100.1(2)
C(2)-Fe(7)-Fe(6)	98.5(2)	C(3)-Fe(8)-Fe(7)	99.4(3)
C(5)-Fe(7)-Fe(6)	156.2(2)	C(9)-Fe(8)-Fe(7)	155.9(2)
Fe(4)-Fe(7)-Fe(6)	55.44(4)	Fe(2)-Fe(8)-Fe(7)	55.18(4)
Fe(1)-Fe(7)-Fe(6)	55.01(4)	Fe(1)-Fe(8)-Fe(7)	54.94(4)
Fe(2)-Fe(7)-Fe(6)	102.83(5)	Fe(3)-Fe(8)-Fe(7)	102.87(5)
C(12)-Fe(7)-Fe(8)	157.8(2)	C(6)-Fe(8)-Fe(6)	156.6(2)
C(2)-Fe(7)-Fe(8)	101.3(3)	C(3)-Fe(8)-Fe(6)	100.9(3)
C(5)-Fe(7)-Fe(8)	99.0(2)	C(9)-Fe(8)-Fe(6)	100.2(3)
Fe(4)-Fe(7)-Fe(8)	103.33(5)	Fe(2)-Fe(8)-Fe(6)	103.28(5)
Fe(1)-Fe(7)-Fe(8)	54.71(4)	Fe(1)-Fe(8)-Fe(6)	55.01(4)
Fe(2)-Fe(7)-Fe(8)	54.47(4)	Fe(3)-Fe(8)-Fe(6)	54.71(4)
Fe(6)-Fe(7)-Fe(8)	60.09(4)	Fe(7)-Fe(8)-Fe(6)	59.95(4)
C(12)-Fe(7)-Fe(5)	101.4(2)	C(6)-Fe(8)-Fe(5)	100.4(2)
C(2)-Fe(7)-Fe(5)	156.2(3)	C(3)-Fe(8)-Fe(5)	156.9(3)
C(5)-Fe(7)-Fe(5)	100.8(2)	C(9)-Fe(8)-Fe(5)	98.8(2)
Fe(4)-Fe(7)-Fe(5)	54.55(4)	Fe(2)-Fe(8)-Fe(5)	55.04(4)
Fe(1)-Fe(7)-Fe(5)	103.21(5)	Fe(1)-Fe(8)-Fe(5)	103.66(5)
Fe(2)-Fe(7)-Fe(5)	54.73(4)	Fe(3)-Fe(8)-Fe(5)	54.42(4)
Fe(6)-Fe(7)-Fe(5)	60.14(3)	Fe(7)-Fe(8)-Fe(5)	60.46(4)
Fe(8)-Fe(7)-Fe(5)	60.14(4)	Fe(6)-Fe(8)-Fe(5)	60.21(3)
C(6)-Fe(8)-C(3)	94.0(4)	Fe(1)-C(1)-Fe(6)	66.2(2)
C(6)-Fe(8)-C(9)	95.4(3)	Fe(1)-C(2)-Fe(7)	65.7(2)
C(3)-Fe(8)-C(9)	97.7(4)	Fe(1)-C(3)-Fe(8)	65.0(2)
C(6)-Fe(8)-Fe(2)	53.3(2)	Fe(2)-C(4)-Fe(5)	66.2(2)
C(3)-Fe(8)-Fe(2)	124.9(3)	Fe(2)-C(5)-Fe(7)	65.6(2)
C(9)-Fe(8)-Fe(2)	125.0(2)	Fe(2)-C(6)-Fe(8)	65.1(2)
C(6)-Fe(8)-Fe(1)	125.8(2)	Fe(3)-C(7)-Fe(5)	65.2(2)
C(3)-Fe(8)-Fe(1)	53.3(3)	Fe(3)-C(8)-Fe(6)	65.3(2)
C(9)-Fe(8)-Fe(1)	127.2(2)	Fe(3)-C(9)-Fe(8)	65.1(2)
Fe(2)-Fe(8)-Fe(1)	106.97(6)	Fe(4)-C(10)-Fe(5)	65.9(2)
C(6)-Fe(8)-Fe(3)	126.8(2)	Fe(4)-C(11)-Fe(6)	66.6(2)

Fe(4)-C(12)-Fe(7)	65.1(2)	C(14)-C(15)-C(16)	101.7(5)
O(3)-Mg(1)-O(5)	175.3(2)	C(14)-C(15)-H(15A)	111.4
O(3)-Mg(1)-O(1)	87.41(19)	C(16)-C(15)-H(15A)	111.4
O(5)-Mg(1)-O(1)	88.08(18)	C(14)-C(15)-H(15B)	111.4
O(3)-Mg(1)-O(2)	88.9(2)	C(16)-C(15)-H(15B)	111.4
O(5)-Mg(1)-O(2)	89.4(2)	H(15A)-C(15)-H(15B)	109.3
O(1)-Mg(1)-O(2)	86.24(18)	O(1)-C(16)-C(15)	104.3(5)
O(3)-Mg(1)-O(4)	91.1(2)	O(1)-C(16)-H(16A)	110.9
O(5)-Mg(1)-O(4)	90.13(19)	C(15)-C(16)-H(16A)	110.9
O(1)-Mg(1)-O(4)	87.44(18)	O(1)-C(16)-H(16B)	110.9
O(2)-Mg(1)-O(4)	173.7(2)	C(15)-C(16)-H(16B)	110.9
O(3)-Mg(1)-Cl(1)	91.9(3)	H(16A)-C(16)-H(16B)	108.9
O(5)-Mg(1)-Cl(1)	92.6(3)	C(17)-O(2)-C(20)	109.3(5)
O(1)-Mg(1)-Cl(1)	178.8(3)	C(17)-O(2)-Mg(1)	124.8(4)
O(2)-Mg(1)-Cl(1)	92.7(3)	C(20)-O(2)-Mg(1)	125.6(4)
