Electronic Supplementary Information (ESI)

Heterometallic uranium/molybdenum nitride synthesis via partial N-atom transfer

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Experimental Procedures

General Considerations. Unless otherwise noted, all manipulations were carried out at ambient temperature under an inert dinitrogen atmosphere using Schlenk techniques and an MBraun glovebox equipped with a purifier unit. The water and oxygen levels were always kept at less than 0.1 ppm. Glassware was dried overnight at 140°C before use.

NMR experiments were carried out using NMR tubes adapted with J-Young valves. NMR spectra were recorded on a Bruker 400 MHz or 600 MHz spectrometers. NMR chemical shifts are reported in ppm with solvent as internal reference.

Elemental analyses were performed under nitrogen using a Thermo Scientific Flash 2000 Organic Elemental Analyzer at the Institute of Chemistry and Chemical Engineering at EPFL.

Starting materials Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Tris(tert-butoxy)silanol was purified by sublimation. Anhydrous solvents were purchased from Aldrich and further distilled from K/benzophenone (thf, hexane). Deuterated solvents for NMR spectroscopy (d_8-thf, d_8-toluene) were purchased from Cortecnet, freeze-degassed and distilled over K/benzophenone. d_6-DMSO was freeze-degassed and dried over 3 Å molecular sieves for several days. ^{13}CO (93.13% ^{13}C) was purchased from Cortecnet and transferred to a flask equipped with a J-Young valve containing activated 3 Å molecular sieves prior to use.
Precise amounts of labelled gases are added to reaction flasks or NMR tubes equipped with a J-Young valve using a short connector of known volume adapted on a Schlenk line equipped with a pressure sensor. Depleted uranium was purchased from Ibilabs, Florida, USA, $[U^{III}(OSi(O^tBu)_3)_3]_2$ [1] (used as source of the monomeric complex $[U(OSi(O^tBu)_3)_3(thf)_2]$), $[Cl(N)Mo^{IV}P2]$ [2] and $[P2Mo^{II}(N)Na]$ [3] were prepared according to the published procedure.

Caution: Depleted uranium (primary isotope ^{238}U) is a weak α-emitter (4.197 MeV) with a half-life of 4.47×10^9 years. Manipulations and reactions should be carried out in monitored fume hoods or in an inert atmosphere glovebox in a radiation laboratory equipped with α- and β-counting equipment.

Synthesis of [Na{(U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], 1. A cold (-40°C) brown-red solution of $[U^{III}(OSi(O^tBu)_3)_3]_2$ (53.9 mg, 0.0262 mmol, 1 equiv) in thf (3.0 mL) was added to a cold (-40°C) orange-red solution of $[P2Mo^{II}(N)Na]$ (30.9 mg, 0.0524 mmol, 2 equiv) in thf (3.0 mL) and stirred at -40°C. The colour of the reaction mixture changed rapidly from dark red to dark brown. The ^1H NMR spectrum of the reaction mixture measured immediately after the addition showed the presence of $[U^{IV}(OSi(O^tBu)_3)_4]$ and complex **1.** (Figure S1) The $^{31}P\{^1H\}$ NMR of the reaction mixture showed only traces of [P2MoNNa] (Figure S2). $^{31}P\{^1H\}$ NMR studies revealed that the reaction is complete after 3 hs stirring.

The reaction mixture was filtered and all volatiles were removed under vacuum. The resultant solid was dissolved in hexane (0.4 mL) and stored at -40°C affording after 15 hs large dark brown crystals of complex **1** in 72% yield (58.0 mg, 0.0381 mmol). Anal. Calcd. for $[Na\{U(OSi(O^tBu)_3(\mu\text{-}N)(MoP2)\}](C_6H_{14})_{0.1}$: C: 49.12%, H: 7.33%, N: 0.86%. Found: C:49.45%, H: 7.43%, N:0.96%.

Complex **1** shows moderate stability at room temperature both in solid state and in a thf solution, fully decomposing to an intractable mixture of unidentified species over the course of 12 hours. Decomposition is significantly slower at -40°C in thf solution and the solid can be stored at -40°C in the solid state at least up to a month.

^1H NMR (d_8-thf, 400 MHz, 233 K): δ = 10.5 ppm (br), -10.5 ppm (br). (Figure S3)

^1H NMR (d_8-thf, 400 MHz, 298 K): δ = 12.7 ppm (br), 8.7 ppm (br), 0.42 ppm (s), -0.61 ppm (s), -2.4 ppm (br). (Figure S4)

$^{31}P\{^1H\}$ NMR (d_8-thf, 162 MHz, 233 K): Silent

$^{31}P\{^{1}H\}$ NMR (d_8-thf, 162 MHz, 298 K): Silent
^{1}H NMR studies in d_8-thf showed full decomposition of **1** over the course of 12 hs at room temperature to yield $[U^{IV}\{OSi(O^tBu)_3\}_4]$ and multiple unidentified species. (Figure S5)
^{1}H NMR studies in d_8-thf showed only a traces decomposition of **1** over the course of 5 days at -40°C (Figure S6).
^{31}P NMR studies in d_8-thf showed the appearance of a new resonance at δ = -19.3 ppm after 5 days at -40°C (Figure S7).

Reaction of 1 equiv. of [P2Mo^{II}(N)Na] with 1 equiv of [U^{III}(OSi(O^{t}Bu)$_3$)$_3$]$_2$ at -40°C. A cold (-40°C) red-brown solution of $[U^{III}(OSi(O^tBu)_3)_3]_2$ (11.3 mg, 0.0053 mmol, 1 equiv) in d_8-thf (0.3 mL) was added to a cold (-40°C) orange-red solution of [P2Mo^{II}(N)Na] (3.2 mg, 0.0052 mmol, 1 equiv) in d_8-thf (0.2 mL). The reaction mixture was stirred at -40°C for 3 days. ^{1}H NMR studies show that the reaction only leads to the formation of complex **1** and unreacted $[U^{III}(OSi(O^tBu)_3)_3(thf)_2]$ (Figure S8).The $^{31}P\{^{1}H\}$ NMR spectrum of the reaction mixture shows the appearance of two new resonances at δ= 75.3 ppm, and -7.1 ppm over the course of 3 days that were assigned to decomposition products (Figure S9).
The reaction mixture was filtered and all volatiles were removed under vacuum. The resultant solid was dissolved in hexane (0.2 mL) and stored at -40°C affording after 15 hs large dark brown crystals of complex **1**.

