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Supplementary information

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Supplementary information for

Nitrogen Reduction by the Fe Sites of Synthetic [Mo_3S_4Fe] Cubes

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Materials and Methods.

General considerations. Unless otherwise noted, all reactions were performed under an inert nitrogen or argon atmosphere using Schlenk techniques and glove boxes. Hexane, toluene, and tetrahydrofuran (THF) were dried and deoxygenated by passing over columns of activated alumina and supported copper catalyst purchased from Hansen & Co., Ltd. ^{1}H, ^{13}C{^{1}H}, and ^{15}N{^{1}H} NMR spectra were recorded on a JEOL ECA-600 or a Bruker Avance 400 spectrometer. Detected ^{1}H NMR signals were referenced to the residual peaks of the deuterated solvents. The ^{15}N NMR chemical shifts were referenced to an external standard CH_3NO_2 ($\delta = 0$). Fourier-transform infrared spectroscopy (FT-IR) was performed using Bruker Optics ALPHA FT-IR equipped with Diamond ATR. Electrospray ionization mass spectrometry (ESI-MS) was performed using a JEOL JMS-100 at room temperature. Elemental analyses were carried out using an Elementar Analytical vario MICRO cube elemental analyzer, where crystalline samples were sealed in tin capsules under an inert atmosphere. Mössbauer measurements were performed in a conventional transmission mode on a Mössbauer spectrometer (Topologic Systems Co. Model-222) with a ^{57}Co(Rh) source (925 MBq). The spectral curve fitting was carried out by using MossWinn 4.0Pre on the assumption of the sum of the Lorentzian curves. The Doppler velocity scale was calibrated with respect to α-iron at room temperature, and the isomer shifts are given relative to α-iron. Cyclic voltammograms were recorded on a BAS ALS-660A electrochemical analyzer. GC/GC-MS analyses were acquired on a Shimadzu GCMS-2010SE. Synthetic procedures for [$Cp^R_3Mo_3S_4FeCl$] (Cp^R = C_5Me_5 (**1a**),[11] $C_5Me_4SiMe_3$ (**1b**), and $C_5Me_4SiEt_3$ (**1c**))[12] and $Cp^R_3Mo_3S_4$ (Cp^R = C_5Me_5 (**4a**), $C_5Me_4SiMe_3$ (**4b**), and $C_5Me_4SiEt_3$ (**4c**))[12] were described elsewhere. Potassium graphite (KC_8),[34] sodium naphthalenide ($Na(C_{10}H_8)$),[35] $[H(OEt_2)_2][BAr^F_4]$ (Ar^F = $(C_6H_3\text{-}3,5\text{-}(CF_3)_2)$,[36] $[PPh_4]_2[Fe_4S_4(SEt)_4]$,[37] $[Fe_4S_4(STip)_2(tmtu)_2]$ (Tip = $C_6H_2\text{-}2,4,6\text{-}^{i}Pr_3$, tmtu = 1,1,3,3-teramethyl-2-thiourea),[38] $Na[Fe_4S_4(STip)_4]$,[39] and $[\{N(SiMe_3)_2\}(tmtu)Fe_4S_3]_2(\mu_6\text{-}S)\{\mu\text{-}N(SiMe_3)_2\}_2$[40] were prepared according to the literature procedures. Low-temperature experiments in glove boxes were carried out using a Techno Sigma UCR-150GB. UV irradiation was conducted using an Asahi Spectra REX-250. Deuterated solvents were dried over sodium metal (for C_6D_6, toluene-d_8, and THF-d_8) before use. $[N^nBu_4][PF_6]$ was recrystallized from THF prior to use. All other chemicals were purchased from commercial sources and used without further purification.

Synthesis of $[K(THF)_2]_2[\{Cp^*_3Mo_3S_4Fe\}_2(\mu\text{-}N_2)]$ (2a). In a nitrogen-filled glove box, a black solid of **1a** (206 mg, 0.226 mmol) was dissolved in THF (20 mL) and cooled to –100˚C. KC_8 (69 mg, 0.510 mmol) was added to the cold solution, and the mixture was gradually heated up to room temperature with stirring overnight. The resultant suspension was filtered, followed by layering hexane on top of the filtrate. Black crystals of

$[K(THF)_2]_2[\{Cp^*{}_3Mo_3S_4Fe\}_2(\mu\text{-}N_2)]$ (**2a**, 37.4 mg, 0.0174 mmol, 15% yield based on **1a**). ^{1}H NMR (THF-d_8): δ 1.87 ($C_5\mathit{Me}_5$). $^{13}C\{^1H\}$ NMR (THF-d_8): δ 99.67 (C_5Me_5), 12.35 ($C_5\mathit{Me}_5$). ^{57}Fe Mössbauer spectrum (mm/s, 78 K): δ = 0.479(4), $|\Delta E_Q|$ = 1.258(8). Anal. Calcd. for $C_{76}Fe_2H_{122}K_2Mo_6N_2O_4S_8$: C, 42.46; H, 5.72; N, 1.30; S, 11.93. Found: C, 42.60; H, 6.03; N, 1.45; S, 12.27.

Synthesis of $^{15}N_2$-labeled 2a ($^{15}N_2$-2a). A black solid of **1a** (206 mg, 0.226 mmol) and KC_8 (69 mg, 0.510 mmol) were mixed as solids, and THF (20 mL) was vacuum-transferred. After filling $^{15}N_2$ into the gas phase, the mixture was allowed to warm to room temperature. Vigorous stirring was initiated when a part of THF melted, and stirring was continued overnight. The resultant suspension was filtered, and hexane was layered on the filtrate. $^{15}N_2$-labeled **2a** ($^{15}N_2$-**2a**) was obtained as a black crystalline powder. $^{15}N\{^1H\}$ NMR (toluene-d_8): δ –40.9.

Synthesis of [Na(15-crown-5)(THF)][$(C_5Me_4SiMe_3)_3Mo_3S_4Fe(N_2)$] (2b). In a nitrogen-filled glove box, THF (20 mL) was frozen by liquid nitrogen. Onto the frozen solvent, a black solid of **1b** (500 mg, 0.460 mmol) was added, followed by careful addition of sodium naphthalenide (19.8 mM in THF, 54.3 mL, 1.07 mmol). The mixture was stirred overnight with gradually warming up to room temperature. The resultant dark-green solution was filtered, and the filtrate was treated with 15-crown-5 (90.5 µL, 0.510 mmol) for a few minutes. After evaporation of the solvent, the black residue was washed with a small amount of hexane. The product was extracted with a mixture of hexane (10 mL) and THF (9 mL). The extract was stored at –35˚C for a few days, leading to the precipitation of [Na(15-crown-5)(THF)][$(C_5Me_4SiMe_3)_3Mo_3S_4Fe(N_2)$] (**2b**, 197 mg, 0.141 mmol, 31% yield based on **1b**) as a black powder. ^{1}H NMR (C_6D_6): δ 2.25 (CMe), 2.03 (CMe), 0.60 (SiMe_3). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 110.9 (CMe), 105.1 (CMe), 82.8 ($\mathit{C}SiMe_3$), 16.1 (CMe), 13.2 (CMe), 3.5 (SiMe_3). FT-IR (ATR, cm^{-1}): 1896 (N≡N). ^{57}Fe Mössbauer spectrum (mm/s, 78 K): δ = 0.410(2), $|\Delta E_Q|$ = 1.422(5).

Synthesis of [Na(15-crown-5)(THF)][$(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2)$] (2c). In a nitrogen-filled glove box, THF (20 mL) was frozen by liquid nitrogen. Onto the frozen solvent, a black solid of **1c** (500 mg, 0.412 mmol) was added, followed by careful addition of sodium naphthalenide (19.8 mM in THF, 48.8 mL, 0.961 mmol). The mixture was stirred overnight with gradually warming up to room temperature. The resultant dark-green solution was filtered, and the filtrate was treated with 15-crown-5 (81.3 µL, 0.458 mmol) for a few minutes. After evaporation of the solvent, the black residue was washed with a small amount of hexane. The product was extracted with a mixture of hexane (10 mL) and THF (6 mL). The extract was stored at –35˚C for a few days, leading to the precipitation of [Na(15-crown-5)(THF)][$(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2)$] (**2c**,

253 mg, 0.158 mmol, 38% yield based on **1c**) as black crystals. ^{1}H NMR (C_6D_6): δ 2.30 (C*Me*), 2.08 (C*Me*), 1.22 (Si*Et*$_3$). ^{13}C{^{1}H} NMR (C_6D_6): δ 110.7 (*C*Me), 105.0 (*C*Me), 82.3 (*C*SiEt$_3$), 16.8 (C*Me*), 13.7 (C*Me*), 9.1 (Si*Et*$_3$), 7.0 (Si*Et*$_3$). FT-IR (ATR, cm^{-1}): 1902 (N≡N). ^{57}Fe Mössbauer spectrum (mm/s, 78 K): δ = 0.401(3), $|\Delta E_Q|$ = 1.466(5).

Synthesis of $^{15}N_2$-labeled 2b and 2c ($^{15}N_2$-2b and $^{15}N_2$-2c). $^{15}N_2$-labeled samples of clusters **2b** and **c** were prepared by using the aforementioned procedures starting from smaller amounts of **1b** (200 mg, 0.184 mmol) or **1c** (200 mg, 0.165 mmol), THF (10 mL), and 15-crown-5 (36.2 µL, 0.204 mmol for **1b**; 32.5 µL, 0.183 mmol for **1c**). Each of the frozen mixtures was exposed to and kept under an $^{15}N_2$ atmosphere during the overnight reaction, followed by filtration and evaporation of the solvent. Resultant black residues of $^{15}N_2$-labeled **2b** and **2c** ($^{15}N_2$-**2b** and $^{15}N_2$-**2c**) were used to measure the ^{15}N NMR and FT-IR without further purification. ^{15}N{H} NMR (Toluene-d_8, 600 MHz): δ 22.0, –5.3 ($^{15}N_2$-**2b**); 22.6, –5.7 ($^{15}N_2$-**2c**). FT-IR (ATR, cm^{-1}): 1847 (N≡N, $^{15}N_2$-**2b**); 1859 (N≡N, $^{15}N_2$-**2c**).

Synthesis of [(C$_5$Me$_4$SiEt$_3$)$_3$Mo$_3$S$_4$Fe(N$_2$SiPh$_3$)] (3). *Method A*. In a nitrogen-filled glove box, THF (20 mL) was frozen by liquid nitrogen. Onto the frozen solvent, a black solid of **1c** (500 mg, 0.412 mmol) and KC_8 (130 mg, 0.961 mmol) were placed. The mixture was allowed to warm to room temperature with stirring overnight. The resultant dark-green solution was filtered and treated with $ClSiPh_3$ (134 mg, 0.455 mmol). After stirring at room temperature overnight, the reaction mixture was dried in vacuo and extracted with hexane (8 mL). Storage of the extract at –35˚C for a few days led to the formation of black crystals of [(C$_5$Me$_4$SiEt$_3$)$_3$Mo$_3$S$_4$Fe(N$_2$SiPh$_3$)] (**3**, 122 mg, 82.9 µmol, 20% yield based on **1c**). It should be noted that one of the ring-^{13}C signals was not observed. ^{1}H NMR (C_6D_6): δ 7.86 (Si*Ph*$_3$), 7.22 (Si*Ph*$_3$), 2.02 (C*Me*), 1.73 (C*Me*), 0.94 (Si*Et*$_3$). ^{13}C{^{1}H} NMR (C_6D_6): δ 135.5 (Si*Ph*$_3$), 113.8 (*C*Me), 105.6 (*C*Me), 16.1 (C*Me*), 12.9 (C*Me*), 8.3 (Si*Et*$_3$), 6.5 (Si*Et*$_3$). FT-IR (ATR, cm^{-1}): 1706 (N=N). ^{57}Fe Mössbauer spectrum (mm/s, 78 K): δ = 0.363(3), $|\Delta E_Q|$ = 0.906(5). *Note*. Preparation of $^{15}N_2$-labeled **3** was unsuccessful in spite of our multiple attempts. ^{15}N{^{1}H} NMR spectrum of cluster **3** is therefore not given here.

Method B. The formation of **3** from **2c** was monitored by the ^{1}H NMR as follows. Cluster **2c** (16.0 mg, 10.0 µmol) and ferrocene (3.8 mg, 0.02 mmol, internal standard for ^{1}H NMR) were dissolved into C_6D_6 (0.5 mL), followed by the addition of $ClSiPh_3$ (3.1 mg, 11 µmol). The reaction mixture was incubated for 2 h at room temperature. A comparison of integrated peak areas of consumed **2c** and produced **3** revealed a 54% conversion yield.

Note for unsuccessful elemental analyses of 2b, 2c, and 3. Elemental analyses of compounds **2b**, **2c**, and **3** were unsuccessful, even though we have measured at least ten times for **2b** and **2c** and five times for **3**. Significantly lower N contents in all cases suggest a loss of binding N_2 prior to or during combustion leading to thermal degradation. The addition of a combustion accelerator (WO_3 powder) did not improve the results, undermining the possibility of incomplete combustion. Despite the lack of the elemental analysis data of these compounds, other spectroscopic data support the isolation. Results are provided below for reference. Anal. Calcd. for $C_{50}FeH_{91}Mo_3N_2NaO_6S_4Si_3$ (**2b**): C, 43.03; H, 6.57; N, 2.01; S, 9.19. Found: C, 38.45-39.94; H, 5.827-5.893; N, 0.17-0.35; S, 7.315-8.307. Anal. Calcd. for $C_{59}FeH_{109}Mo_3N_2NaO_6S_4Si_3$ (**2c**): C, 46.57; H, 7.22; N, 1.841; S, 8.428. Found: C, 44.75-45.43; H, 6.636-6.807; N, 0.23-0.33; S, 6.377-8.101. Anal. Calcd. for $C_{63}FeH_{96}Mo_3N_2S_4Si_4$ (**3**): C, 51.62; H, 6.60; N. 1.91; S, 8.75. Found: C, 50.85-51.50; H, 6.465-6.680; N, 0.96-1.33; S, 6.777-9.386.

General Procedure for the Catalytic Reduction of N_2 into $N(SiMe_3)_3$ in the presence of $[Mo_3S_4Fe]$ cubes. A 100 mL round-bottom flask equipped with a three-way stopcock was charged with sodium dispersion (460 mg, 20.0 mmol), THF (13.4 mL), and a stirring bar to furnish a suspension. Black crystals of cluster **2c** (16.0 mg, 10.0 μmol) and $ClSiMe_3$ (2.54 mL, 195 mg, 20.0 mmol) were added to the mixture sequentially. The flask was attached to a balloon containing N_2 (1 atm), and the mixture was stirred at room temperature for 100 h. Cyclododecane (33.8 mg, 0.200 mmol) was added as an internal standard for gas chromatograph-mass spectrometry (GC-MS) analysis. After stirring for 5 min, the mixture was centrifuged, and the supernatant was subjected to GC-MS analysis.

Typical Procedure for Attempted Synthesis of NH_3 using N_2-clusters 2b and 2c. In a glove box filled with N_2, a 50 mL Schlenk flask was charged with **2c** (3.9 mg, 2.5 μmol), $[H(OEt_2)_2]BAr^F{}_4$ (466 mg, 460 μmol), and KC_8 (67.4 mg, 500 μmol) and then cooled to –78°C. Cold Et_2O (5 mL, −78 °C) was added to the mixture. After stirring at −78 °C for 1 h, the mixture was warmed to room temperature and further stirred at room temperature for 20 min. The amount of dihydrogen of the catalytic reaction was determined by GC analysis. The reaction mixture was evaporated under reduced pressure, and the distillate was trapped in dilute H_2SO_4 solution (0.5 M, 5 mL). Et_2O (2 mL) and aqueous solution of potassium hydroxide (30 wt%, 3 mL) were added to the residue, and the mixture was distilled into the same H_2SO_4 solution. The amounts of $NH_3$and N_2H_4 were determined by means of color reaction.[41,42] As summarized in Supplementary Table 4, the NH_3/N_2H_4 yields remained substoichiometric with respect to the clusters.

Attempted trapping experiment: CO exposure to a catalytic reaction mixture containing $[Mo_3S_4Fe]$ cube. To gain insight into the $[Mo_3S_4Fe]$ species during catalysis, we first conducted a CO trapping experiment

using the original catalytic conditions with 2000 eq. sodium dispersion and $ClSiMe_3$. However after 48 h, the catalytic reaction mixture led to the formation of a significant amount of oily organic products (*e.g*. $Me_3Si(CH_2)_4OSiMe_3$), which were inseparable from the Mo-Fe-S cluster species and hampered spectroscopic characterizations by the ^1H NMR. Thus, the following CO-trapping experiment employed less amounts of sodium dispersion and $ClSiMe_3$ with a shorter reaction time. A THF suspension containing **1c** (10.0 μmol), $ClSiMe_3$ (2.0 mmol), and sodium dispersion (2.0 mmol) was stirred for 24 h under N_2. The reaction mixture was then evaporated into dryness to remove volatile compounds (*e.g.* THF and $ClSiMe_3$) and re-dissolved into THF (1.4 mL). The resultant solution was exposed to 1 atm of CO and stirred for 24 h, followed by removing the solvent in vacuo to leave a brown oil. Its ^1H NMR spectrum in C_6D_6 (Supplementary Fig. 24) exhibited a characteristic signal of the CO-adduct $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (**5**) at δ 12.2 ppm, which corresponds to a yield of 11% to **1c**. This signal was assigned by comparison with an authentic sample, in addition to the CO band in the IR spectrum, and the yield of **5** was calculated based on the peak area relative to the internal standard (ferrocene).