O(4)-Mg(1)-Cl(1)	93.6(3)	O(2)-C(17)-C(18)	104.7(6)
O(3)-Mg(1)-Br(1)	90.8(15)	O(2)-C(17)-H(17A)	110.8
O(5)-Mg(1)-Br(1)	93.7(15)	C(18)-C(17)-H(17A)	110.8
O(1)-Mg(1)-Br(1)	177.9(14)	O(2)-C(17)-H(17B)	110.8
O(2)-Mg(1)-Br(1)	92.6(15)	C(18)-C(17)-H(17B)	110.8
O(4)-Mg(1)-Br(1)	93.7(15)	H(17A)-C(17)-H(17B)	108.9
C(16)-O(1)-C(13)	109.5(5)	C(17)-C(18)-C(19)	102.4(6)
C(16)-O(1)-Mg(1)	124.2(4)	C(17)-C(18)-H(18A)	111.3
C(13)-O(1)-Mg(1)	126.3(4)	C(19)-C(18)-H(18A)	111.3
O(1)-C(13)-C(14)	103.9(5)	C(17)-C(18)-H(18B)	111.3
O(1)-C(13)-H(13A)	111.0	C(19)-C(18)-H(18B)	111.3
C(14)-C(13)-H(13A)	111.0	H(18A)-C(18)-H(18B)	109.2
O(1)-C(13)-H(13B)	111.0	C(20)-C(19)-C(18)	101.8(6)
C(14)-C(13)-H(13B)	111.0	C(20)-C(19)-H(19A)	111.4
H(13A)-C(13)-H(13B)	109.0	C(18)-C(19)-H(19A)	111.4
C(15)-C(14)-C(13)	101.4(5)	C(20)-C(19)-H(19B)	111.4
C(15)-C(14)-H(14A)	111.5	C(18)-C(19)-H(19B)	111.4
C(13)-C(14)-H(14A)	111.5	H(19A)-C(19)-H(19B)	109.3
C(15)-C(14)-H(14B)	111.5	O(2)-C(20)-C(19)	105.1(6)
C(13)-C(14)-H(14B)	111.5	O(2)-C(20)-H(20A)	110.7
H(14A)-C(14)-H(14B)	109.3	C(19)-C(20)-H(20A)	110.7

O(2)-C(20)-H(20B)	110.7	O(4)-C(25)-H(25B)	110.2
C(19)-C(20)-H(20B)	110.7	C(26)-C(25)-H(25B)	110.2
H(20A)-C(20)-H(20B)	108.8	H(25A)-C(25)-H(25B)	108.5
C(24)-O(3)-C(21)	107.6(5)	C(25)-C(26)-C(27)	103.5(6)
C(24)-O(3)-Mg(1)	125.7(4)	C(25)-C(26)-H(26A)	111.1
C(21)-O(3)-Mg(1)	120.7(4)	C(27)-C(26)-H(26A)	111.1
O(3)-C(21)-C(22)	105.6(6)	C(25)-C(26)-H(26B)	111.1
O(3)-C(21)-H(21A)	110.6	C(27)-C(26)-H(26B)	111.1
C(22)-C(21)-H(21A)	110.6	H(26A)-C(26)-H(26B)	109.0
O(3)-C(21)-H(21B)	110.6	C(26)-C(27)-C(28)	101.5(6)
C(22)-C(21)-H(21B)	110.6	C(26)-C(27)-H(27A)	111.5
H(21A)-C(21)-H(21B)	108.7	C(28)-C(27)-H(27A)	111.5
C(23)-C(22)-C(21)	104.1(6)	C(26)-C(27)-H(27B)	111.5
C(23)-C(22)-H(22A)	110.9	C(28)-C(27)-H(27B)	111.5
C(21)-C(22)-H(22A)	110.9	H(27A)-C(27)-H(27B)	109.3
C(23)-C(22)-H(22B)	110.9	O(4)-C(28)-C(27)	103.7(7)
C(21)-C(22)-H(22B)	110.9	O(4)-C(28)-H(28A)	111.0
H(22A)-C(22)-H(22B)	109.0	C(27)-C(28)-H(28A)	111.0
C(22)-C(23)-C(24)	102.3(6)	O(4)-C(28)-H(28B)	111.0
C(22)-C(23)-H(23A)	111.3	C(27)-C(28)-H(28B)	111.0
C(24)-C(23)-H(23A)	111.3	H(28A)-C(28)-H(28B)	109.0
C(22)-C(23)-H(23B)	111.3	C(32)-O(5)-C(29)	107.5(5)
C(24)-C(23)-H(23B)	111.3	C(32)-O(5)-Mg(1)	128.1(4)
H(23A)-C(23)-H(23B)	109.2	C(29)-O(5)-Mg(1)	121.3(4)
O(3)-C(24)-C(23)	103.9(6)	O(5)-C(29)-C(30)	106.4(7)
O(3)-C(24)-H(24A)	111.0	O(5)-C(29)-H(29A)	110.4
C(23)-C(24)-H(24A)	111.0	C(30)-C(29)-H(29A)	110.4