Reaction of 1 equiv. of [P2Mo^{II}(N)Na] with 1 equiv of [U^{III}(OSi(O^{t}Bu)$_3$)$_3$]$_2$ at room temperature. A red-brown solution of $[U^{III}(OSi(O^tBu)_3)_3]_2$ (20.7 mg, 0.010 mmol, 1 equiv) in d_8-thf (0.3 mL) was added to an orange-red solution of [P2Mo^{II}(N)Na] (5.9 mg, 0.010 mmol, 1 equiv) in d_8-thf (0.2 mL) and the reaction mixture was stirred at 25°C. ^{1}H NMR studies revealed the disappearance of the starting materials after 1 h and the formation of $[U^{IV}(OSi(O^tBu)_3)_4]$ as a major product (Figure S10). The $^{31}P\{^{1}H\}$ NMR spectrum of the reaction mixture showed the appearance of three resonances at δ= 75.0 ppm, 47.9 ppm and -7.3 ppm over the course of 30 min and their disappearance after 1 h, affording three new resonances at δ= 77.9 ppm, 76.3 ppm and -4.3 ppm (Figure S11)

Reaction of [Na{(U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], 1 with 1 equiv. of ^{13}CO. [Na{U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], complex **1** (9.1 mg, 0.0060 mmol, 1 equiv) was dissolved in 0.5 mL of d_8-thf and the solution was transferred in an NMR tube. The tube was connected to a Schlenk line and the solution was degassed by three cycles of freeze-pump-thawing. 1 equiv of ^{13}CO was added to the frozen solution. The reaction mixture immediately changed colour from dark brown to dark orange. Multinuclear NMR spectroscopy of the reaction mixture revealed the immediate consumption of the starting material and the formation of a mixture of species (Figures S12-S14) including the previously reported [P2Mo(^{13}CO)] complex [3] and Na^{13}CO. Volatiles were removed and 0.5 mL of D_2O (pD=13) were added to the solid together with few drops of d_6-DMSO affording an orange solution. The ^{13}C NMR spectrum of the reaction mixture revealed the formation of $N^{13}CO^-$ in 10% yield. No peak attributable to [P2Mo(^{13}CO)] was observed, consistently with its insolubility in water. [3] ^{13}C-labelled sodium acetate was used as internal standard for quantification (Figure S15)

Reaction of [Na{(U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], 1 with excess ^{13}CO. [Na{U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}] (5 mg, 0.033 mmol, 1 equiv) was dissolved in 0.5 mL of d_8-thf and the solution was transferred in an NMR tube. The tube was connected to a Schlenk line and the solution was degassed by three cycles of freeze-pump-thawing. 1 atm of ^{13}CO was added to the tube. The reaction mixture immediately changed colour from red-brown to light green. Multinuclear NMR spectroscopy of the reaction mixture revealed the formation of a mixture of species (Figures S16-S18). Volatiles were removed and 0.5 mL of D_2O (pD=13) were added to the light green solid together with few drops of d_6-DMSO affording a light green solution. The ^{13}C NMR spectrum of the reaction mixture revealed the formation of $N^{13}CO^-$. (Figure S19)

Reaction of [Na{(U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], 1 with 10 equiv. of ^{13}CO. [Na{U(OSi(O^{t}Bu)$_3$(μ-N)(MoP2)}], complex **1** (5.0 mg, 0.0033 mmol, 1 equiv) was dissolved in 0.5 mL of d_8-thf and the solution was transferred in an NMR tube. The tube was connected to a Schlenk line and the solution was degassed by three cycles of freeze-pump-thawing. 1 equiv of ^{13}CO was added to the frozen solution. The reaction mixture immediately changed colour from dark brown to dark green. Multinuclear NMR spectroscopy of the reaction mixture revealed the immediate consumption of the starting material and the formation of a mixture of species (Figures S20-S22). The reaction mixture was left to evolve at -40°C for 24 hs and warmed up to 25°C for other 24 hs. Multinuclear NMR spectroscopy of the reaction mixture revealed the formation of the previously reported [P2Mo(^{13}CO)$_3$] complex [3] (Figures S23-S25). Volatiles were removed and 0.5 mL of D_2O (pD=13) were added to the solid together with few drops of d_6-DMSO affording an green solution. The ^{13}C NMR spectrum of the reaction mixture revealed the formation of N^{13}CO$^-$ in 50% yield. No peak attributable to [P2Mo(^{13}CO)$_3$] was observed, consistently with its insolubility in water. [3] ^{13}C-labelled sodium acetate was used as internal standard for quantification (Figure S26)

Reaction of 2 equiv. of [Cl(N)Mo^{IV}P2] with 1 equiv of [U^{III}(OSi(O^{t}Bu)$_3$)$_3$]$_2$ at -40°C and warmed up at room temperature. A cold (-40°C) pink solution of [Cl(N) Mo^{IV}P2] (10.4 mg, 0.017 mmol, 2 equiv) in 0.3 mL of d_8-thf was added to a cold (-40°C) red-brown solution of [U(OSi(O^{t}Bu)$_3$]$_2$ (17.7 mg, 0.0086 mmol, 1 equiv) in 0.3 mL of d_8-thf. The reaction mixture was monitored by ^{1}H NMR spectroscopy and no reaction was observed after 24h at -40°C (Figure S27). The reaction mixture was warmed to 25°C but no reaction was observed after 24h. The reaction with 1 equiv of [Cl(N)Mo P2] also resulted in no reaction.

NMR spectra

Figure S1. ^{1}H NMR spectrum (400 MHz, d_8-thf, 233K) of the evolution of the reaction mixture of 2 equiv. of [P2MoNNa], a) before addition and b) after addition of 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at -40°C.