Synthesis of $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (5). In an argon-filled glove box, a solution of $Fe_2(CO)_9$ (85 mg, 235 μmol) in THF (20 mL) was added to a THF (14 mL) solution of $[(C_5Me_4SiEt_3)_3Mo_3S_4]$ (**4c**; 200 mg, 177 μmol). The reaction mixture was stirred under UV irradiation at room temperature for 24 h. The resultant greenish brown mixture was evaporated to dryness under reduced pressure, followed by dissolving into hexane (5 mL). The solution was filtered and placed onto a column (1.5 x 15 cm) packed with neutral alumina (70-230 mesh, sigma-aldrich). An olive green band eluted by hexane was collected and dried in vacuo, and the resultant residue was dissolved into pentane (4 mL). Crystallization of the solution at –30˚C for a day gave black crystals of $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (**5**, 39 mg, 32 μmol, 18 %). ^1H NMR (C_6D_6, 400 MHz, ppm): δ 12.2 (br, 18H, CCH_3), 6.97 (br, 18H, CCH_3), 1.17 (br, 27H, $SiCH_2CH_3$), 0.57 (br, 18H, $SiCH_2CH_3$). FT-IR (ATR, cm^{-1}): 1877 (CO). Anal. Calcd. for $C_{46}FeH_{81}Mo_3OS_4Si_3$: C, 45.80; H, 6.77; S, 10.63. Found: C, 45.71; H, 6.75; S, 10.28.

X-ray Crystallographic Structure Determinations. Crystal data and refinement parameters of clusters **2a**, **2c**, **3c**, and **5** are listed in Supplementary Table 5. Single crystals were covered with oil (Immersion Oil, type-B: code 1248, Cargile Laboratories, Inc.) and mounted on nylon loops. Diffraction data were collected under a cold N_2 stream (–100˚C for **2a** and **3**, –150˚C for **2c**), on a Rigaku RA-Micro 7 equipped with a PILATUS 200K detector, using graphite-monochromated Mo Kα radiation (λ = 0.710690 Å). Eighteen preliminary images were taken at 0.5˚ increments of ω to evaluate the crystal quality and to determine pre-refined unit cell parameters, followed by full data collection also with 0.5˚ increments of ω. The raw

frame data were processed using CrystalClear program, and the data sets were corrected for absorption using the REQAB program. Calculations were performed with the CrystalStructure program package and Shelxl programs. All structures were solved by direct methods and refined by full-matrix least-square techniques. All non-hydrogen and non-disordered atoms were refined anisotropically. A riding model was used to place hydrogen atoms. The structural analysis of **2a** revealed large thermals for THF molecules on K atoms, giving rise to multiple Alert Bs in automatic cif-check program. Nevertheless, we should not use various restraints to force the thermal parameters low, because these THFs reside in a wide slot and are weakly bound to K. It is natural for these THFs to occupy a lot of space to flop around. In the structural analysis of **2b**, methyl hydrogen atoms on C6 and C38 ($C_5\mathit{Me}_4SiEt_4$) were added at calculated positions, while this process inevitably led to the short H…H contacts and the appearance of an Alert B in the automatic cif-check program. In the unit cell of **3**·(hexane)$_{0.93}$, there are two crystallographically independent molecules of **3**, in addition to one entire solvent (hexane) molecule and five sites for a solvent carbon chain. The five sites span unit cells forming a crystal-transiting helix. In the infinite chain, a hexane molecule and a black fill 7 (6+1) successive sites. The pattern repeats after 5 cycles, and therefore 30 (6x5) carbon atoms are stored in 35 (7x5) sites, leading to the 6/7 (30/35) occupancy for carbon atoms and the formula of **3**·(hexane)$_{0.93}$. Some hydrogen atoms in the infinite chain could not be specified, resulting in the appearance of two Alert Bs in the automatic cif-check program. One of the two independent molecules of **3** revealed residual electron densities for the nitrogen atoms, which were refined to 14.7% occupancy. As the corresponding electron density for silicon was absent around the *distal* nitrogen atom of the minor component, which is also away from the silicon atom of the major component, we concluded that one of two molecules of **3** is partially replaced by **2c** (or its oxidized form) as a minor component. Therefore the metrical parameters of the other molecule of **3** was used for discussion. An OMIT command was used to eliminate nine diffractions, as the diffraction images of **3** showed some patterned spots of satellite crystal(s). In the structure of **5**, the bulky $C_5Me_4SiEt_3$ ligands on Mo prevent the aggregation of the $[Mo_3S_4Fe]$ clusters but instead they lead to weak packing forces. In addition, the longer Si-C bonds compared to carbon-carbon bonds results in smaller intramolecular forces. Thus, many of the thermal parameters of **5** are large, especially for the $SiEt_3$ groups, and some disorder also occurs in these groups. We have used restraints to reduce these thermal parameters, attempting to minimize Alerts appearing in an automatic checkCIF program, with partial success. However, large thermal parameters and some disorder are fundamental properties of this type of compound even though checkCIF Alerts are generated. In this case, two level B alerts remain which refer to thermal parameters of the Si11 and the connected carbon atoms. In spite of these large thermals in the periphery of the molecule, the structure of the

chemically interesting core with an Fe-CO moiety is well established. The atomic coordinates were deposited with the Cambridge Crystallographic Data Centre, Cambridge CB2 1EK, UK under reference numbers CCDC 2079174-2079176 and 2141451.

Computational methods. Geometry optimizations were performed using the density functional theory, including the ZORA scalar relativistic method implemented in the ORCA program (Version 4.2.1)[43]. The BP86 functional[44,45], employing the Grimme's dispersion with Becke-Johnson damping[46,47], ZORA-def2-TZVP basis sets and SARC/J auxiliary basis sets were used[48-50]. The increased integration grids (Grid6) and the tight SCF criteria were applied for all calculations. The Conductor-like continuum polarization model (C-PCM) was used as the implicit solvent model, where tetrahydrofuran solvent was applied[51]. Vibrational frequency calculations were performed to confirm that the optimized structures were local minima (*i.e.* no imaginary frequencies). The Mössbauer parameters were computed using the B3LYP functional[52-55], CP(PPP) basis sets for Fe[32,56], and DKH-def2-TZVP for the remaining atoms[49,50]. For the isomer-shift calculations, α = 0.1706325, β = 0.332 26751, and C = 23615 values were employed[57]. Kohn-Sham orbitals and Mayer bond orders[58] were calculated using the ADF program[59]. The BP86-D3BJ functional, TZ2P[49,50] basis sets for all electrons in the system, and the relativistic Scalar ZORA[60] approach was applied for Mo and Fe. The COSMO[61-63] method, employing tetrahydrofuran solvent, was used as the implicit solvent model.

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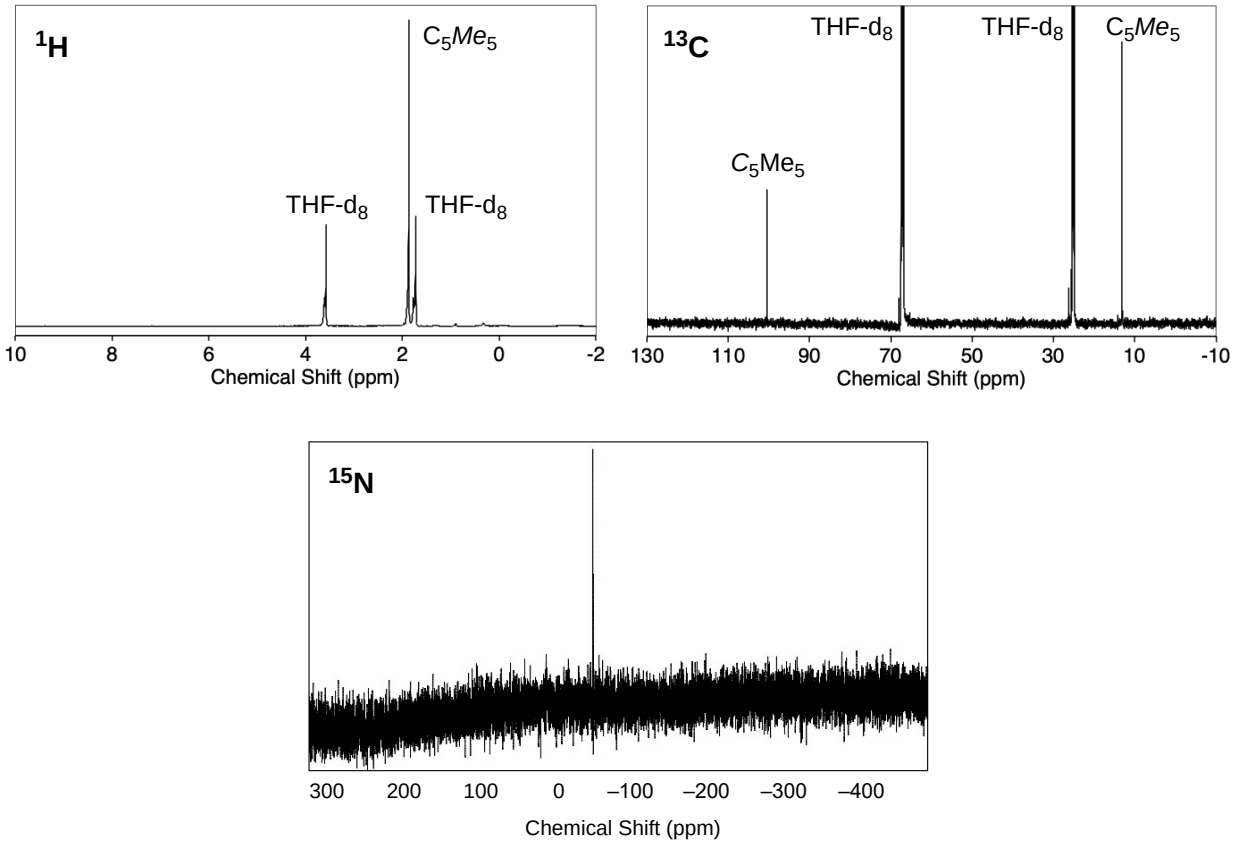
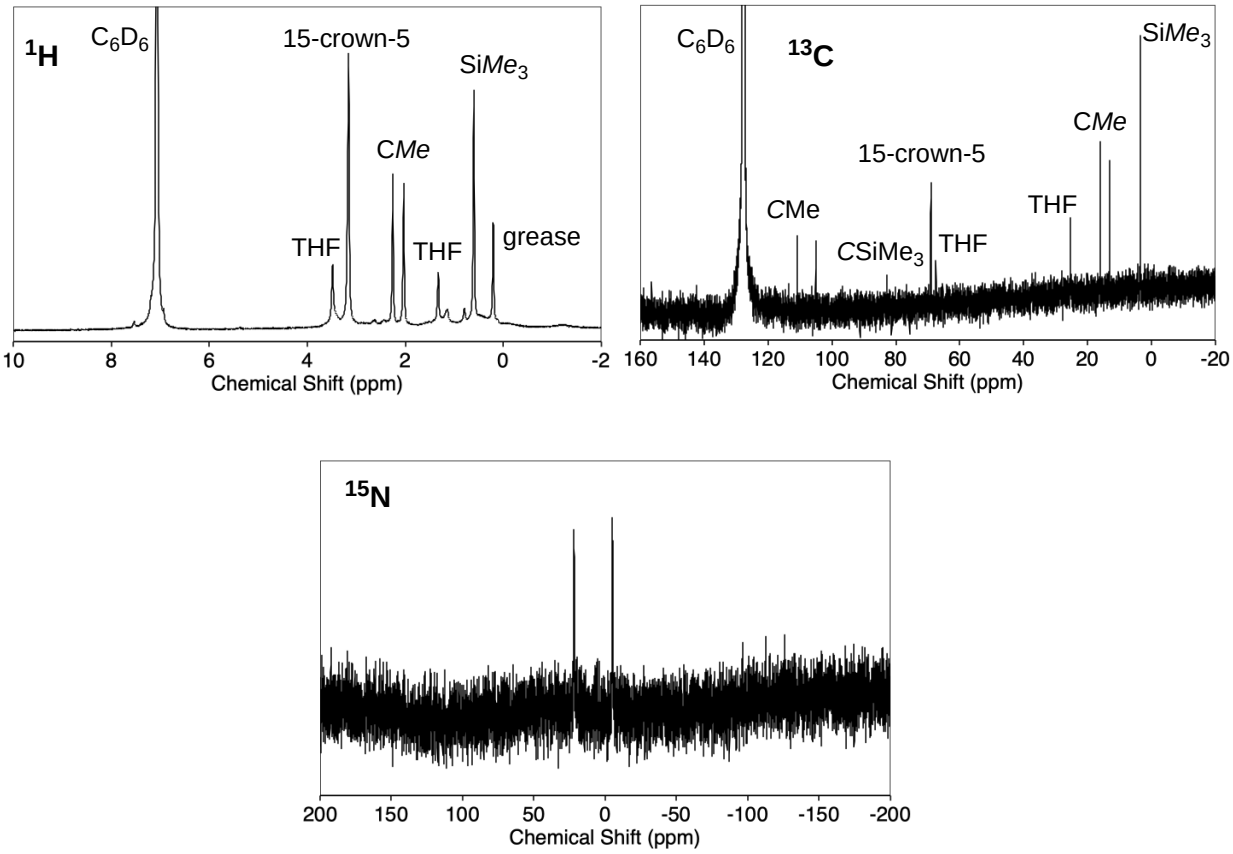
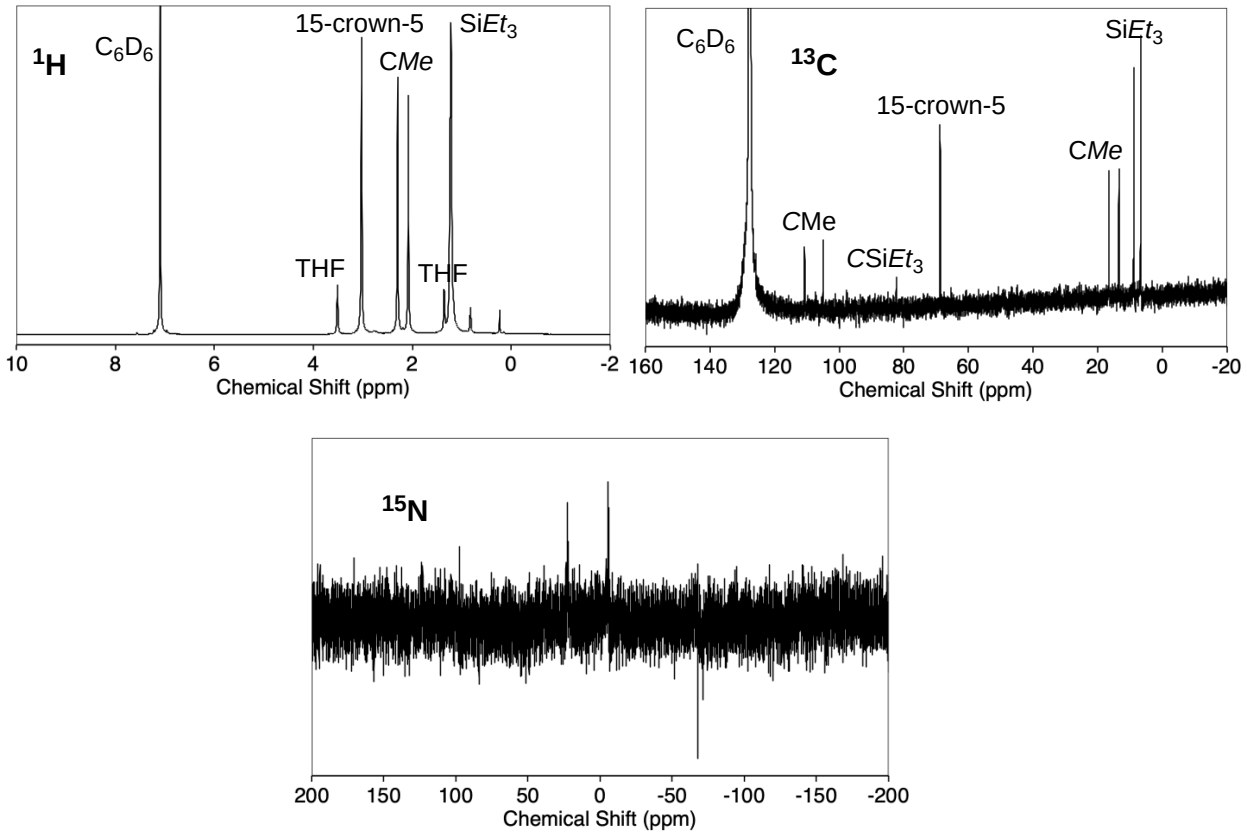


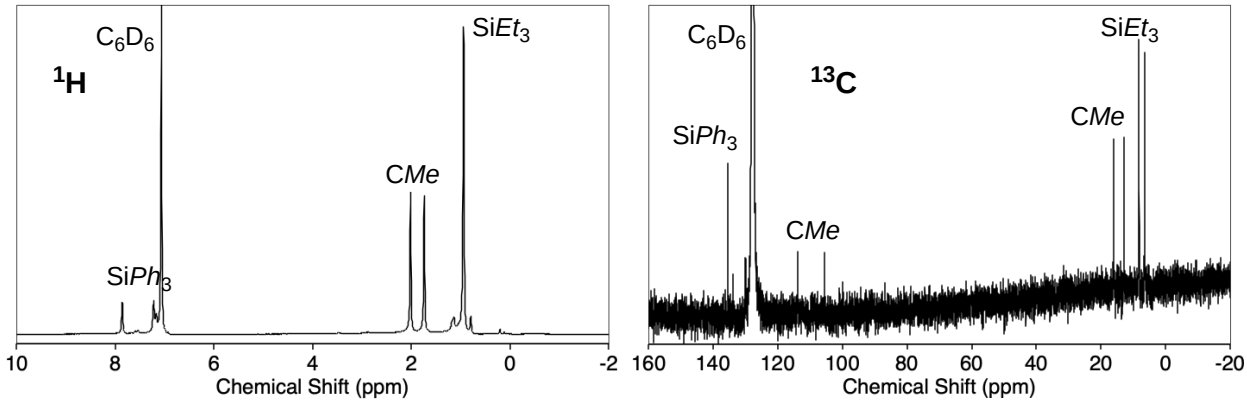
Supplementary Fig. 1. NMR spectra of $[K(THF)_2]_2[\{Cp^*_3Mo_3S_4Fe\}_2(\mu\text{-}N_2)]$ (**2a**); ^1H and $^{13}C\{^1H\}$ NMR in THF-d_8 at room temperature and $^{15}N\{^1H\}$ NMR spectrum in toluene-d_8 at –50°C.