O(3)-C(24)-H(24B)	111.0	O(5)-C(29)-H(29B)	110.4
C(23)-C(24)-H(24B)	111.0	C(30)-C(29)-H(29B)	110.4
H(24A)-C(24)-H(24B)	109.0	H(29A)-C(29)-H(29B)	108.6
C(25)-O(4)-C(28)	107.7(5)	C(31)-C(30)-C(29)	103.8(7)
C(25)-O(4)-Mg(1)	127.2(4)	C(31)-C(30)-H(30A)	111.0
C(28)-O(4)-Mg(1)	125.0(4)	C(29)-C(30)-H(30A)	111.0
O(4)-C(25)-C(26)	107.7(6)	C(31)-C(30)-H(30B)	111.0
O(4)-C(25)-H(25A)	110.2	C(29)-C(30)-H(30B)	111.0
C(26)-C(25)-H(25A)	110.2	H(30A)-C(30)-H(30B)	109.0

C(30)-C(31)-C(32)	102.2(7)	C(36)-O(6)-C(33)	106.0(7)
C(30)-C(31)-H(31A)	111.3	C(36)-O(6)-Mg(2)	125.9(5)
C(32)-C(31)-H(31A)	111.3	C(33)-O(6)-Mg(2)	128.1(5)
C(30)-C(31)-H(31B)	111.3	O(6)-C(33)-C(34)	102.8(9)
C(32)-C(31)-H(31B)	111.3	O(6)-C(33)-H(33A)	111.2
H(31A)-C(31)-H(31B)	109.2	C(34)-C(33)-H(33A)	111.2
O(5)-C(32)-C(31)	104.0(6)	O(6)-C(33)-H(33B)	111.2
O(5)-C(32)-H(32A)	110.9	C(34)-C(33)-H(33B)	111.2
C(31)-C(32)-H(32A)	110.9	H(33A)-C(33)-H(33B)	109.1
O(5)-C(32)-H(32B)	110.9	C(33)-C(34)-C(35)	103.8(10)
C(31)-C(32)-H(32B)	110.9	C(33)-C(34)-H(34A)	111.0
H(32A)-C(32)-H(32B)	109.0	C(35)-C(34)-H(34A)	111.0
O(6)-Mg(2)-O(6)#1	91.2(4)	C(33)-C(34)-H(34B)	111.0
O(6)-Mg(2)-O(7)#1	90.2(2)	C(35)-C(34)-H(34B)	111.0
O(6)#1-Mg(2)-O(7)#1	178.4(3)	H(34A)-C(34)-H(34B)	109.0
O(6)-Mg(2)-O(7)	178.4(3)	C(36)-C(35)-C(34)	104.2(9)
O(6)#1-Mg(2)-O(7)	90.2(2)	C(36)-C(35)-H(35A)	110.9
O(7)#1-Mg(2)-O(7)	88.4(4)	C(34)-C(35)-H(35A)	110.9
O(6)-Mg(2)-Cl(2)	89.5(6)	C(36)-C(35)-H(35B)	110.9
O(6)#1-Mg(2)-Cl(2)	89.3(6)	C(34)-C(35)-H(35B)	110.9
O(7)#1-Mg(2)-Cl(2)	90.0(6)	H(35A)-C(35)-H(35B)	108.9
O(7)-Mg(2)-Cl(2)	91.2(6)	O(6)-C(36)-C(35)	107.6(8)
O(6)-Mg(2)-Cl(2)#1	89.3(6)	O(6)-C(36)-H(36A)	110.2
O(6)#1-Mg(2)-Cl(2)#1	89.5(6)	C(35)-C(36)-H(36A)	110.2
O(7)#1-Mg(2)-Cl(2)#1	91.2(6)	O(6)-C(36)-H(36B)	110.2
O(7)-Mg(2)-Cl(2)#1	90.0(6)	C(35)-C(36)-H(36B)	110.2
Cl(2)-Mg(2)-Cl(2)#1	178.4(11)	H(36A)-C(36)-H(36B)	108.5
O(6)-Mg(2)-Br(2)	89.6(12)	C(40)-O(7)-C(37)	107.0(7)
O(6)#1-Mg(2)-Br(2)	88.5(11)	C(40)-O(7)-Mg(2)	127.0(5)
O(7)#1-Mg(2)-Br(2)	90.8(11)	C(37)-O(7)-Mg(2)	125.9(5)
O(7)-Mg(2)-Br(2)	91.2(12)	O(7)-C(37)-C(38)	106.7(8)
O(6)-Mg(2)-Br(2)#1	88.5(11)	O(7)-C(37)-H(37A)	110.4
O(6)#1-Mg(2)-Br(2)#1	89.6(12)	C(38)-C(37)-H(37A)	110.4
O(7)#1-Mg(2)-Br(2)#1	91.2(12)	O(7)-C(37)-H(37B)	110.4
O(7)-Mg(2)-Br(2)#1	90.8(11)	C(38)-C(37)-H(37B)	110.4
Br(2)-Mg(2)-Br(2)#1	177(2)	H(37A)-C(37)-H(37B)	108.6

C(37)-C(38)-C(39)	102.0(9)	H(43A)-C(43)-H(43B)	109.5
C(37)-C(38)-H(38A)	111.4	O(8)-C(44)-C(43)	108.0(8)