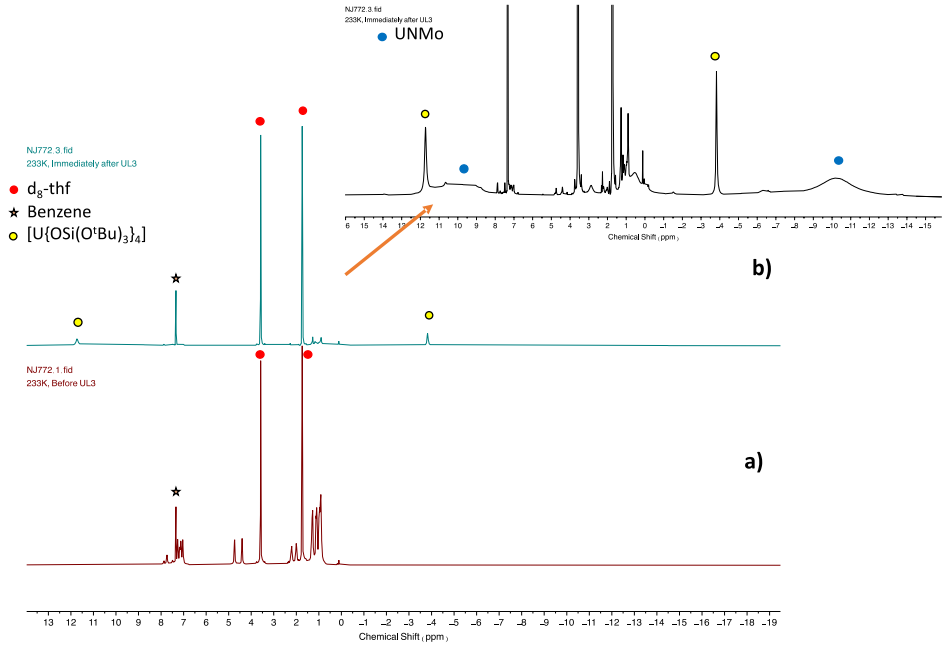


Figure S2. $^{31}P\{^{1}H\}$ NMR spectra (162 MHz, d_8-thf, 233K) of the evolution of the reaction mixture of 2 equiv. of [P2MoNNa] a) before addition, b) immediately after addition, and c) 3 hs after addition of 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at -40°C.

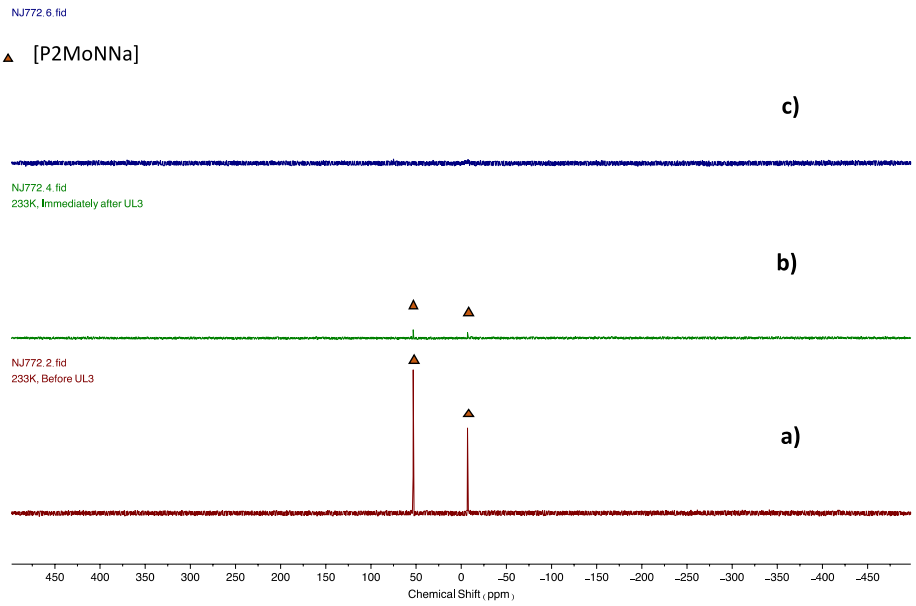


Figure S3. ^{1}H NMR spectrum (400 MHz, d_8-thf, 233K) of complex **1**.

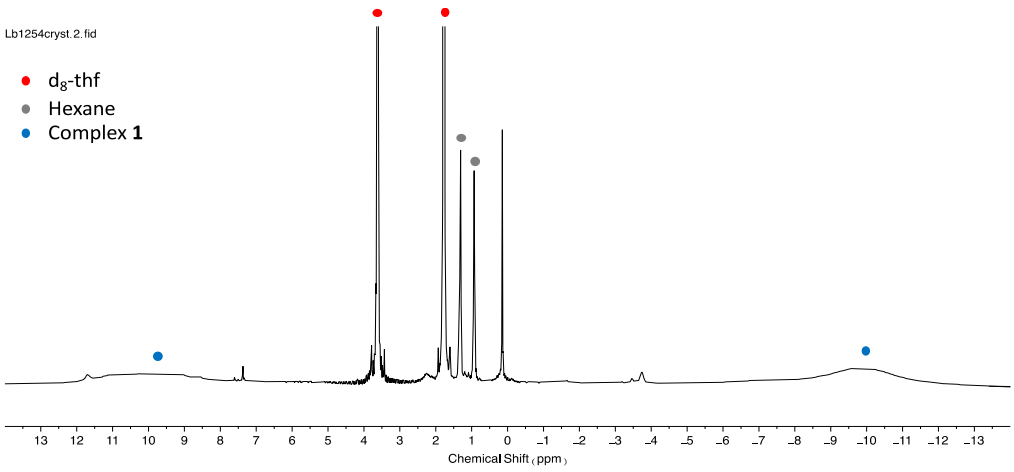


Figure S4. ^{1}H NMR spectrum (400 MHz, d_8-thf, 298K) of complex **1**.