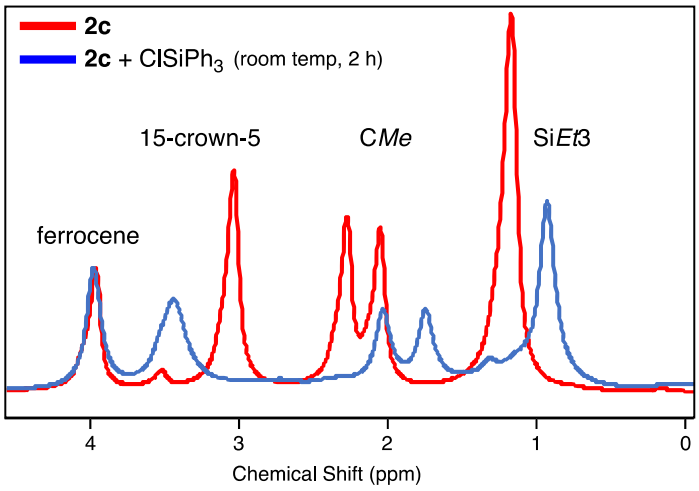
Supplementary Fig. 2. NMR spectra of [Na(15-crown-5)(THF)][($C_5Me_4SiMe_3$)$_3$$Mo_3S_4Fe(N_2)$] (**2b**); H and $^{13}C\{^1H\}$ NMR in C_6D_6 and $^{15}N\{^1H\}$ NMR spectrum in toluene-d_8 at room temperature.



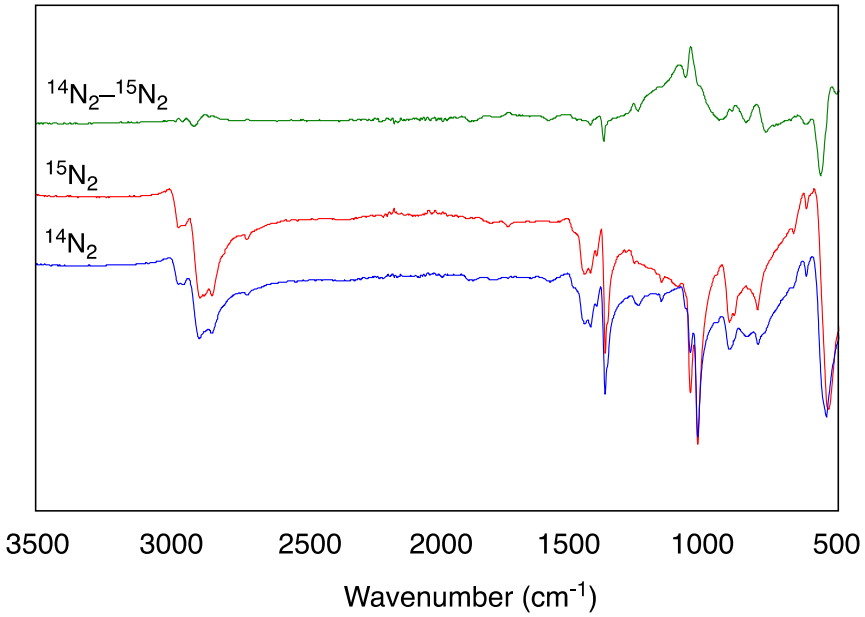
Supplementary Fig. 3. NMR spectra of [Na(15-crown-5)(THF)][$(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2)$] (**2c**); ^{1}H and $^{13}C\{^{1}H\}$ NMR in C_6D_6 and $^{15}N\{^{1}H\}$ NMR spectrum in toluene-d_8 at room temperature. The methylene and methyl signals of $SiEt_3$ were overlapped in the ^{1}H NMR.



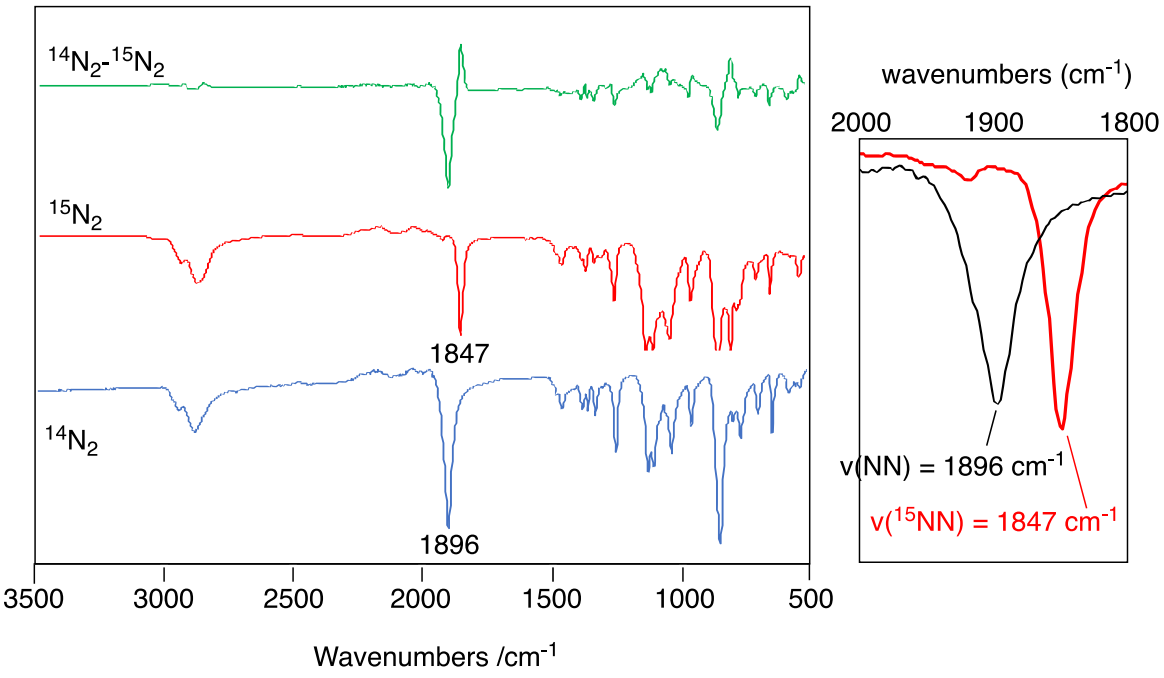
Supplementary Fig. 4. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2SiPh_3)]$ (**3**) in C_6D_6 at room temperature. Preparation of $^{15}N_2$-labeled **3** was unsuccessful in spite of our multiple attempts. $^{15}N\{^{1}H\}$ NMR spectrum of cluster **3** is therefore not given here. The methylene and methyl signals of $SiEt_3$ were overlapped in the ^{1}H NMR.



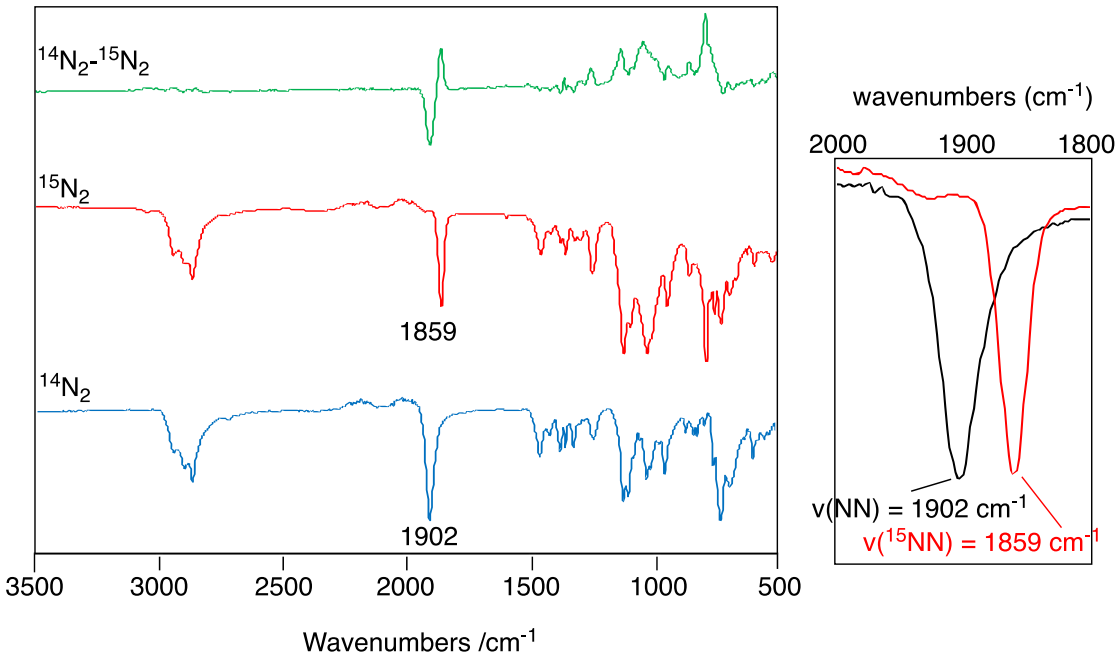
Supplementary Fig. 5. ^{1}H NMR monitoring experiment of the reaction of **2c** with $ClSiPh_3$ (1.1 equiv.) in C_6D_6 at room temperature, leading to the formation of **3** after 2 h. Ferrocene is added as an internal standard.



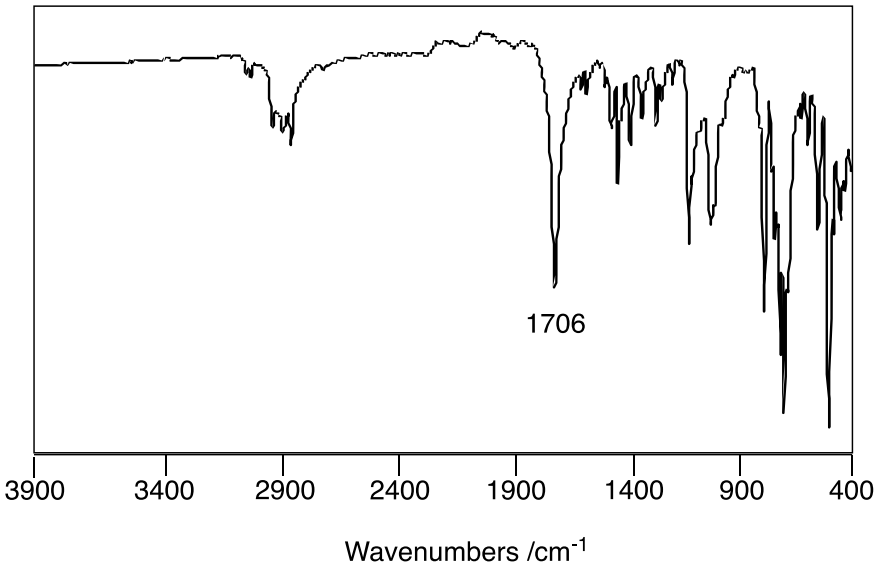
Supplementary Fig. 6. IR spectra of **2a** (blue), ^{15}N-labeled **2a** (red), as well as the corresponding difference spectrum (green). Note that the N-N band for the symmetric Fe-NN-Fe moiety is inactive in the IR spectrum, and thus does not clearly appear in the difference spectrum (green). Despite our effort to record a resonance-Raman spectrum of **2a** and ^{15}N-labeled **2a**, we have been unsuccessful to detect a meaningful N–N stretching band.



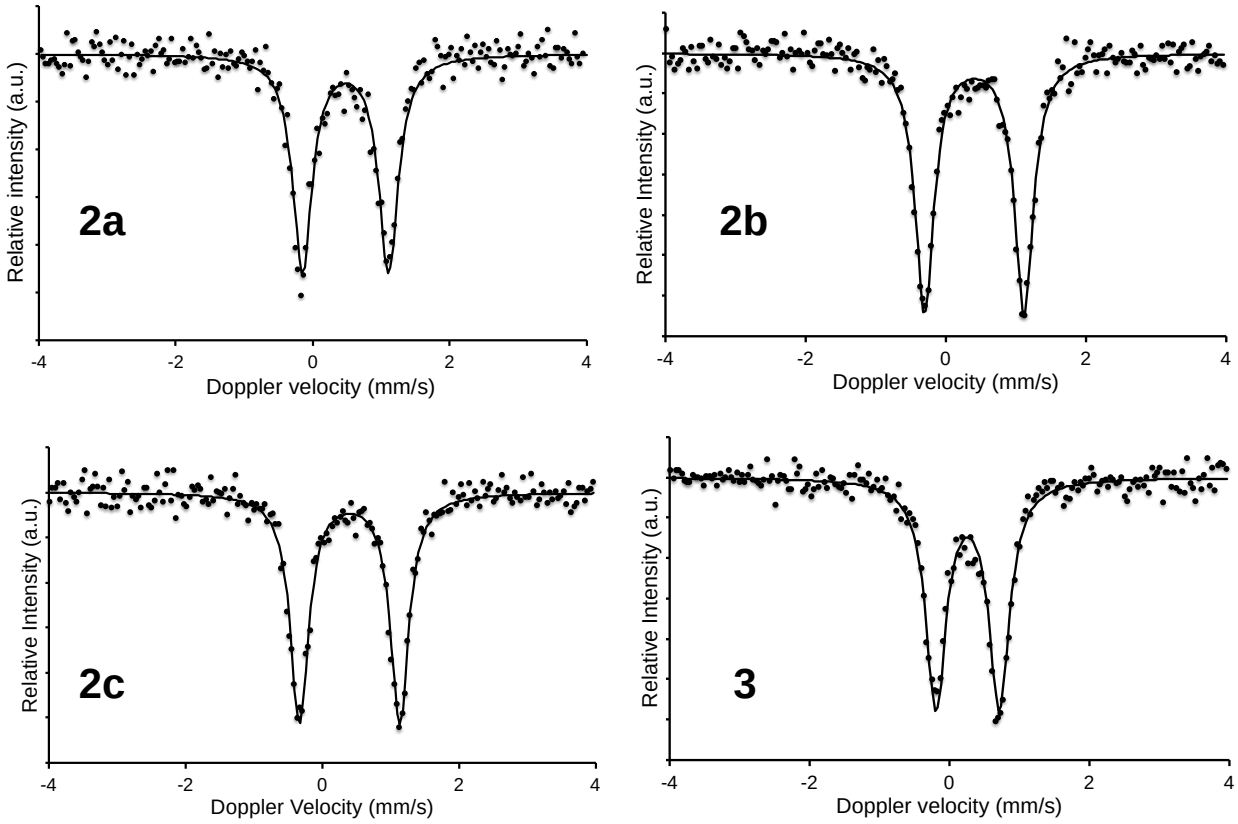
Supplementary Fig. 7. IR spectra of **2b** (blue), ^{15}N-labeled **2b** (red), as well as the corresponding difference spectrum (green). Expanded spectrum of the N-N band is shown in the right figure.