C(39)-C(38)-H(38A)	111.4	O(8)-C(44)-H(44A)	110.1
C(37)-C(38)-H(38B)	111.4	C(43)-C(44)-H(44A)	110.1
C(39)-C(38)-H(38B)	111.4	O(8)-C(44)-H(44B)	110.1
H(38A)-C(38)-H(38B)	109.2	C(43)-C(44)-H(44B)	110.1
C(40)-C(39)-C(38)	101.9(9)	H(44A)-C(44)-H(44B)	108.4
C(40)-C(39)-H(39A)	111.4	C(48)-O(9)-C(45)	110(2)
C(38)-C(39)-H(39A)	111.4	O(9)-C(45)-C(46)	104.6(17)
C(40)-C(39)-H(39B)	111.4	O(9)-C(45)-H(45A)	110.8
C(38)-C(39)-H(39B)	111.4	C(46)-C(45)-H(45A)	110.8
H(39A)-C(39)-H(39B)	109.2	O(9)-C(45)-H(45B)	110.8
O(7)-C(40)-C(39)	108.7(8)	C(46)-C(45)-H(45B)	110.8
O(7)-C(40)-H(40A)	110.0	H(45A)-C(45)-H(45B)	108.9
C(39)-C(40)-H(40A)	110.0	C(45)-C(46)-C(47)	99.7(14)
O(7)-C(40)-H(40B)	110.0	C(45)-C(46)-H(46A)	111.8
C(39)-C(40)-H(40B)	110.0	C(47)-C(46)-H(46A)	111.8
H(40A)-C(40)-H(40B)	108.3	C(45)-C(46)-H(46B)	111.8
C(41)-O(8)-C(44)	107.3(7)	C(47)-C(46)-H(46B)	111.8
O(8)-C(41)-C(42)	110.9(9)	H(46A)-C(46)-H(46B)	109.6
O(8)-C(41)-H(41A)	109.5	C(48)-C(47)-C(46)	106.8(16)
C(42)-C(41)-H(41A)	109.5	C(48)-C(47)-H(47A)	110.4
O(8)-C(41)-H(41B)	109.5	C(46)-C(47)-H(47A)	110.4
C(42)-C(41)-H(41B)	109.5	C(48)-C(47)-H(47B)	110.4
H(41A)-C(41)-H(41B)	108.1	C(46)-C(47)-H(47B)	110.4
C(41)-C(42)-C(43)	101.2(9)	H(47A)-C(47)-H(47B)	108.6
C(41)-C(42)-H(42A)	111.5	O(9)-C(48)-C(47)	106.2(17)
C(43)-C(42)-H(42A)	111.5	O(9)-C(48)-H(48A)	110.5
C(41)-C(42)-H(42B)	111.5	C(47)-C(48)-H(48A)	110.5
C(43)-C(42)-H(42B)	111.5	O(9)-C(48)-H(48B)	110.5
H(42A)-C(42)-H(42B)	109.4	C(47)-C(48)-H(48B)	110.5
C(44)-C(43)-C(42)	100.0(8)	H(48A)-C(48)-H(48B)	108.7
C(44)-C(43)-H(43A)	111.8	C(48')-O(9')-C(45')	108(2)
C(42)-C(43)-H(43A)	111.8	O(9')-C(45')-C(46')	111(2)
C(44)-C(43)-H(43B)	111.8	O(9')-C(45')-H(45C)	109.5
C(42)-C(43)-H(43B)	111.8	C(46')-C(45')-H(45C)	109.5

O(9')-C(45')-H(45D)	109.5	C(52)-C(51)-H(51A)	111.1
C(46')-C(45')-H(45D)	109.5	C(50)-C(51)-H(51B)	111.1
H(45C)-C(45')-H(45D)	108.1	C(52)-C(51)-H(51B)	111.1
C(45')-C(46')-C(47')	102.4(19)	H(51A)-C(51)-H(51B)	109.0
C(45')-C(46')-H(46C)	111.3	O(10)-C(52)-C(51)	112.6(18)
C(47')-C(46')-H(46C)	111.3	O(10)-C(52)-H(52A)	109.1
C(45')-C(46')-H(46D)	111.3	C(51)-C(52)-H(52A)	109.1
C(47')-C(46')-H(46D)	111.3	O(10)-C(52)-H(52B)	109.1
H(46C)-C(46')-H(46D)	109.2	C(51)-C(52)-H(52B)	109.1
C(48')-C(47')-C(46')	103.0(17)	H(52A)-C(52)-H(52B)	107.8
C(48')-C(47')-H(47C)	111.2	C(52')-O(10')-C(49')	93(3)
C(46')-C(47')-H(47C)	111.2	O(10')-C(49')-C(50')	116(2)
C(48')-C(47')-H(47D)	111.2	O(10')-C(49')-H(49C)	108.3