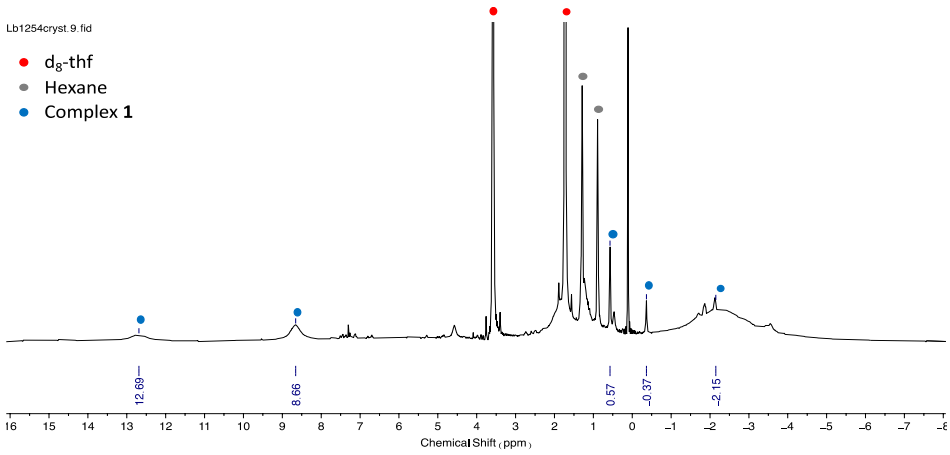


Figure S5. ^{1}H NMR spectra (400 MHz, d_8-thf, 298K) of complex **1** at room temperature immediately after dissolving (bottom) and after 12 hs at room temperature (top) showing complete decomposition of **1**.

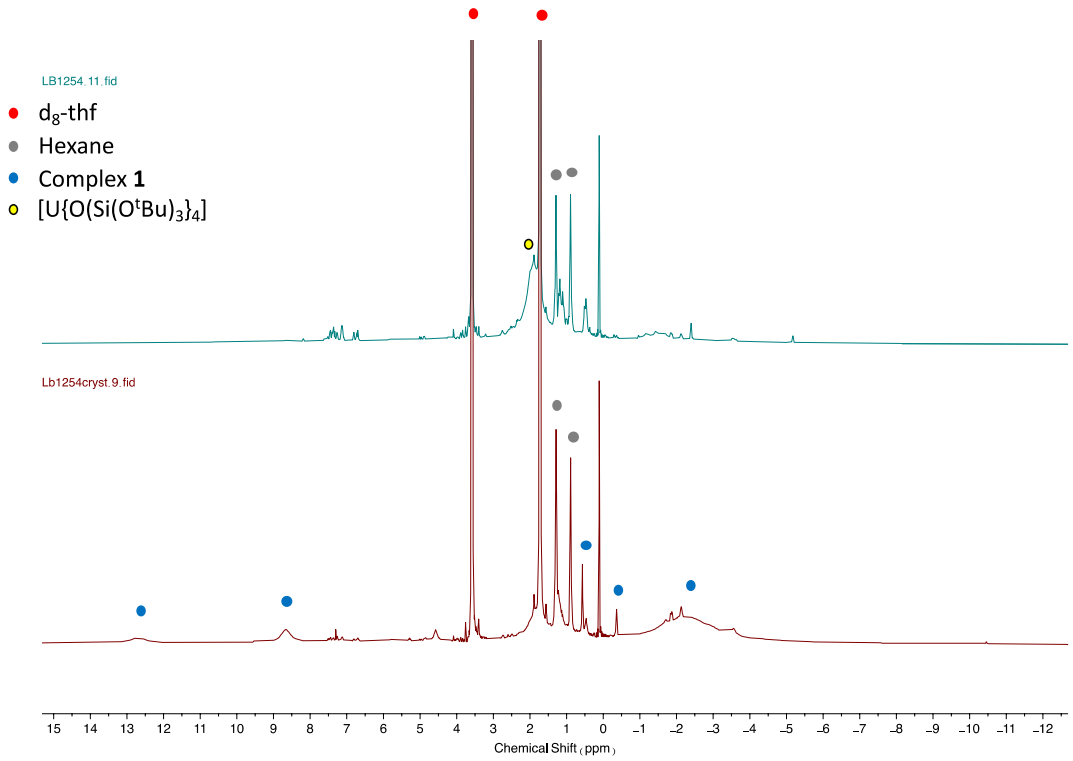


Figure S6. ^{1}H NMR spectra (400 MHz, d_8-thf, 233K) of the evolution of a solution of complex **1** in THF at -40°C a) immediately b) 24 hs after, c) 48 hs after and d) 5 days after dissolving

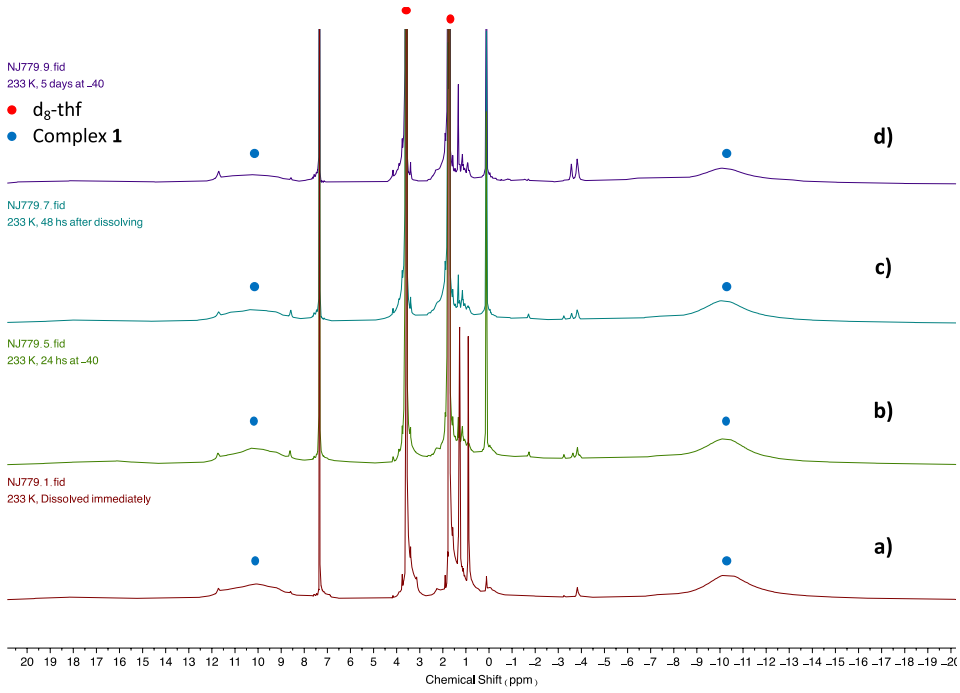


Figure S7. $^{31}P\{^{1}H\}$ NMR spectra (162 MHz, d_8-thf, 233K) of the evolution of a solution of complex **1** in THF at -40°C a) immediately b) 24 hs after, c) 48 hs after and d) 5 days after dissolving