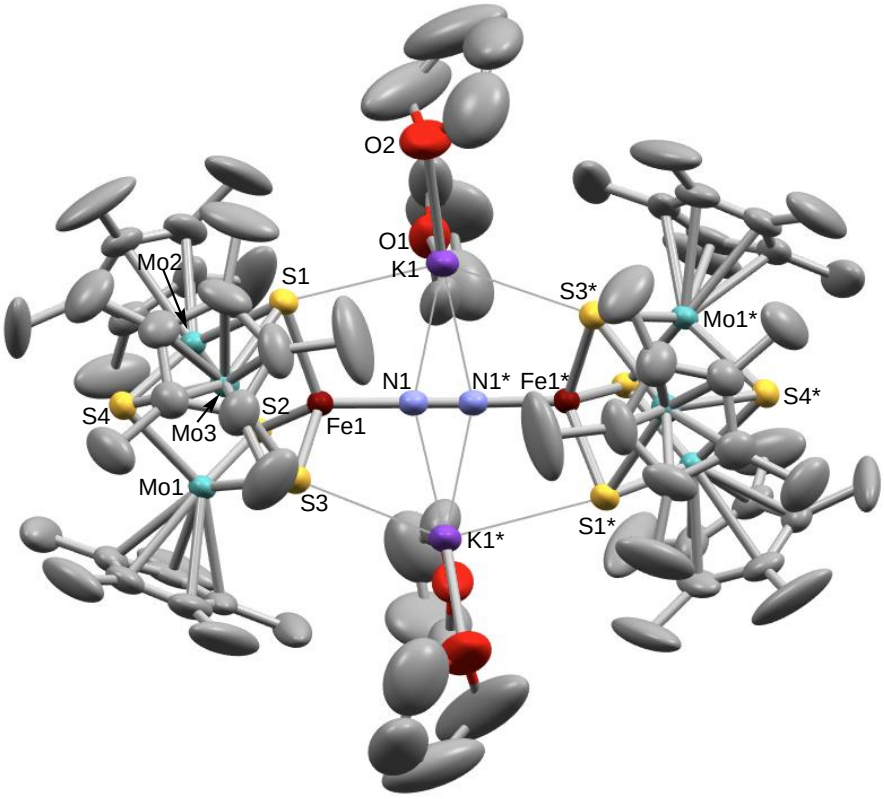
Supplementary Fig. 8. IR spectra of **2c** (blue), ^{15}N-labeled **2c** (red), as well as the corresponding difference spectrum (green). Expanded spectrum of the N-N band is shown in the right figure.



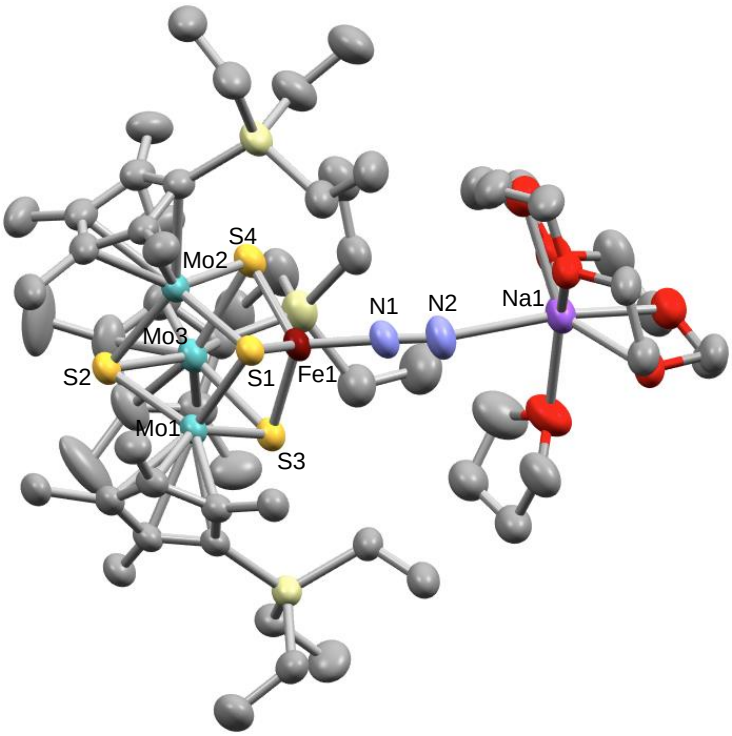
Supplementary Fig. 9. IR spectrum of **3**. Preparation of $^{15}N_2$-labeled **3** was unsuccessful in spite of our multiple attempts.



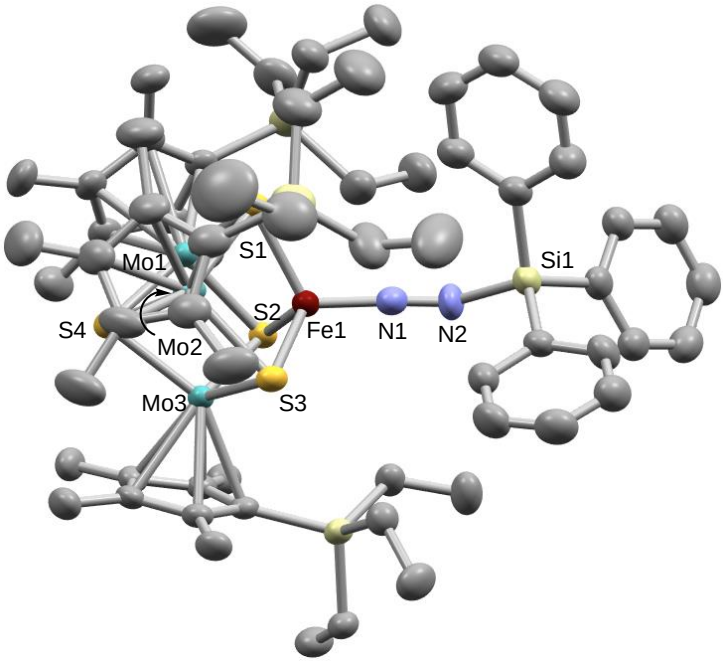
Supplementary Fig. 10. ^{57}Fe Mössbauer spectra of **2a**, **2b**, **2c**, and **3** at 78 K and zero-field.



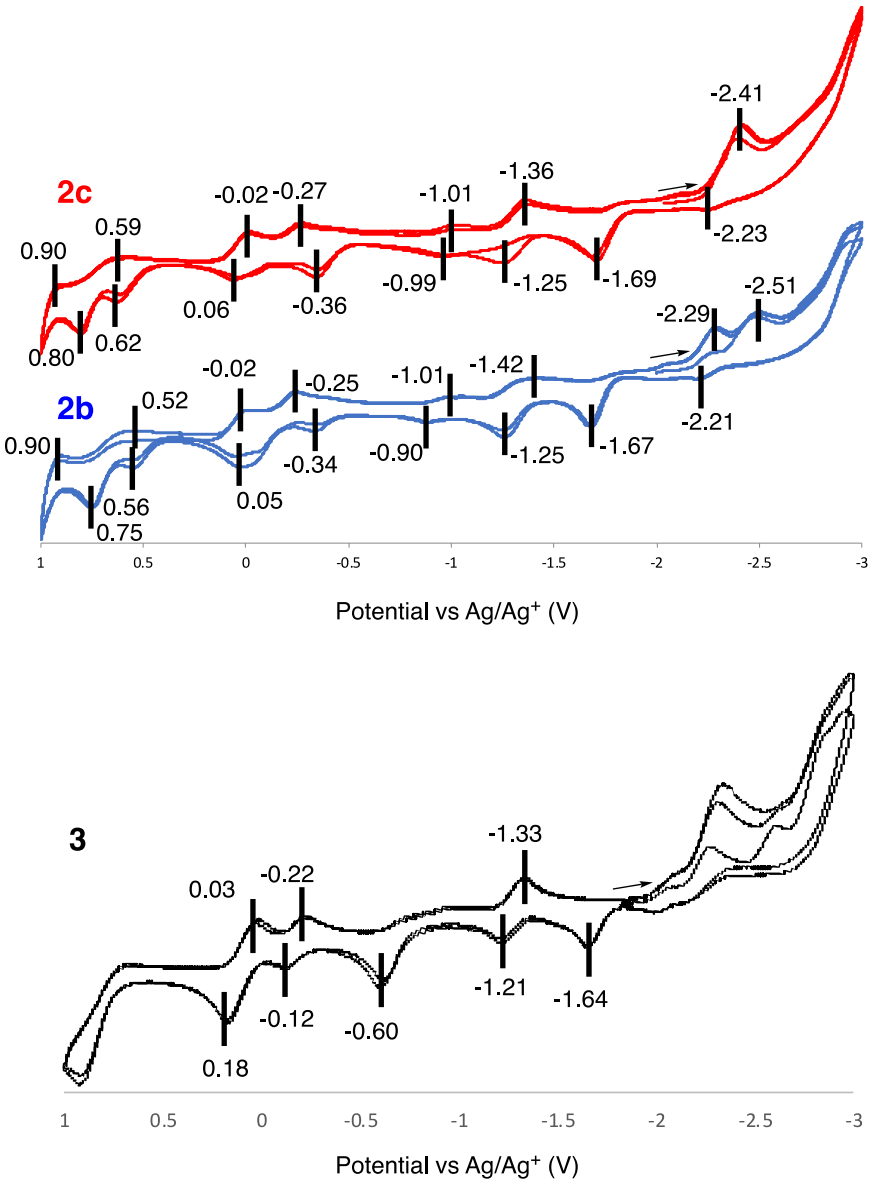
Supplementary Fig. 11. Structure of **2a** with thermal ellipsoids set at the 50% probability level. Selected Bond lengths (Å) and angles (˚): Fe1-N1 1.817(3), N1-N1* 1.151(6), Fe1-S1 2.1968(12), Fe1-S2 2.186(2), Fe1-S3 2.1958(16), Fe1-Mo1 2.7878(7), Fe1-Mo2 2.7851(10), Fe1-Mo3 2.7773(18), Mo1-S2 2.3547(17), Mo1-S3 2.3562(16), Mo1-S4 2.3400(12), Mo2-S1 2.3521(14), Mo2-S2 2.3556(12), Mo2-S4 2.3444(14), Mo3-S1 2.3521(13), Mo3-S3 2.3568(12), Mo3-S4 2.3389(13), N1-K1 2.786(3), N1*-K1 2.793(3), S1-K1 3.1969(16), S3-K1* 3.2820(19), N1*-N1-Fe1 171.77(12), N1-Fe1-S1 111.39(11), N1-Fe1-S2 114.66(12), N1-Fe1-S3 109.27(11).



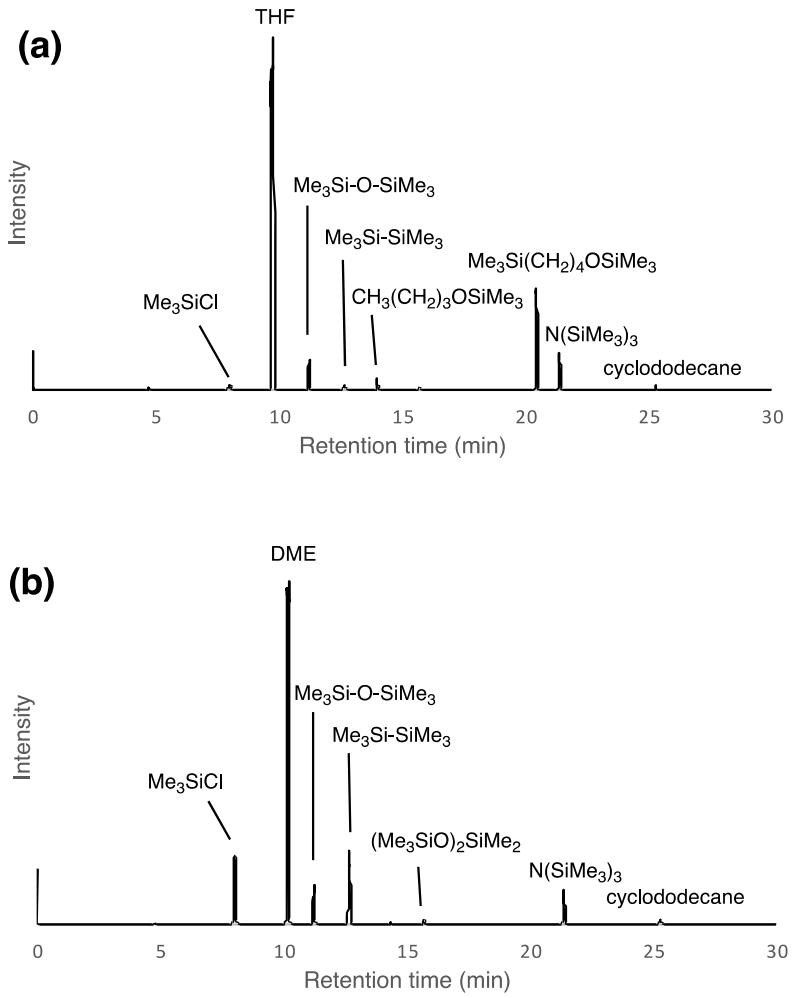
Supplementary Fig. 12. Structure of **2c** with thermal ellipsoids set at the 50% probability level. Selected Bond lengths (Å) and angles (˚): Fe1-N1 1.763(4), N1-N2 1.136(5), N2-Na1 2.496(5), Fe1-S1 2.1921(12), Fe1-S3 2.1898(13), Fe1-S4 2.1991(14), Fe1-Mo1 2.7773(7), Fe1-Mo2 2.7955(8), Fe1-Mo3 2.7823(8), Mo1-S1 2.3473(11), Mo1-S2 2.3338(12), Mo1-S3 2.3659(12), Mo2-S1 2.3535(12), Mo2-S2 2.3387(11), Mo2-S4 2.3497(12), Mo3-S2 2.3389(12), Mo3-S3 2.3374(13), Mo3-S4 2.3603(12), N2-N1-Fe1 178.1(4), N1-N2-Na1 164.9(4), N1-Fe1-S1 113.22(14), N1-Fe1-S3 108.47(14), N1-Fe1-S4 113.87(15).



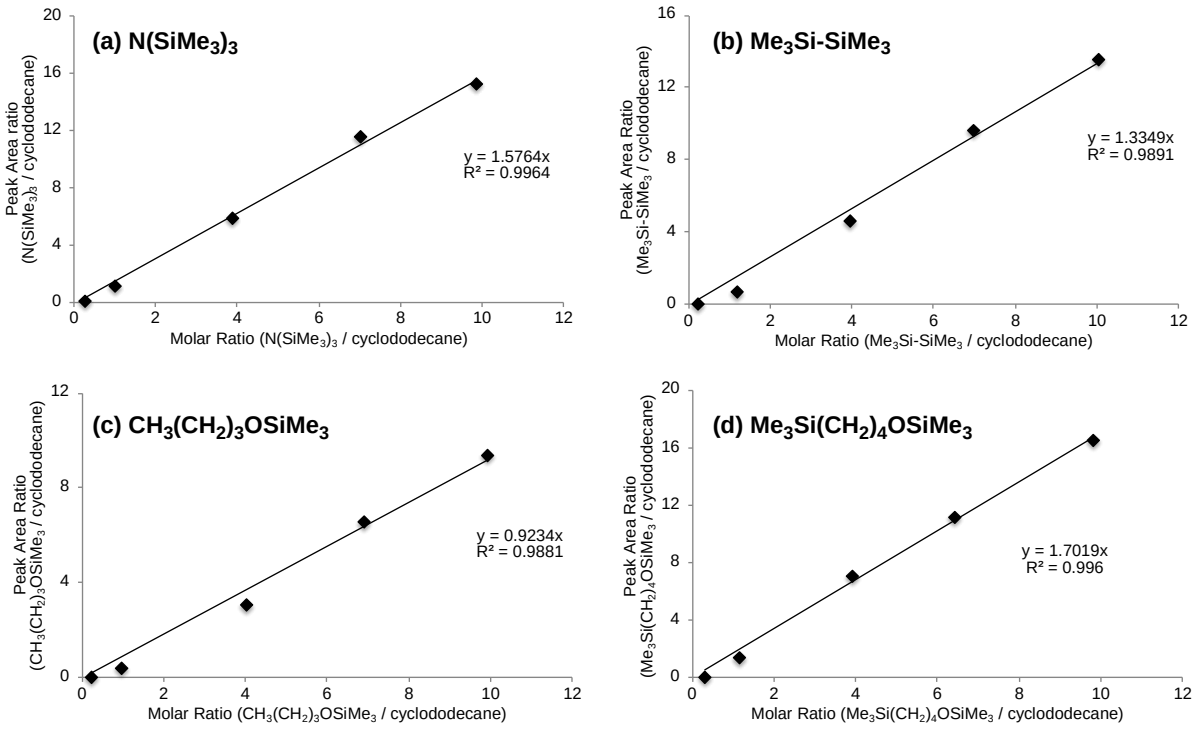
Supplementary Fig. 13. Structure of **3** with thermal ellipsoids set at the 50% probability level. One of two crystallographically independent molecules is shown. Selected Bond lengths (Å) and angles (˚): Fe1-N1 1.687(5), N1-N2 1.193(7), N2-Si1 1.755(5), Fe1-S1 2.2140(15), Fe1-S2 2.1910(15), Fe1-S3 2.2042(15), Fe1-Mo1 2.7818(9), Fe1-Mo2 2.8070(9), Fe1-Mo3 2.7601(9), Mo1-S1 2.3493(15), Mo1-S2 2.3308(13), Mo1-S4 2.3424(14), Mo2-S1 2.3434(14), Mo2-S3 2.3408(14), Mo2-S4 2.3525(15), Mo3-S2 2.3265(13), Mo3-S3 2.3465(14), Mo3-S1 2.3428(13), N2-N1-Fe1 171.8(5), N1-N2-Si1 133.4(5), N1-Fe1-S1 117.12(16), N1-Fe1-S2 106.33(17), N1-Fe1-S3 113.51(17).