C(46')-C(47')-H(47D)	111.2	C(50')-C(49')-H(49C)	108.3
H(47C)-C(47')-H(47D)	109.1	O(10')-C(49')-H(49D)	108.3
O(9')-C(48')-C(47')	110(2)	C(50')-C(49')-H(49D)	108.3
O(9')-C(48')-H(48C)	109.7	H(49C)-C(49')-H(49D)	107.4
C(47')-C(48')-H(48C)	109.7	C(51')-C(50')-C(49')	95(2)
O(9')-C(48')-H(48D)	109.7	C(51')-C(50')-H(50C)	112.7
C(47')-C(48')-H(48D)	109.7	C(49')-C(50')-H(50C)	112.7
H(48C)-C(48')-H(48D)	108.2	C(51')-C(50')-H(50D)	112.7
C(49)-O(10)-C(52)	99.7(19)	C(49')-C(50')-H(50D)	112.7
O(10)-C(49)-C(50)	116.0(17)	H(50C)-C(50')-H(50D)	110.2
O(10)-C(49)-H(49A)	108.3	C(50')-C(51')-C(52')	101.1(19)
C(50)-C(49)-H(49A)	108.3	C(50')-C(51')-H(51C)	111.6
O(10)-C(49)-H(49B)	108.3	C(52')-C(51')-H(51C)	111.6
C(50)-C(49)-H(49B)	108.3	C(50')-C(51')-H(51D)	111.6
H(49A)-C(49)-H(49B)	107.4	C(52')-C(51')-H(51D)	111.6
C(51)-C(50)-C(49)	99.8(13)	H(51C)-C(51')-H(51D)	109.4
C(51)-C(50)-H(50A)	111.8	O(10')-C(52')-C(51')	119(2)
C(49)-C(50)-H(50A)	111.8	O(10')-C(52')-H(52C)	107.6
C(51)-C(50)-H(50B)	111.8	C(51')-C(52')-H(52C)	107.6
C(49)-C(50)-H(50B)	111.8	O(10')-C(52')-H(52D)	107.6
H(50A)-C(50)-H(50B)	109.5	C(51')-C(52')-H(52D)	107.6
C(50)-C(51)-C(52)	103.5(14)	H(52C)-C(52')-H(52D)	107.0
C(50)-C(51)-H(51A)	111.1		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for neism18h. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe1	31(1)	39(1)	50(1)	6(1)	2(1)	4(1)
Fe2	39(1)	34(1)	45(1)	1(1)	5(1)	-3(1)
Fe3	41(1)	40(1)	37(1)	-6(1)	4(1)	0(1)
Fe4	46(1)	40(1)	36(1)	4(1)	-4(1)	2(1)
Fe5	29(1)	32(1)	38(1)	-2(1)	1(1)	0(1)
Fe6	30(1)	29(1)	35(1)	1(1)	1(1)	1(1)
Fe7	37(1)	33(1)	34(1)	-2(1)	5(1)	2(1)
Fe8	36(1)	37(1)	36(1)	7(1)	1(1)	1(1)
C1	34(3)	44(4)	70(6)	13(4)	-1(4)	-8(3)
C2	50(5)	40(4)	82(7)	-7(4)	29(5)	6(4)
C3	47(5)	72(6)	71(6)	22(5)	-12(5)	13(5)
C4	37(4)	56(5)	59(6)	2(4)	2(4)	-18(4)
C5	62(5)	33(4)	64(6)	-13(4)	11(5)	2(4)
C6	62(6)	48(5)	55(5)	17(4)	6(4)	-6(4)
C7	40(4)	60(5)	63(6)	-15(5)	16(4)	6(4)
C8	60(5)	42(4)	50(5)	-15(4)	0(4)	-3(4)
C9	61(5)	80(7)	28(4)	2(4)	3(4)	-2(5)
C10	52(5)	67(6)	69(6)	-7(5)	-28(5)	19(5)
C11	62(5)	37(4)	47(4)	19(4)	8(4)	-3(4)
C12	80(6)	57(5)	29(4)	-4(4)	11(4)	3(5)
Mg1	26(1)	24(1)	27(1)	2(1)	1(1)	-2(1)
Cl1	39(1)	29(2)	57(1)	-1(3)	6(1)	-10(2)
Br1	39(1)	29(2)	57(1)	-1(3)	6(1)	-10(2)
O1	22(2)	26(2)	27(2)	-1(2)	-1(2)	-2(2)
C13	30(3)	33(3)	40(4)	-5(3)	-3(3)	3(3)
C14	29(3)	37(4)	49(4)	-6(3)	2(3)	-5(3)
C15	34(3)	27(3)	43(4)	-4(3)	3(3)	2(3)
C16	37(3)	27(3)	39(4)	2(3)	3(3)	2(3)