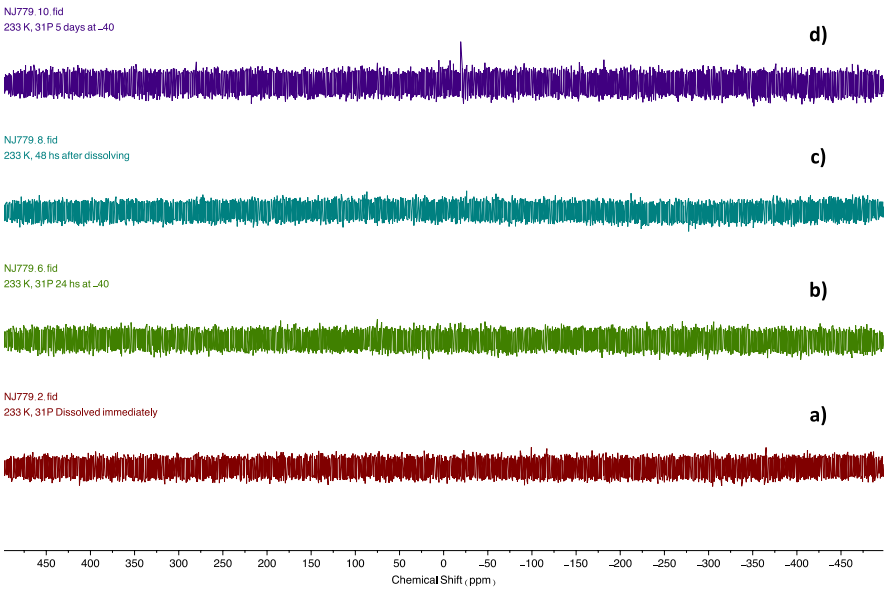


Figure S8. ^{1}H NMR spectra (400 MHz, d_8-thf, 233K) of the evolution of the reaction mixture of 1 equiv. of [P2MoNNa] with 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at -40°C, a) immediately after addition, b) 3 days after addition.

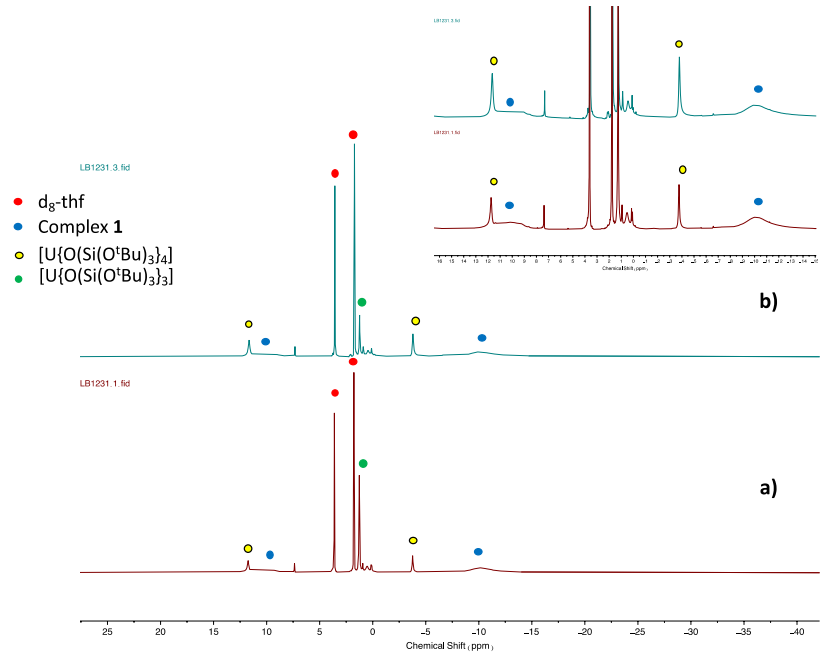


Figure S9. $^{31}P\{^{1}H\}$ NMR spectra (162 MHz, d_8-thf, 233K) of the evolution of the reaction mixture of 1 equiv. of [P2MoNNa] with 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at -40°C, b) immediately after addition, c) 3 days after addition versus a) pure [P2MoNNa].

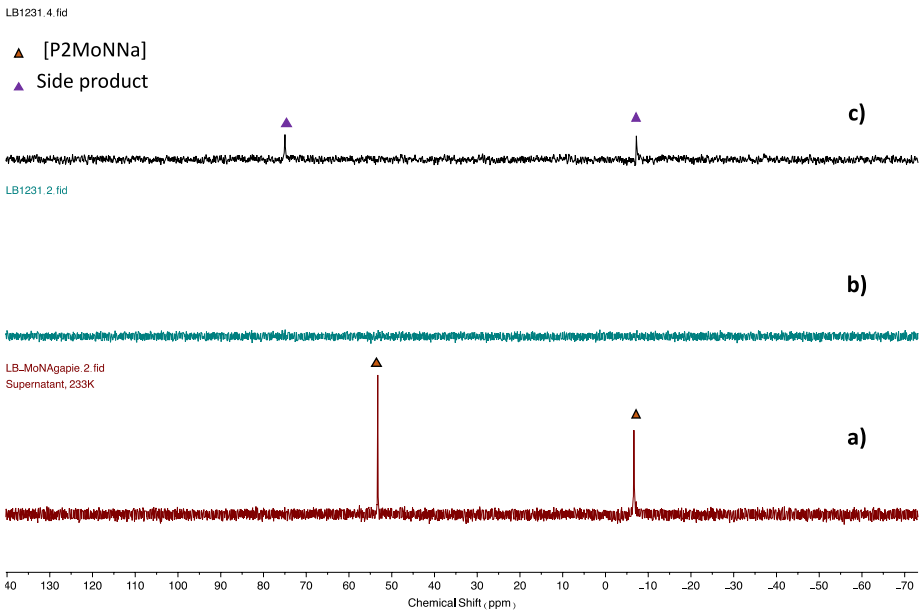


Figure S10. ^{1}H NMR spectra (400 MHz, d_8-thf, 298K) of the evolution of the reaction mixture of 1 equiv. of [P2MoNNa] with 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at room temperature, a) immediately after addition, b) 30 min after addition, c) 1 h after addition.