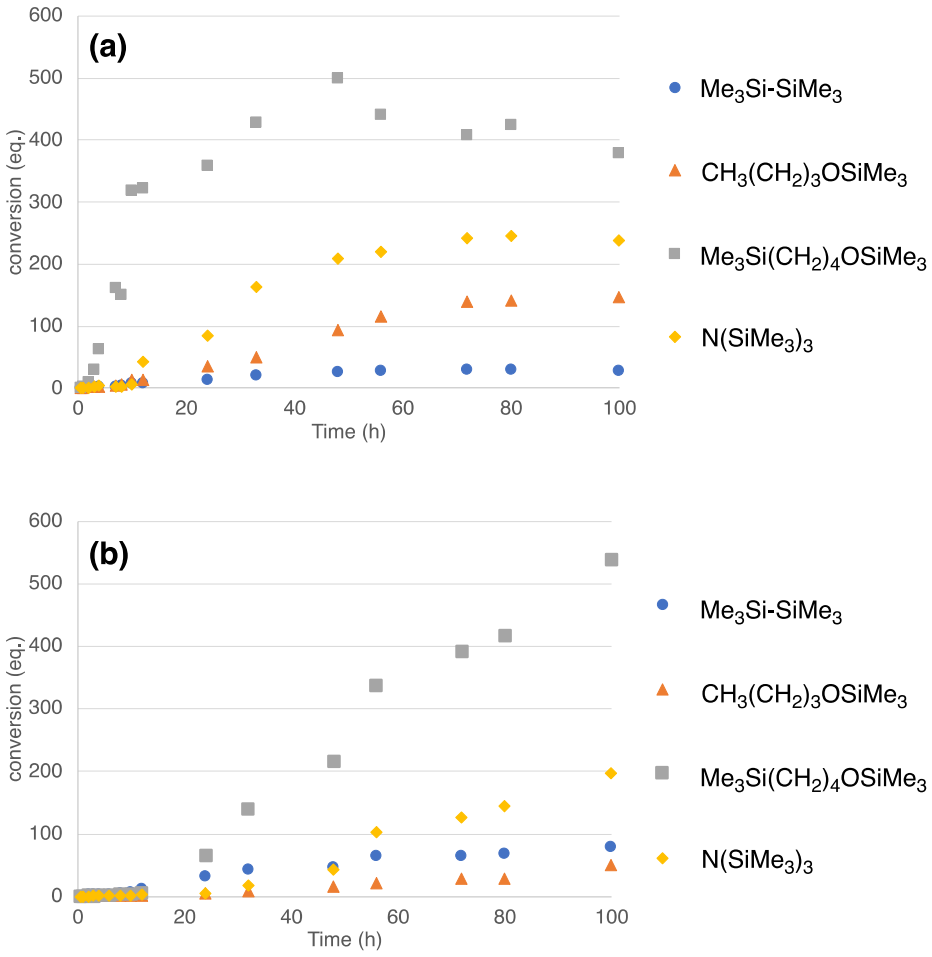
Supplementary Fig. 14. Preliminary cyclic voltammograms of clusters **2b**, **2c**, and **3** in THF at room temperature. Partial decomposition of the N_2-clusters may occur in the presence of large excess of electrolyte. The voltammogram of **2a** was not measured. Although we have been unable to assign complicated waves in the voltammograms, similarity between **2b** and **2c** supports their homology and indicates analogous electronic structures. Conditions: sample concentration, 4 mM; solvent, THF; working electrode, glassy carbon; counter electrode, Pt; reference electrode, Ag/Ag(NO_3) (0.01 M in acetonitrile) separated from the working compartment by a Vycor glass membrane; scan rate, 0.02 V/s (**2b** and **2c**) or 0.1 V/s (**3**); supporting electrolyte, [N^nBu_4][PF_6] (0.2 M).



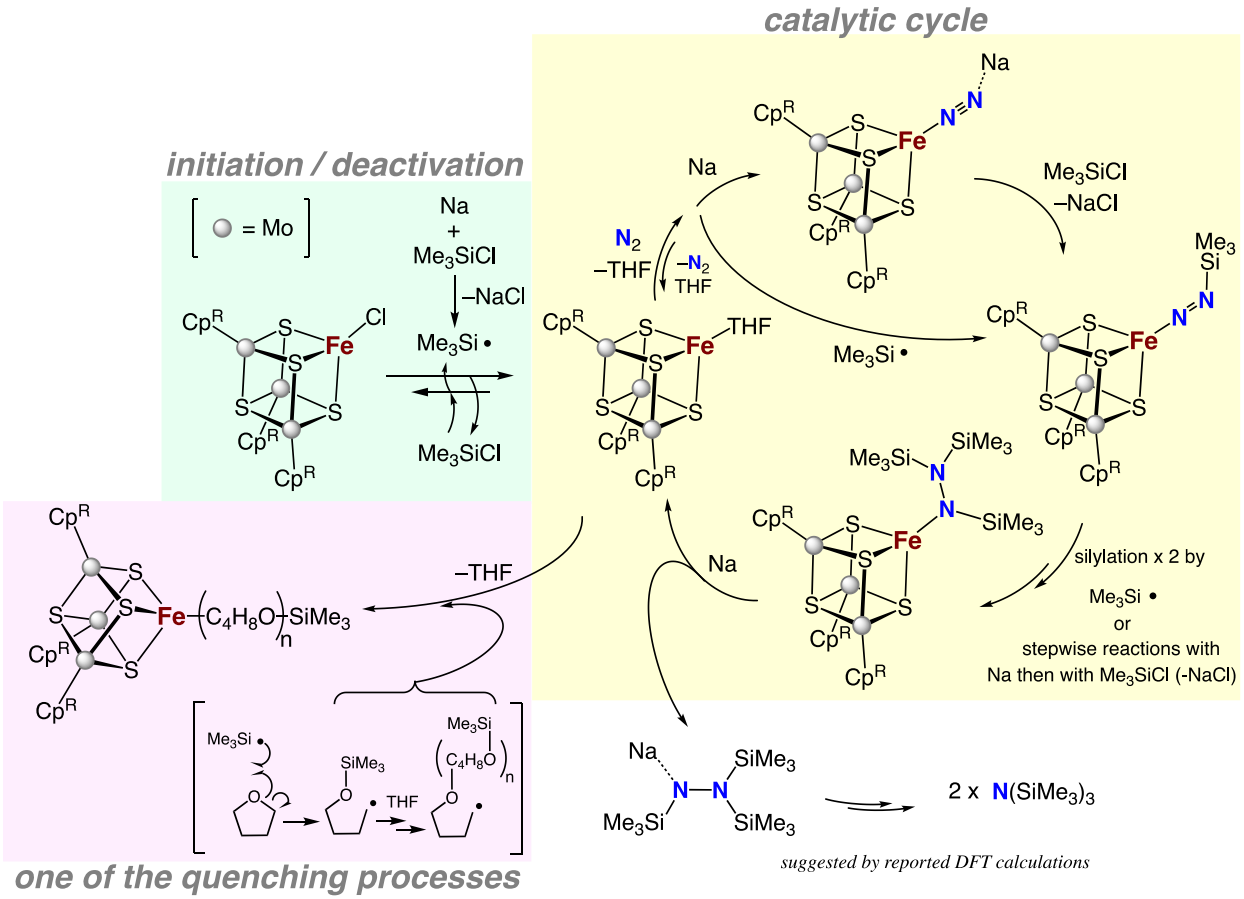
Supplementary Fig. 15. Representative GC charts of the reaction products of (a) Supplementary Table 1, entry 3, and (b) Supplementary Table 1, entry 4.



Supplementary Fig. 16. Calibration curves for quantification of (a) $N(SiMe_3)_3$, (b) $Me_3Si\text{-}SiMe_3$, (c) $CH_3(CH_2)_3OSiMe_3$, and (d) $Me_3Si(CH_2)_4OSiMe_3$.

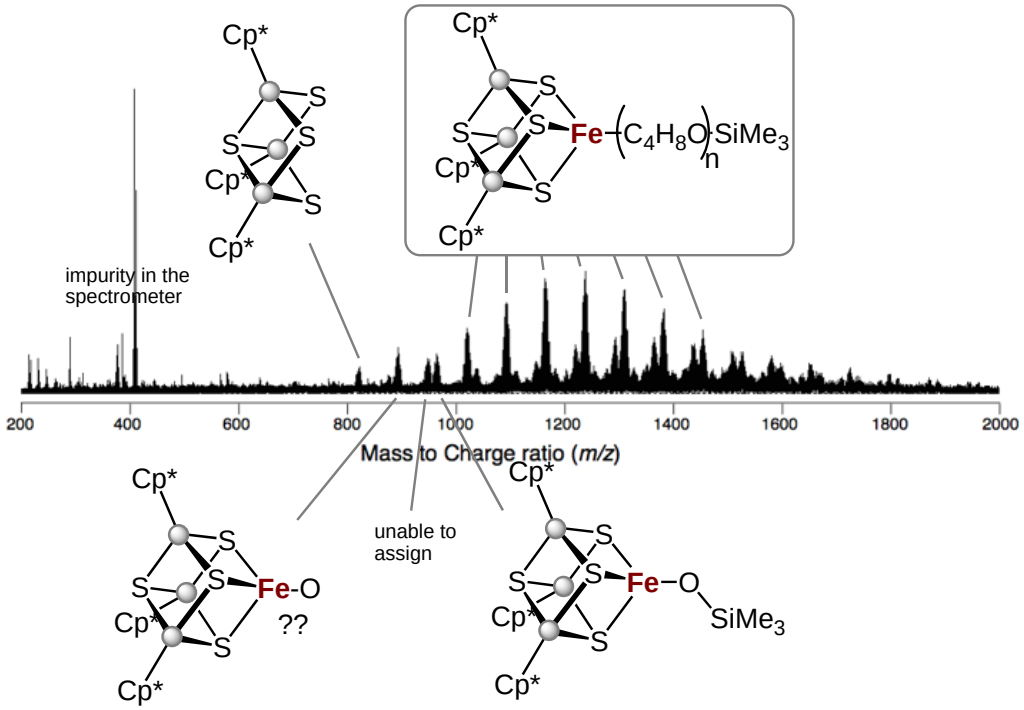


Supplementary Fig. 17. Time-profiles for the formation of silylated products in the reaction of N_2 (1 atm) with Na and $ClSiMe_3$ in the presence of catalytic amounts of (a) cluster **1b** or (b) cluster **2c** in THF. The same conditions as for entries 2 and 7 in Supplementary Table 1 were applied.

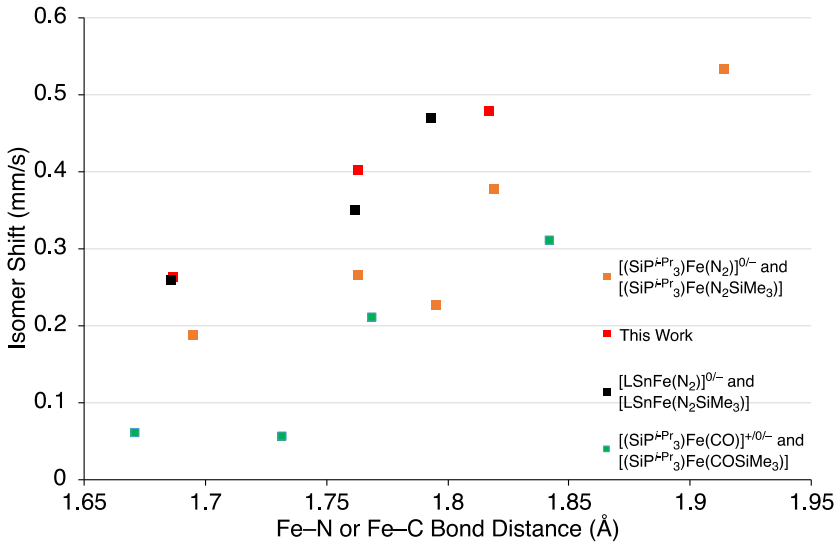


Supplementary Fig. 18. Proposed catalytic cycle for silylation of N_2 by [Mo_3S_4Fe] cubes.

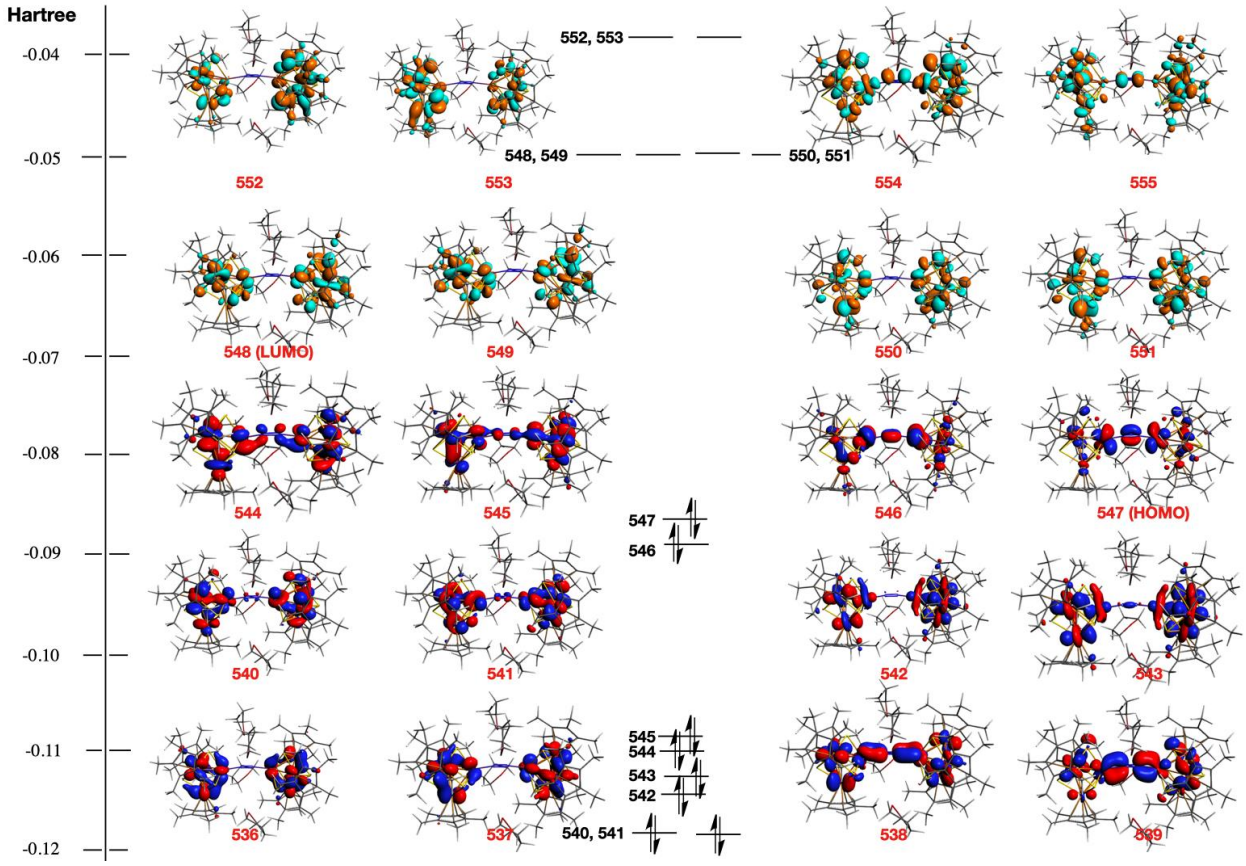
In the proposed catalytic cycle (yellow background), the Fe-NN···Na cluster (top in the cycle) has been synthesized as **2b** and **2c**. An analogue of the Fe-NN-$SiMe_3$ intermediate (right in the cycle) has been obtained in the form of Fe-NN-$SiPh_3$ cluster **3**. The Fe-N($SiMe_3$)-N($SiMe_3$)$_2$ cluster (bottom in the cycle) is a speculated intermediate, based on the reported DFT studies on Mo-[25] and Co-catalyzed[27] silylation of N_2. The formation of Fe-THF (or Fe-N_2) cluster species (left or upper left in the cycle) has been implied by the CO-trapping experiment (Supplementary Fig. 24), where a low yield of Fe-CO cluster **5** was observed. A quenching process (pink background) was indicated by the ESI-MS measurement of the reaction mixture after catalysis (Supplementary Fig. 19).