O2	27(2)	30(2)	34(2)	-7(2)	5(2)	-6(2)
C17	38(4)	33(4)	42(4)	-9(3)	7(3)	-4(3)
C18	50(4)	34(4)	40(4)	-10(3)	9(3)	4(3)

C19	37(4)	43(4)	36(4)	5(3)	10(3)	5(3)
C20	30(3)	35(3)	37(4)	-3(3)	-1(3)	-4(3)
O3	40(3)	32(2)	29(2)	5(2)	-1(2)	4(2)
C21	46(4)	35(4)	37(4)	1(3)	-1(3)	10(3)
C22	46(4)	48(5)	44(4)	6(4)	-3(4)	11(4)
C23	49(5)	41(4)	41(4)	6(3)	-13(3)	4(4)
C24	42(4)	42(4)	37(4)	1(3)	-1(3)	10(3)
O4	32(2)	32(2)	32(2)	-3(2)	8(2)	-6(2)
C25	46(4)	29(3)	39(4)	-4(3)	5(3)	2(3)
C26	67(6)	42(5)	53(5)	-8(4)	32(5)	2(4)
C27	41(4)	73(6)	45(5)	3(4)	9(4)	-2(4)
C28	40(4)	47(4)	41(4)	-5(3)	12(3)	-16(4)
O5	24(2)	37(2)	29(2)	2(2)	-3(2)	-2(2)
C29	30(3)	43(4)	54(5)	-3(4)	0(3)	1(3)
C30	43(5)	103(8)	51(5)	4(6)	-15(4)	2(5)
C31	41(4)	60(5)	41(4)	11(4)	-10(4)	4(4)
C32	40(4)	62(5)	29(4)	-1(4)	-2(3)	4(4)
Mg2	28(2)	59(2)	36(2)	0	0	3(2)
Cl2	19(3)	74(3)	53(2)	10(2)	1(3)	-6(3)
Br2	19(3)	74(3)	53(2)	10(2)	1(3)	-6(3)
O6	33(3)	81(4)	53(4)	-20(3)	-7(2)	13(3)
C33	47(5)	113(9)	50(5)	-29(6)	-13(4)	14(6)
C34	69(7)	103(10)	83(8)	-39(7)	2(6)	-8(7)
C35	81(8)	92(9)	87(8)	-14(7)	-14(7)	30(7)
C36	40(5)	106(8)	58(6)	-30(6)	-5(4)	20(5)
O7	44(3)	57(4)	47(3)	-7(3)	11(3)	-12(3)
C37	69(6)	53(5)	62(6)	-2(5)	14(5)	-4(5)
C38	104(10)	52(6)	99(9)	3(6)	35(8)	5(6)
C39	63(6)	82(8)	72(7)	-2(6)	22(5)	-1(6)
C40	55(5)	73(6)	48(5)	-11(5)	18(4)	-16(5)
O8	74(4)	70(4)	54(4)	-7(3)	11(3)	17(4)
C41	46(5)	65(6)	61(6)	-16(5)	-8(4)	5(4)
C42	109(9)	74(7)	54(6)	-8(5)	15(6)	-34(7)
C43	66(6)	58(6)	44(5)	-11(4)	3(4)	12(5)
C44	59(5)	53(5)	44(4)	1(4)	5(4)	13(4)
O9	82(10)	94(10)	123(12)	-34(9)	-14(11)	5(9)

C45	43(8)	62(9)	107(14)	-10(9)	-19(9)	14(7)
C46	59(11)	127(15)	123(15)	-13(13)	-22(11)	-3(10)
C47	61(10)	111(13)	99(12)	8(12)	-6(10)	-23(8)
C48	47(14)	105(10)	115(12)	-48(9)	18(9)	-34(9)
O9'	82(10)	94(10)	123(12)	-34(9)	-14(11)	5(9)
C45'	43(8)	62(9)	107(14)	-10(9)	-19(9)	14(7)
C46'	59(11)	127(15)	123(15)	-13(13)	-22(11)	-3(10)
C47'	61(10)	111(13)	99(12)	8(12)	-6(10)	-23(8)
C48'	47(14)	105(10)	115(12)	-48(9)	18(9)	-34(9)
O10	183(16)	135(13)	149(12)	-42(10)	-19(14)	18(14)
C49	168(16)	57(9)	113(14)	-13(10)	10(13)	-24(11)
C50	131(14)	80(11)	133(14)	31(11)	26(13)	-4(10)
C51	134(16)	84(13)	175(15)	45(12)	11(14)	39(12)
C52	131(15)	91(13)	155(15)	-7(11)	6(13)	14(11)
O10'	131(15)	91(13)	155(15)	-7(11)	6(13)	14(11)
C49'	134(16)	84(13)	175(15)	45(12)	11(14)	39(12)
C50'	131(14)	80(11)	133(14)	31(11)	26(13)	-4(10)
C51'	168(16)	57(9)	113(14)	-13(10)	10(13)	-24(11)