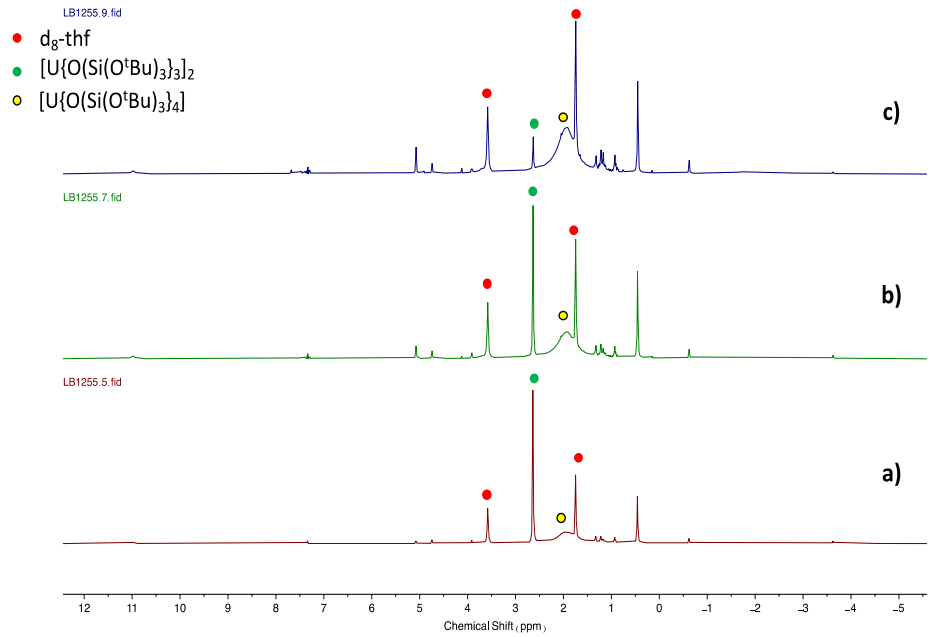


Figure S11. $^{31}P\{^{1}H\}$ NMR spectra (162 MHz, d_8-thf, 298K) of the evolution of the reaction mixture of 1 equiv. of [P2MoNNa] with 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at room temperature, a) immediately after addition, b) 30 min after addition, c) 1 h after addition.

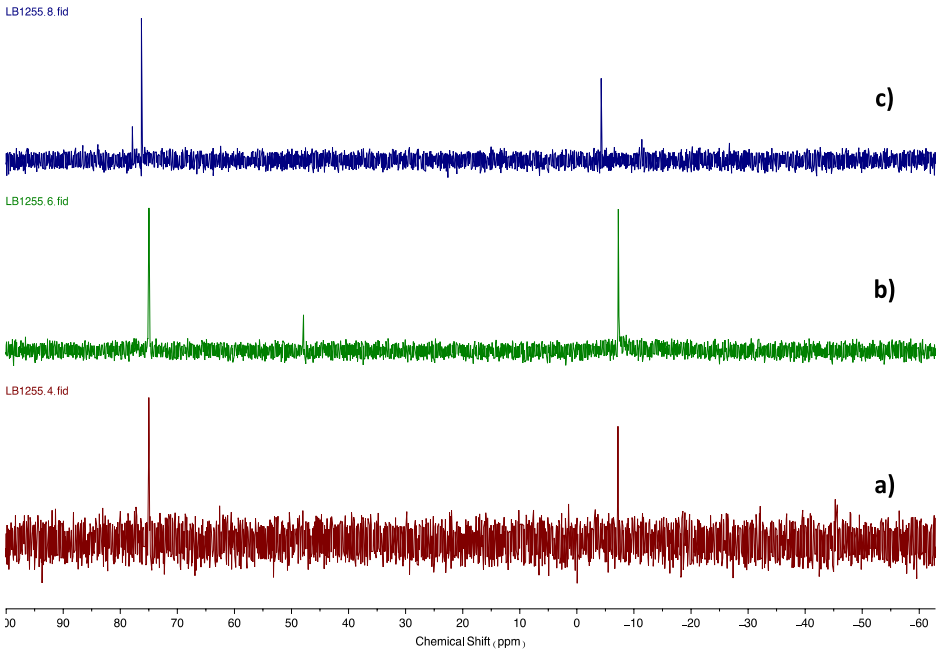


Figure S12. ^{1}H NMR spectra (400 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 1 equiv of ^{13}CO a) before and b) immediately after addition.

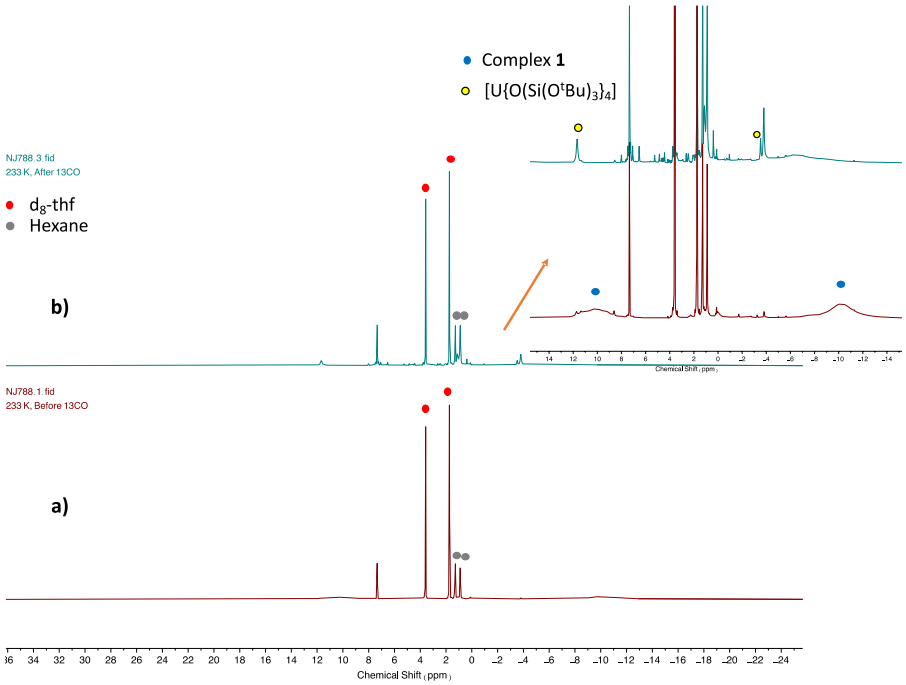


Figure S13. $^{31}P\{^{1}H\}$ NMR (162 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 1 equiv of ^{13}CO a) before and b) immediately after addition.