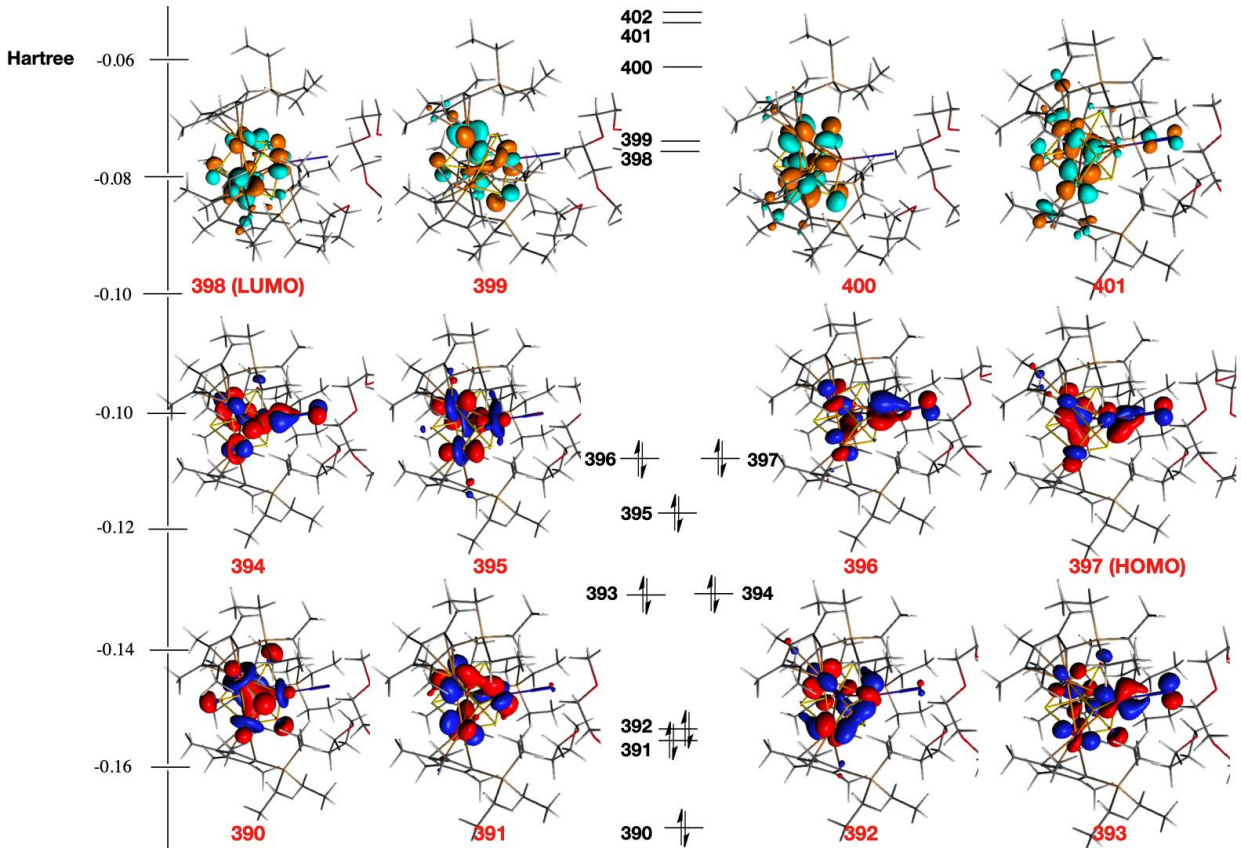
Supplementary Fig. 19. Electro-Spray-Ionization mass spectrum (ESI-MS) of the mixture after 100 h catalysis with **1a**. The same condition as for entry 1 in Supplementary Table 1 was applied. A series of signals with repeated patterns are assignable as [Mo_3S_4Fe] cubes binding ring-opened products of THF (-$(C_4H_8O)_nSiMe_3$).



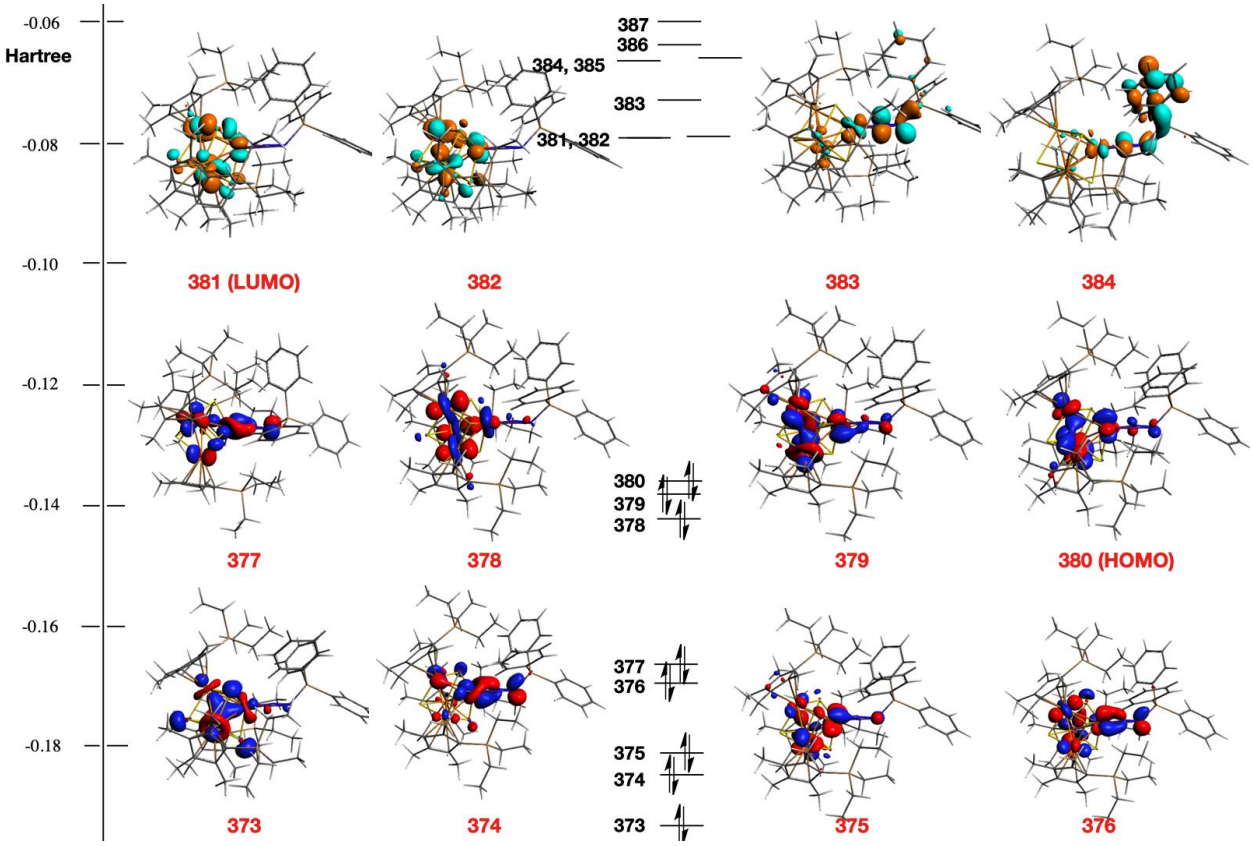
Supplementary Fig. 20. Pseudo-linear relationship between the isomer shifts (Mössbauer spectrum) and the Fe-N or Fe-C distances. SiP$^{i\text{-}Pr}_3$ = [Si(*o*-C$_6$H$_4$P^{i}Pr$_2$)$_3$]$^-$,[29,64] L = [N(*o*-(NCH$_2$P^{i}Pr$_2$)(C$_6$H$_4$)$_3$]$^{3-}$.[32]



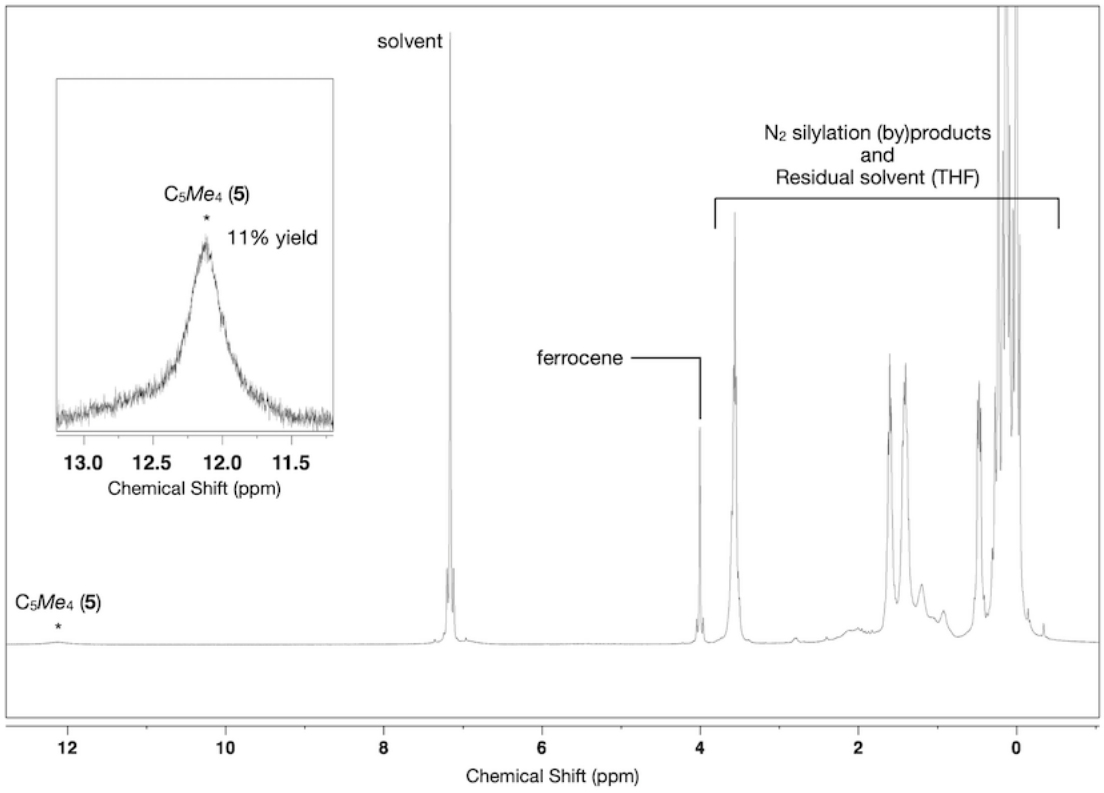
Supplementary Fig. 21. Kohn-Sham frontier orbitals of the *S* = 0 state optimized structure of **2a**. The degenerate 548, 549, 550, and 551 Kohn-Sham orbitals show some Fe-d_{xy} or Fe-d_{x2-y2} characters, which are unoccupied and mixed with the Mo orbitals. As the occupied orbitals are delocalized mainly on Mo to store reducing equivalents derived from reductants, we tentatively assign that Fe is close to Fe^{II} but slightly reduced.



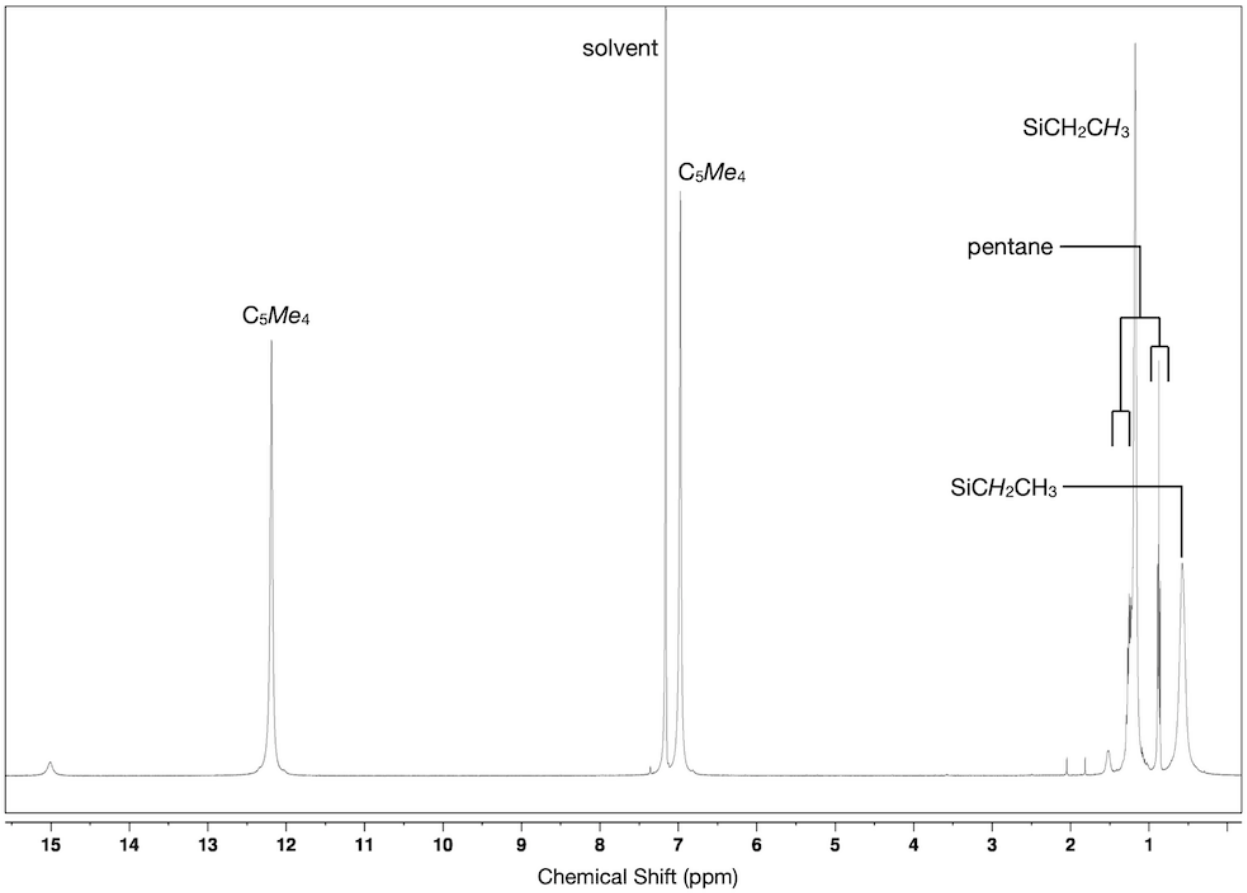
Supplementary Fig. 22. Kohn-Sham frontier orbitals of the *S* = 0 state optimized structure of **2c**. Two lowest unoccupied and nearly degenerated Kohn-Sham orbitals (398 and 399) show Fe-d_{xy} or Fe-d_{x2-y2} characters, which are mixed with the Mo orbitals. As the occupied orbitals are delocalized mainly on Mo to store reducing equivalents derived from reductants, we tentatively assign that Fe is close to Fe^{II} but slightly reduced.



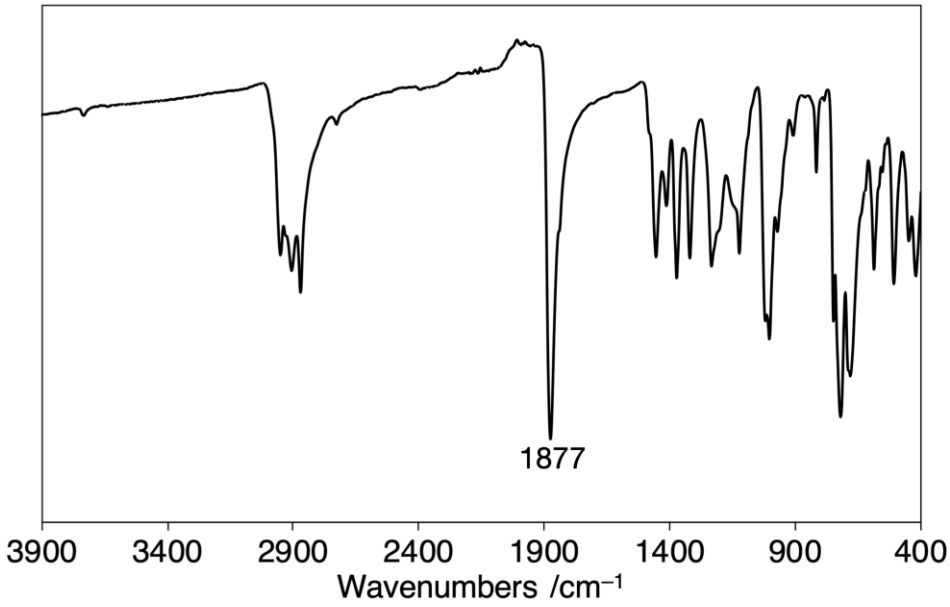
Supplementary Fig. 23. Kohn-Sham frontier orbitals of the *S* = 0 state optimized structure of **3**. Two lowest unoccupied and nearly degenerated Kohn-Sham orbitals (381 and 382) show Fe-d_{xy} or Fe-d_{x2-y2} characters, which are mixed with the Mo orbitals. As the occupied orbitals are delocalized mainly on Mo to store reducing equivalents derived from reductants, we tentatively assign that Fe is close to Fe^{II} but slightly reduced.