C52'	183(16)	135(13)	149(12)	-42(10)	-19(14)	18(14)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for neism18h.

	x	y	z	U(eq)
H13A	6504	3716	-1336	41
H13B	6262	4344	-581	41
H14A	6168	2902	392	46
H14B	6170	2392	-686	46
H15A	6758	1981	-567	42
H15B	6610	1685	503	42
H16A	6810	3198	1196	41
H16B	7112	3011	399	41
H17A	6647	7306	1615	45
H17B	6924	6655	2244	45
H18A	6328	7095	3015	50
H18B	6503	5996	3253	50
H19A	5971	5513	2573	47
H19B	5990	6407	1756	47
H20A	6392	4560	1824	41
H20B	6206	5054	878	41
H21A	6535	7506	-314	47
H21B	6218	6736	-93	47
H22A	5957	7409	-1420	55
H22B	6312	7951	-1776	55
H23A	6274	6685	-2930	52
H23B	6091	5894	-2180	52
H24A	6664	5338	-2180	48
H24B	6812	6496	-2185	48
H25A	7080	4015	-2032	46
H25B	7319	3507	-1198	46
H26A	7529	4211	-3050	65
H26B	7726	3395	-2356	65
H27A	7986	5214	-2524	64
H27B	7996	4670	-1462	64

H28A	7684	6164	-1131	51
H28B	7478	6102	-2156	51
H29A	7816	5462	615	51
H29B	7767	4297	249	51
H30A	8082	3845	1564	79
H30B	8032	4957	2064	79
H31A	7678	4011	3046	57
H31B	7568	3251	2166	57
H32A	7095	4362	2242	52
H32B	7342	5344	2431	52
H33A	4991	3950	-2766	84
H33B	4651	3847	-2081	84
H34A	4878	2240	-2873	102
H34B	4761	2170	-1742	102
H35A	5323	1657	-1505	104
H35B	5457	2221	-2486	104
H36A	5466	2994	-645	82
H36B	5607	3547	-1620	82
H37A	5112	7395	415	73
H37B	5305	6885	1339	73
H38A	4680	8055	1354	102
H38B	5000	8124	2116	102
H39A	4844	6624	2882	87
H39B	4465	7082	2618	87
H40A	4656	5323	1957	70
H40B	4399	6045	1338	70
H41A	7222	4774	4839	69
H41B	6862	4900	4260	69
H42A	6914	5206	6116	95
H42B	6619	5762	5459	95
H43A	6915	7217	6005	67
H43B	7284	6624	6032	67
H44A	6915	7328	4356	63
H44B	7325	7429	4562	63
H45A	5509	5064	4946	85
H45B	5199	5845	5215	85

H46A	5920	6227	5283	123
H46B	5629	6542	6083	123
H47A	5429	7880	5156	108
H47B	5819	7867	4733	108
H48A	5255	7522	3721	107
H48B	5646	7324	3352	107
H45C	5438	4869	4131	85
H45D	5092	5433	4509	85
H46C	5661	5246	5496	123
H46D	5350	6032	5754	123
H47C	5753	7280	5399	108
H47D	5986	6505	4750	108
H48C	5418	7651	4204	107
H48D	5747	7314	3558	107
H49A	6224	9374	-458	135
H49B	6331	10217	334	135
H50A	5803	10901	303	137
H50B	5713	10142	-600	137
H51A	5382	9265	426	157
H51B	5534	9887	1354	157
H52A	5796	8391	1638	151
H52B	5791	8070	507	151
H49C	5527	10495	932	157
H49D	5220	9671	911	157
H50C	5423	8962	-562	137
H50D	5461	10192	-721	137
H51C	6037	10182	-315	135
H51D	6017	9014	-710	135
H52C	6042	8400	770	187
H52D	6142	9526	1128	187

Table S6. Torsion angles [°] for neism18h.