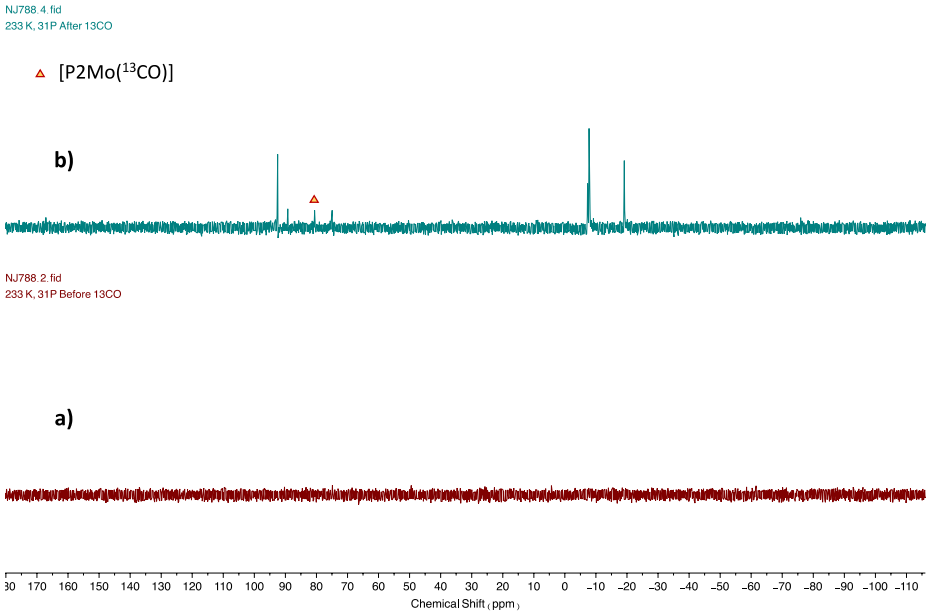


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 1 equiv. of ^{13}CO immediately after addition.

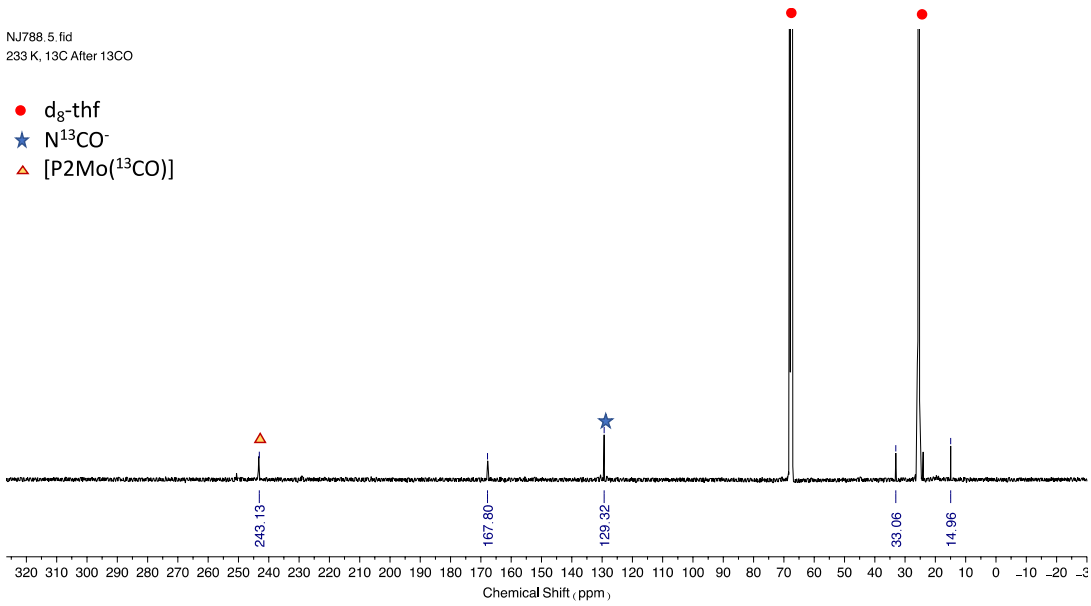


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, D_2O, 298K) of the hydrolysis with pD=13 D_2O of the reaction mixture between complex **1** and 1 equiv of ^{13}CO.