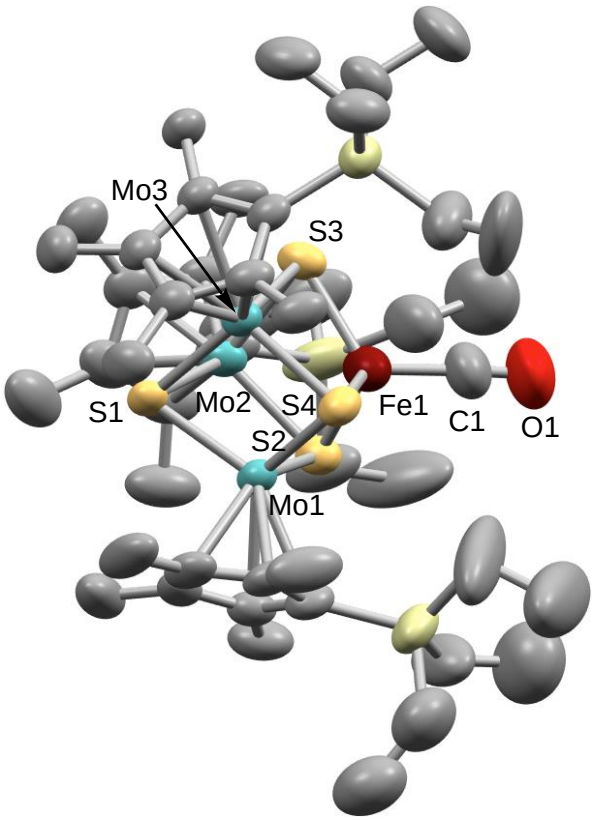
Supplementary Fig. 24. ^{1}H NMR of a CO-exposed catalytic reaction mixture after filtration and evaporation. The inset shows a small signal assignable as $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (**5**) appeared at δ 12.2 in C_6D_6. The NMR yield was calculated based on the peak area relative to the internal standard (ferrocene).



Supplementary Fig. 25. ^{1}H NMR spectrum of $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (**5**) in C_6D_6 at room temperature. Single crystals of **5** contains pentane, and thereby the signals of pentane appear together.



Supplementary Fig. 26. IR spectrum of [$(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)$] (**5**).



Supplementary Fig. 27. Structure of $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]$ (**5**) with thermal ellipsoids set at the 50% probability level. For clarity, disordered atoms (ethyl moieties of $SiEt_3$) are shown with one each groups. Selected Bond lengths (Å) and angles (˚): Fe1-C1 1.768(8), C1-O1 1.091(10), Fe1-S2 2.1928(17), Fe1-S3 2.2151(18), Fe1-S4 2.1897(18), Fe1-Mo1 2.7548(10), Fe1-Mo2 2.7787(12), Fe1-Mo3 2.7590(10), Mo1-S1 2.3389(13), Mo1-S2 2.3218(13), Mo1-S4 2.3307(15), Mo2-S1 2.3357(12), Mo2-S2 2.3371(15), Mo2-S3 2.3409(14), Mo3-S1 2.3318(13), Mo3-S3 2.3429(13), Mo3-S4 2.3419(14), O1-C1-Fe1 178.0(10), C1-Fe1-S2 105.7(3), C1-Fe1-S3 119.4(3), C1-Fe1-S4 110.7(3).

Supplementary Table 1. Summary of N_2 silylation reactions catalyzed by [Mo_3S_4Fe] clusters.[a]

Entry	Precatalysts	Run	Amount of reactants[b]		time (h)	Solvent	$N(SiMe_3)_3$ yield[b]	Ave. yield[b]
			Na	Me_3SiCl				Error[c]
1	**1a**	1	2000	2000	100	THF	166.9	127.0
		2					109	
		3					105	34.6
2	**1b**	1	2000	2000	100	THF	240.5	248.0
		2					265.9	
		3					237.5	15.6
3	**1c**	1	2000	2000	100	THF	124.6	122.9
		2					119.4	
		3					124.6	3.0
4	**1c**	1	2000	2000	100	DME	105.8	74.4
		2					64.7	
		3					52.7	27.8
5	**2b**	1	2000	2000	100	THF	160.6	142.5
		2					136.4	
		3					130.4	16.0
6	**2b**	1	2000	2000	100	DME	105.8	119.1
		2					125.1	
		3					126.5	11.6
7	**2c**	1	2000	2000	100	THF	180	227.1
		2					251.6	
		3					249.6	40.8
8	**2c**	1	2000	2000	100	DME	95.5	78.3
		2					66.9	
		3					72.4	15.2
9	**3**	1	2000	2000	100	THF	264.1	258.3
		2					258.7	
		3					252	6.1
10	$Cp^*_3Mo_3S_4$ (**4a**)	1	2000	2000	100	THF	5	6.5
		2					7.9	
		3					6.6	1.5
11	$Cp^L_3Mo_3S_4$ (**4b**)	1	2000	2000	100	THF	7.4	9.6
		2					12.6	
		3					8.7	2.7
12	$Cp^{XL}_3Mo_3S_4$ (**4c**)	1	2000	2000	100	THF	22.6	12.9
		2					5.7	
		3					10.4	8.7

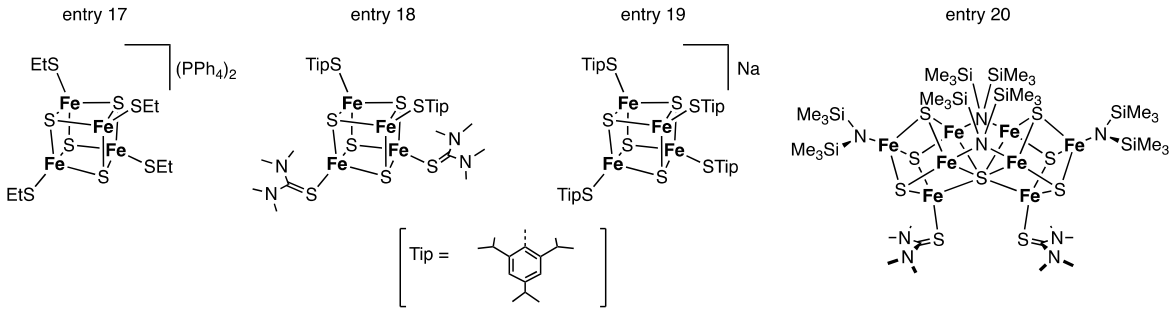
[a] Reactions with cluster **2a** were not examined due to the low isolated yield and the lower performance of the Cp* (C_5Me_5) system. [b] Values are shown in a scale of equivalence relative to cluster. [c] Error is shown as standard deviations of three independent experiments (n = 3).

Supplementary Table 2. Conditions for the GC analysis.

Instrument	Shimadzu GC-2010 Plus		
Column	Agilent J&W No. 123-1055		
Film thickness	50 m, 0.32 mm, 5.0 µm		
He (primary)	566 kPa	He (carrier)	48.4 kPa
INIT TEMP	50 °C	INIT TIME	0 min.
PROG RATE	10℃/min.	FINAL TEMP	280 °C
FINAL TIME	30 min.	INJ TEMP	260 °C
DET TEMP	200 °C	SPLIT ratio	50.0
Amount of solution	1.0 µL		

Supplementary Table 3. Representative yields of $N(SiMe_3)_3$ from N_2 by small-molecule Fe precatalysts under ambient pressure. CAAC = cyclic (alkyl)(amino)carbene.[22] dmpe = 1,2-bis(dimethylphosphino)ethane.[24] ^{xyl}pda = *N,N'*-bis(2,6-dimethylphenyl)-*o*-phenylenediamine.[25] tmtu = tetramethylthiourea. Tip = 2,4,6-$^{i}Pr_3C_6H_2$. Errors shown in this table are calculated as standard deviations of three independent experiments (n = 3).

Entry	Precatalyst	$N(SiMe_3)_3$ yield (equiv/Fe atom)	Reference
1	$[Cp^*_3Mo_3S_4FeCl]$ (**1a**)	127.0 ± 34.6	This work
2	$[Cp^L_3Mo_3S_4FeCl]$ (**1b**)	248.0 ± 15.6	This work
3	$[Cp^{XL}_3Mo_3S_4FeCl]$ (**1c**)	122.9 ± 3.0	This work
4	$[Cp^L_3Mo_3S_4Fe(N_2)]^-$ (**2b**)	142.5 ± 16.0	This work
5	$[Cp^{XL}_3Mo_3S_4Fe(N_2)]^-$ (**2c**)	227.1 ± 40.8	This work
6	$Fe(CO)_5$	25	21
7	Cp_2Fe	13	21
8	Cp^L_2Fe	23	21
9	$\{C_5H_2(SiMe_3)_2\}_2Fe$	34	21
10	$(CAAC)_2Fe$	24.4 ± 2.7	22
11	$[(CAAC)_2Fe]^+$	19.4 ± 3.0	22
12	$Fe_4(\mu\text{-}H)_4(\mu_3\text{-}H)_2\{N(SiMe_3)_2\}_2(PMe_2Ph)_4$	40 ± 5	23
13	$Fe_4(\mu\text{-}H)_4(\mu_3\text{-}H)_2\{N(SiMe_3)_2\}_2(PEt_3)_4$	40 ± 3	23
14	$Fe(dmpe)_2(N_2)$	47	24
15	$Fe(dmpe)_2\{NN(SiMe_3)_2\}$	56	24
16	$[Fe_2S_2(^{xyl}pda^{\bullet-})_2]$	88	25
17	$[PPh_4]_2[Fe_4S_4(SEt)_4]$	4.3 ± 0.7	This work
18	$[Fe_4S_4(STip)_2(tmtu)_2]$	0.9 ± 0.3	This work
19	$Na[Fe_4S_4(STip)_4]$	3.1 ± 0.5	This work
20	$[\{N(SiMe_3)_2\}(tmtu)Fe_4S_3]_2(\mu_6\text{-}S)\{\mu\text{-}N(SiMe_3)_2\}_2$	4.7 ± 1.5	This work
21	$FeCl_2$	Not detected	21



Kanatzidis *et al.* reported sub-stoichiometric conversion of N_2 into NH_3 in the presence of porous Fe-S gels under continuous light irradiation,[66] and one may wonder the possible application of Fe-S species in catalytic N_2 silylation. Therefore, some synthetic Fe-S clusters were tested as potential precatalysts for N_2 silylation (entries 17-20). Among three $[Fe_4S_4]$ clusters listed in entries 17-19, $[Fe_4S_4(SEt)_4]^{2-}$ (entry 17)[37] in the formal $Fe(II)_2Fe(III)_2$ oxidation state is the representative one, while its solubility is very low in the solvent for catalysis (THF). In order to check the influence of the solubility, two THF-soluble $[Fe_4S_4]$ clusters in different oxidation states ($Fe(II)_2Fe(III)_2$ for entry 18 and $Fe(II)Fe(III)_3$ for entry 19)[38,39] were additionally tested. As we have previously reported an $[Fe_8S_7]$ cluster model of the nitrogenase P-cluster[40], this cluster was also added as a catalyst candidate (entry 20). All of the cubic or fused-cuboidal $[Fe_4S_4]$ and $[Fe_8S_7]$ clusters (entries 17-20) showed significantly lower catalytic activities than the cubic $[Mo_3S_4Fe]$ clusters (entries 1-5), undermining the possibility to generate highly catalytically active but yet unidentified Fe-S species from the $[Mo_3S_4Fe]$ cubes. Significantly low catalytic activities of the platform $[Mo_3S_4]$ clusters $Cp^R{}_3Mo_3S_4$ (**4a**-**4c**) (Table 1, entries 7-9) indicate the difficulty to generate Mo-based catalytically active species via cleavage of the Mo-Cp^R or Mo-S bonds. Soon after we submitted this article, Song *et al.* reported a $[Fe_2S_2]$ cluster and silylation of N_2 in the presence of KC_8 and $ClSiMe_3$ (entry 16). In this case, neither N_2 binding nor N_2 activation has been shown.[25] Given the absence of the N_2-binding abilities of the $[Fe_2S_2]$ species and facile decomposition of its diferrous form, which can be readily generated in the presence of excess KC_8 in the catalytic reaction mixture, it is reasonable to assume that degradation of the $[Fe_2S_2]$ cluster is necessary to generate the catalytically active species.

Supplementary Table 4. Summary of the reactions of **2b** or **2c** with reducing agents and proton sources under N_2.

$$N_2\ (1\ atm) + \text{reductant}\ (0.50\ mmol) + \text{proton source}\ (0.46\ mmol) \xrightarrow[\substack{Et_2O\ (5\ mL)\\ -78\ °C,\ 1\ h\\ \text{then rt, 20 min}}]{\text{cat.}} NH_3 + NH_2NH_2 + H_2$$

entry	cat. (μmol)	reductant (equiv/cat.)	proton source (equiv/cat.)	NH_3 (equiv/cat.)	NH_2NH_2 (equiv/cat.)	H_2 (equiv/cat.)
1	**2b** (10)	KC_8 (50)	$[H(OEt_2)_2]BAr^F{}_4$ (46)	0.9	n.d.	12
2	**2c** (10)	KC_8 (50)	$[H(OEt_2)_2]BAr^F{}_4$ (46)	1.3	n.d.	11
3[a]	**2b** (10)	$CoCp^*{}_2$ (50)	$[H_2NPh_2]OTf$ (46)	0.6	n.d.	10
4[a]	**2c** (10)	$CoCp^*{}_2$ (50)	$[H_2NPh_2]OTf$ (46)	0.8	trace	11
5	**2c** (2.5)	KC_8 (200)	$[H(OEt_2)_2]BAr^F{}_4$ (184)	1.6	n.d.	48
6[a]	**2c** (2.5)	$CoCp^*{}_2$ (200)	$[H_2NPh_2]OTf$ (184)	1.3±0.2	trace	37±7
7[b]	**2c** (2.5)	$CoCp^*{}_2$ (200)	$[H_2NPh_2]OTf$ (184)	1.5±0.7	trace	38±4
8[a]	**2c** (5.0)	$CoCp^*{}_2$ (100)	$[H_2NPh_2]OTf$ (92)	1.6±0.1	n.d.	37±7
9[a]	**2c** (5.0)	$CoCp^*{}_2$ (100)	$[H_2NPh_2]BAr^F{}_4$ (92)	0.5	n.d.	22
10[a]	**2c** (5.0)	$CoCp^*{}_2$ (100)	$[H_2N(2,5\text{-}Cl_2C_6H_3)]OTf$ (92)	1.1	0.1	22

n.d. = not detected, rt = room temperature. [a] At −78 °C for 3 h then at rt for 15 h.
[b] Et_2O was added by trap-to-trap distilation, at −196 °C to −78 °C for 3 h then at rt for 15 h.

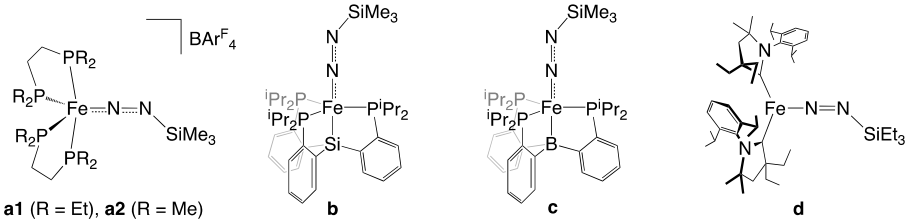
Supplementary Table 5. Crystal data and refinement summary for $[K(THF)_2]_2[\{Cp^*_3Mo_3S_4Fe\}_2(\mu\text{-}N_2)]$ (**2a**), $[Na(15\text{-crown-5})(THF)][(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2)]\cdot(THF)_{0.5}\cdot(hexane)_{0.5}$ (**2c**$\cdot(THF)_{0.5}\cdot(hexane)_{0.5}$), $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(N_2SiPh_3)]\cdot(hexane)_{0.93}$ (**3**$\cdot(hexane)_{0.93}$), and $[(C_5Me_4SiEt_3)_3Mo_3S_4Fe(CO)]\cdot(pentane)$ (**5**$\cdot$(pentane)).