C16-O1-C13-C14	16.4(7)	C30-C31-C32-O5	40.5(9)
Mg1-O1-C13-C14	-162.8(4)	C36-O6-C33-C34	38.1(11)
O1-C13-C14-C15	-37.3(7)	Mg2-O6-C33-C34	-140.1(8)
C13-C14-C15-C16	43.2(7)	O6-C33-C34-C35	-38.0(12)
C13-O1-C16-C15	10.6(7)	C33-C34-C35-C36	24.3(14)
Mg1-O1-C16-C15	-170.2(4)	C33-O6-C36-C35	-22.8(12)
C14-C15-C16-O1	-33.9(7)	Mg2-O6-C36-C35	155.5(8)
C20-O2-C17-C18	10.6(8)	C34-C35-C36-O6	-1.2(14)
Mg1-O2-C17-C18	-174.0(4)	C40-O7-C37-C38	-17.0(11)
O2-C17-C18-C19	-31.8(7)	Mg2-O7-C37-C38	166.1(7)
C17-C18-C19-C20	40.6(7)	O7-C37-C38-C39	33.4(13)
C17-O2-C20-C19	15.3(7)	C37-C38-C39-C40	-35.8(13)
Mg1-O2-C20-C19	-160.1(4)	C37-O7-C40-C39	-6.7(11)
C18-C19-C20-O2	-34.6(7)	Mg2-O7-C40-C39	170.1(7)
C24-O3-C21-C22	12.4(8)	C38-C39-C40-O7	27.1(12)
Mg1-O3-C21-C22	166.4(5)	C44-O8-C41-C42	1.3(11)
O3-C21-C22-C23	13.5(8)	O8-C41-C42-C43	-22.3(11)
C21-C22-C23-C24	-32.9(8)	C41-C42-C43-C44	32.6(10)
C21-O3-C24-C23	-33.4(8)	C41-O8-C44-C43	21.8(10)
Mg1-O3-C24-C23	174.2(5)	C42-C43-C44-O8	-34.2(10)
C22-C23-C24-O3	41.1(8)	C48-O9-C45-C46	-32(4)
C28-O4-C25-C26	8.3(8)	O9-C45-C46-C47	34(3)
Mg1-O4-C25-C26	-172.0(5)	C45-C46-C47-C48	-27(3)
O4-C25-C26-C27	16.9(9)	C45-O9-C48-C47	14(4)
C25-C26-C27-C28	-34.1(9)	C46-C47-C48-O9	9(4)
C25-O4-C28-C27	-30.2(8)	C48'-O9'-C45'-C46'	-2(7)
Mg1-O4-C28-C27	150.1(5)	O9'-C45'-C46'-C47'	-13(5)
C26-C27-C28-O4	39.6(8)	C45'-C46'-C47'-C48'	22(5)
C32-O5-C29-C30	10.4(9)	C45'-O9'-C48'-C47'	17(7)
Mg1-O5-C29-C30	172.0(6)	C46'-C47'-C48'-O9'	-24(6)
O5-C29-C30-C31	15.1(10)	C52-O10-C49-C50	22(3)
C29-C30-C31-C32	-33.3(10)	O10-C49-C50-C51	-7(3)
C29-O5-C32-C31	-31.6(8)	C49-C50-C51-C52	-11(3)
Mg1-O5-C32-C31	168.4(5)	C49-O10-C52-C51	-30(3)

C50-C51-C52-O10	27(4)	C49'-C50'-C51'-C52'	27(5)
C52'-O10'-C49'-C50'	35(6)	C49'-O10'-C52'-C51'	-13(7)
O10'-C49'-C50'-C51'	-43(5)	C50'-C51'-C52'-O10'	-11(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,z

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