	2a	**2c**	**3**	**5**
Formula	$C_{76}H_{122}Fe_2K_2Mo_6N_2O_4S_8$	$C_{64}H_{120}FeMo_3N_2NaO_6{}_{.5}S_4Si_3$	$C_{69.4}H_{113.89}FeMo_3N_2S_4Si_{3.93}$	$C_{51}H_{93}FeMo_3OS_4Si_3$
Formula weight (g/mol)	2149.77	1600.78	1558.53	1267.40
Crystal system	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	*C*2/*c* (#15)	*P*-1 (#2)	*P*-1 (#2)	*P*-1 (#2)
a (Å)	27.434(6)	14.7538(18)	13.6929(12)	10.7438(12)
b (Å)	11.217(12)	15.4577(16)	22.552(2)	13.2463(15)
c (Å)	29.288(2)	17.654(2)	26.911(3)	22.469(3)
α (˚)	90	79.971(5)	110.411(2)	104.907(8)
β (˚)	100.20(3)	89.180(7)	90.389(2)	97.158(11)
γ (˚)	90	82.974(6)	93.2421(17)	102.887(9)
V (Å^3)	8870(10)	3936.0(8)	7772.8(14)	2955.5(6)
Z	4	2	4	2
D_{calcd} (g/cm3)	1.610	1.351	1.332	1.437
Max 2θ (˚)	55.06	55.268	55.08	55.17
No. of reflections (measured)	10186	18169	35440	13562
No. of data (used) ($I > 2.00\sigma(I)$)	8570	11331	29953	10170
No. of parameters refined	444	804	1508	616
R_1 [a]	0.0408	0.0565	0.0573	0.0590
wR_2 [b]	0.1030	0.1532	0.1610	0.1945
GOF [c]	1.123	0.893	1.159	1.104

[a] $I > 2\sigma(I)$, $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] refined with all data, $wR_2 = [\{\Sigma w(F_o^2-F_c^2)^2\}/\Sigma w(F_o^2)^2]^{1/2}$. [c] GOF = $[\{\Sigma w(F_o^2-F_c^2)^2\}/(N_o-N_p)]^{1/2}$, where N_o and N_p denote the numbers of reflection data and parameters.

Supplementary Table 6. N-N bond distances, N-N stretching frequencies, and Mössbauer parameters of reported Fe complexes bearing [N_2SiR_3] ligands. depe = 1,2-bis(diethylphosphino)ethane,[29] dmpe = 1.2-bis(dimethylphosphino)ethane, $SiP^{i\text{-}Pr}_3$ = [Si(*o*-$C_6H_4P^iPr_2)_3]^-$,[30] $BP^{i\text{-}Pr}_3$ = [B(*o*-$C_6H_4P^iPr_2)_3]^-$,[64] CAAC = cyclic (alkyl)(amino)carbene.[22]

compound	d (N-N) (Å)	d (Fe-N) (Å)	ν_{NN} (cm^{-1})	δ (mm/s)	ΔE_Q (mm/s)	note
cluster **3**	1.193(7)	1.687(5)	1706	0.363(3)	0.906(5)	this work
[$Fe(depe)_2NNSiMe_3$][BAr^F_4] (**a1**)	1.194(8)	1.691(6)	1732	—	—	Fe^{2+}
[$Fe(dmpe)_2NNSiMe_3$][BAr^F_4] (**a2**)	1.197(5) 1.203(5)	1.692(3)	1727	—	—	Fe^{2+}
[($SiP^{i\text{-}Pr}_3$)Fe($NNSiMe_3$)] (**b**)	1.195(3)	1.695(3)	1748	0.188	1.26	Fe^{2+}
[($BP^{i\text{-}Pr}_3$)Fe($NNSiMe_3$)] (**c**)	1.225(3)	1.6960(8)	1741	—	—	—
[$(CAAC)_2FeNNSiEt_3$] (**d**)	—	—	1690	0.59	1.60	—



a1 (R = Et), **a2** (R = Me) **b** **c** **d**

Supplementary Table 7. Spin densities, $<S^2>$ values, relative energies of the optimized S = 0 and 2 states of **2a**. Ground state of **2a** is S = 0 . The S = 2 state is 24.8 kcal/mol higher in energy.

Atom	***S* = 0**	***S* = 2**[a]
1 N	-	-0.11
2 Fe	-	1.26
3 S	-	0.01
4 S	-	0.02
5 S	-	0.01
6 S	-	0.00
7 Mo	-	-0.07
8 Mo	-	-0.10
9 Mo	-	-0.13
110 N	-	-0.12
111 Fe	-	1.25
112 S	-	0.03
113 S	-	0.06
114 S	-	0.09
115 S	-	0.04
116 Mo	-	-0.09
117 Mo	-	-0.14
118 Mo	-	-0.12
$<S^2>$	-	6.33
Relative Energy/kcal mol^{-1}	0.0	**24.8**

[a] In the S = 2 state, computed spin density, ρ(2Fe) of 1.26 and ρ(2Fe) of 1.25, suggested that the unpaired electrons are manly localized on Fe centers.

Supplementary Table 8. Spin densities, $\langle S^2 \rangle$ values, relative energies of the optimized S = 0, 1, and 2 states of **2c**. Ground state of **2c** is S = 0. The S = 1 and 2 states are 20.8 and 39.4 kcal/mol higher in energy, respectively.[a]

Atom	***S* = 0**	***S* = 1**[b]	***S* = 2**[c]
1 Mo	-	0.53	0.76
2 Mo	-	0.01	0.36
3 Mo	-	0.05	0.41
4 Fe	-	1.21	1.95
5 S	-	0.04	0.14
6 S	-	0.02	0.05
7 S	-	0.04	0.15
8 S	-	0.04	0.02
19 N	-	-0.04	-0.04
20 N	-	-0.06	-0.08
$\langle S^2 \rangle$	-	2.08	6.10
Relative Energy/kcal mol^{-1}	0.0	**20.8**	**39.4**

[a] Computed $\langle S^2 \rangle$ values, 2.08 of the S = 1 state and 6.10 of the S = 2 state, are closer to their ideal values (2.00 of the S = 1 state and 6.00 of the S = 2 state), suggesting only minor spin contaminations.

[b] According to the computed spin densities, two unpaired electrons of the S = 1 state are delocalized between 1Mo and 4Fe. [ρ(1Mo) = 0.53 and ρ(4Fe) = 1.21].

[c] In the case of the S = 2 state, four unpaired electrons are delocalized in the [Mo_3S_4Fe] cube.

Supplementary Table 9. Spin densities, $<S^2>$ values, relative energies of the optimized S = 0, 1 and 2 states of **3**. Ground state of **3** is S = 0. The S = 1 and 2 states are 20.7 and 42.8 kcal/mol higher in energy, respectively.[a]

Atom	***S* = 0**	***S* = 1**[b]	***S* = 2**[c]
1 Fe	-	1.19	1.86
2 Mo	-	0.04	0.56
3 Mo	-	0.71	0.87
4 Mo	-	0.01	0.37
5 S	-	0.03	0.18
6 S	-	0.03	0.02
7 S	-	0.05	0.12
8 S	-	0.01	0.04
172 N	-	-0.09	-0.12
173 N	-	-0.09	-0.13
$<S^2>$	-	2.10	6.14
Relative Energy/kcal mol^{-1}	0.0	**20.7**	**42.8**

[a] Computed $<S^2>$ values, 2.10 of the S = 1 state and 6.14 of the S = 2 state, are closer to their ideal values, indicating only minor spin contaminations.

[b] Computed spin densities of the S = 1 state, ρ(3Mo) = 0.71 and ρ(4Fe) = 1.19, suggested that two unpaired electrons are delocalized between 1Fe and 3Mo; [ρ(1Mo) = 0.53 and ρ(4Fe) = 1.21].

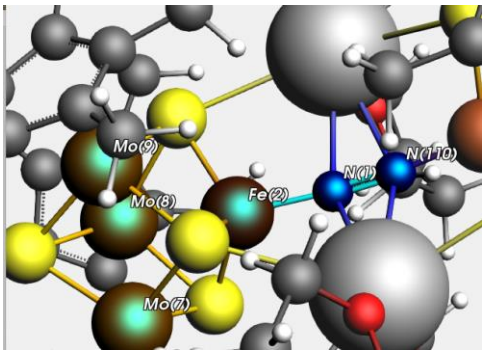
[c] In the case of the S = 2 state, four unpaired electrons are delocalized in the $[Mo_3S_4Fe]$ cube.

Supplementary Table 10. Computed Mössbauer parameters. X-ray structures and the ground state optimized structures were used for the Mössbauer parameter calculations. Experimental values are in parenthesis. Calculated isomer shift (IS) values of three systems are in agreement with the experimental data. Calculated quadrupole splitting (QS) values are larger than the experimental values.

	ρ_{00} (AU^{-3})	IS (mm/s)	QS (mm/s)
2a, optimized	23614.91922, 23614.90547	0.35, 0.35 *(0.48)*	0.84, 0.84 *(1.26)*
2a, X-ray	23614.24868, 23614.24013	0.46, 0.46	0.68, 0.64
2c, optimized	23615.42574	0.26 *(0.40)*	0.84 *(1.47)*
2c, X-ray	23614.64413	0.39	0.74
3, optimized	23616.141535316	0.14 *(0.26)*	0.47 *(0.91)*
3, X-ray	23615.437893828	0.26	0.48

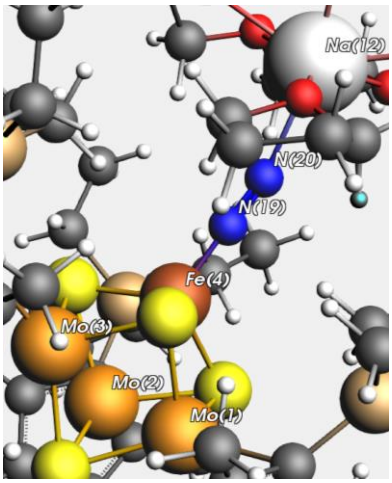
Supplementary Table 11. Calculated Mayer bond orders of the selected bonds of the optimized ground state (*S* = 0) of **2a**. The computed Mayer bond orders of the N-N is 2.00, suggesting a N=N double bond. The Mayer bond orders of Fe-N is 0.89. The computed Mayer bond orders Fe-Mo (0.57-0.58) and Mo-Mo (0.67-0.68) indicate metal-metal bonding character.

	Atom		Atom	Bond Order
1	N	2	Fe	0.89
1	N	110	N	2.00
2	Fe	7	Mo	0.58
2	Fe	8	Mo	0.57
2	Fe	9	Mo	0.58
7	Mo	8	Mo	0.68
7	Mo	9	Mo	0.68
8	Mo	9	Mo	0.67



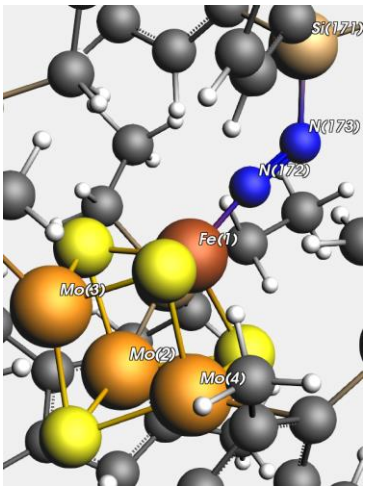
Supplementary Table 12. Calculated Mayer bond orders of the selected bonds of the optimized ground state (*S* = 0) of **2c**. The computed Mayer bond orders of N-N (2.31) is larger than **2a**. The Fe-N bond order (1.12) is relatively large in comparison with **2a**. The computed Mayer bond orders Fe-Mo (0.54-0.55) and Mo-Mo (0.69-0.73) indicate metal-metal bonding character.

	Atom		Atom	Bond Order
4	Fe	1	Mo	0.54
4	Fe	2	Mo	0.55
4	Fe	3	Mo	0.55
4	Fe	19	N	1.12
1	Mo	2	Mo	0.69
1	Mo	3	Mo	0.73
2	Mo	3	Mo	0.71
19	N	20	N	2.31



Supplementary Table 13. Calculated Mayer bond orders of the selected bonds of the optimized ground state (*S* = 0) of **3**. Computed Mayer bond order of N-N (1.68) is smaller than those of **2a** and **2c**, while the bond order of Fe-N (1.49) is larger. The Fe-Mo (0.48-0.50) and Mo-Mo (0.70-0.75) indicate metal-metal bonding character.

	Atom		**Atom**	**Bond Order**
1	Fe	2	Mo	0.50
1	Fe	3	Mo	0.48
1	Fe	4	Mo	0.50
1	Fe	172	N	1.49
2	Mo	3	Mo	0.75
2	Mo	4	Mo	0.70
3	Mo	4	Mo	0.72
172	N	173	N	1.68



Cartesian coordinates of the optimized structures

Cluster 2a

S=0

Fe	2.21950411477942	4.12988228142792	5.77850420518142
Mo	1.37729001465722	1.70267172172028	4.79477113804593
Mo	0.55916600013346	4.14273163758024	3.55737028279340
Mo	-0.40303580030081	3.49912053509632	6.19551924592633
S	2.74812774792465	3.33222258029927	3.81627723184327
S	1.53618011473935	2.47650358752840	6.98045400152009
S	0.56200477208125	5.49790949570352	5.45238870834114
S	-0.80403110673242	2.34066789109714	4.19575408303613
C	3.05361725087933	0.07258022091612	4.74692855404755
C	2.03890646914309	-0.39109784758903	5.66580121384417
C	2.23438558294279	-0.73366051837352	7.10944546224507
H	1.33298170673786	-0.52381218684762	7.70008083865971
H	3.06315616945500	-0.17299531995902	7.55546936138138
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C	7.77540145	6.15660937	3.24064339
C	7.03190825	5.09337483	2.62426886
C	6.44611404	4.28411752	3.66767807
C	6.36361167	4.39133232	6.27055705
H	7.10673190	4.62515492	7.04489209
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C	8.24946194	6.88578859	5.71710933

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Cluster 2c

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C	5.22899106847997	1.83731493554853	-0.33446631874628
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H	8.19365799524226	2.07934405460486	6.29502044616766
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H	3.98987462215463	-0.34137077874179	8.07647962782641
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H	5.56765444343828	-0.58639000317251	7.30922912703021
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C	2.32298951776386	5.81632343913446	7.24285220697349
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Cluster 3

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H	7.85718567140311	1.82496655514592	3.28826824570464
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C	4.94737848757747	1.66988970153401	6.66926489192914
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H	1.95855061588146	8.53159063164918	0.96556108162065
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C	-0.87181074490593	1.80033886217828	9.23760079203471
H	-1.49993872170485	1.82129701928633	10.14268739002353
H	0.16624330603744	1.95749367226874	9.54343486510296
H	-0.94459025707289	0.79526956585673	8.80264795070653
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C	-1.05742175900338	5.83561431635742	10.88014585646090
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H	-1.69710521546820	6.63462383527098	10.46764777617005
C	-1.92722587612580	4.74201461541128	11.51682112237021
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H	-2.56809431272263	5.13700044504182	12.32043005593140
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H	0.93306656137294	3.38485802252053	10.96675768580597
H	1.80775059322250	3.44621095868617	9.43424583383358
C	2.55230665692476	4.83394295681035	10.91971017609634
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H	2.19478243359433	5.49670068277415	11.72250973611706
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H	1.87563890610018	6.24751846456785	8.22858607137063
H	0.36893019244388	6.99618973463888	7.79533750518977
C	1.27613799455297	7.84620627002723	9.56876290375373
H	0.36272967594748	8.32548370912245	9.95162492423955
H	1.84789696337790	8.60795744590968	9.01673162238902
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C	5.72026995832613	7.46360042395658	10.08853069338660
H	4.66154523110411	7.73206505556560	10.06286225071448
C	6.43360262361508	7.60581642790984	11.28022344324152
H	5.93238208746968	7.97819827172620	12.17523499454813
C	7.79196967395348	7.27231285973681	11.32375124356680
H	8.35220425543645	7.38620391878133	12.25336020907503
C	8.43087803735960	6.79421699213785	10.17572116059517
H	9.49013101974528	6.53348322743720	10.20804678085111
C	7.71139319676120	6.64800406962494	8.98586876636677
H	8.21709366647532	6.26931917451019	8.09508331662233
C	6.39327532110333	6.37665547299174	5.87367492417373
C	7.38565606377315	7.29673609431747	5.48558307715306
H	7.55981794847794	8.19649736479662	6.08136997381372
C	8.15177246262349	7.08284874671443	4.33824480548428
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C	7.92934381418951	5.94641497675086	3.55339661379720
H	8.51960980960541	5.78194266698472	2.65048133926803
C	6.94490195842585	5.02723081273304	3.92358485893956
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H	5.40749984470775	4.51894906619857	5.33619281890250
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C	4.54559602703192	9.49857000776465	7.51821136157559
H	5.47443185548867	9.66691163993497	8.06789644157661
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H	1.83398876574813	11.21973426622181	6.36829359653949
C	2.15011677297349	9.09203369080937	6.13789793876200
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C	2.99951405074741	8.01735998019398	6.39661249393815
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