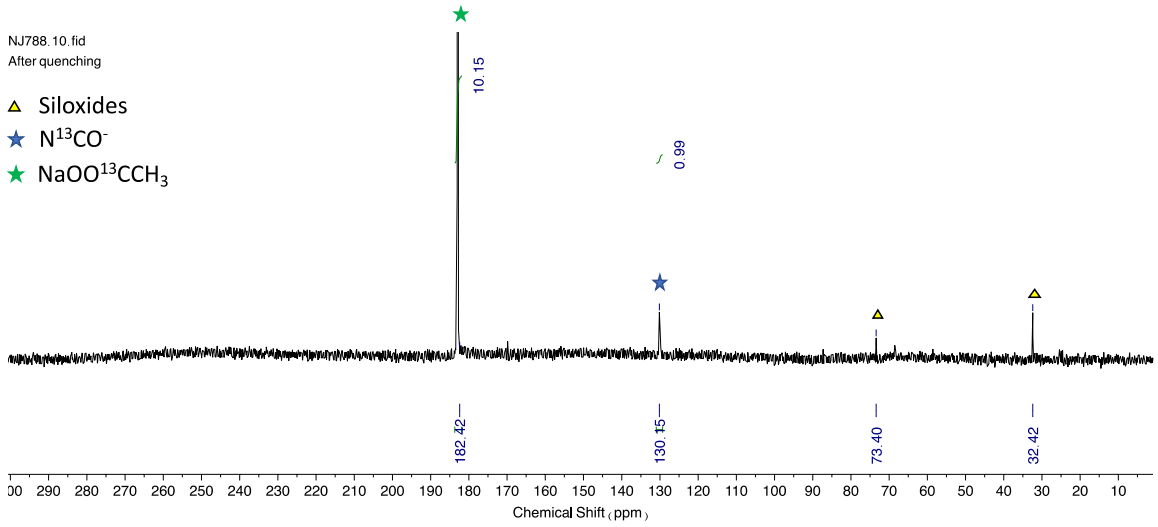


Figure S16. ^{1}H NMR spectrum (400 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 1 atm of ^{13}CO immediately after addition.

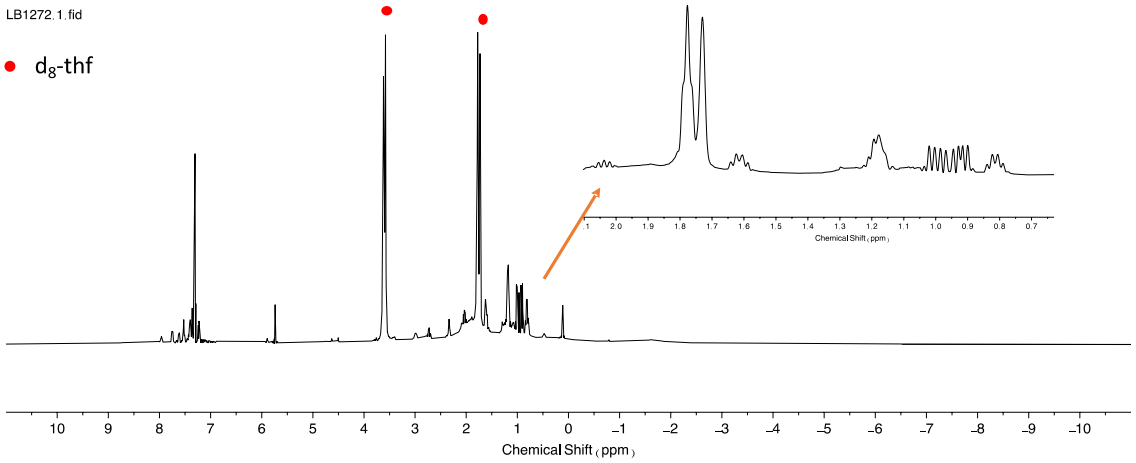


Figure S17. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 1 atm of ^{13}CO immediately after addition.

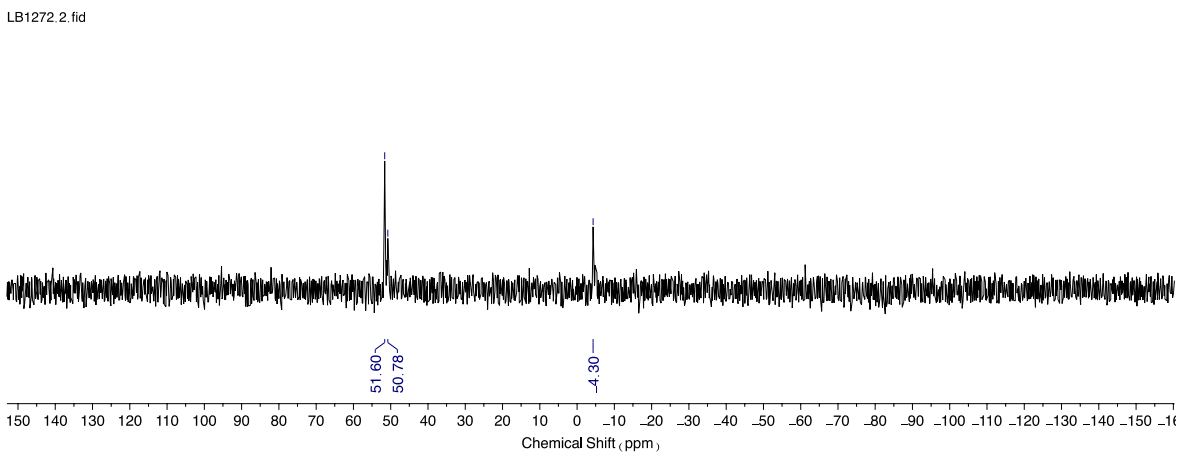


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 1 atm of ^{13}CO immediately after addition.

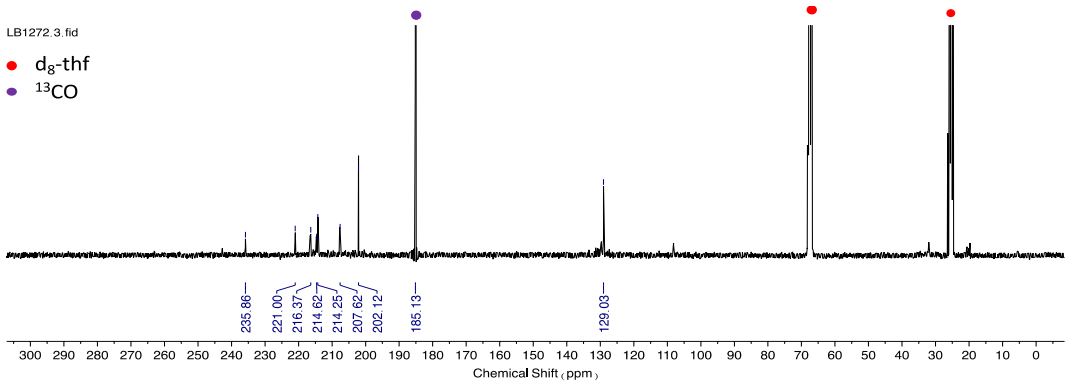


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, D_2O, 298K) of the hydrolysis with pD=13 D_2O of the reaction mixture between complex **1** and 1 atm of ^{13}CO.

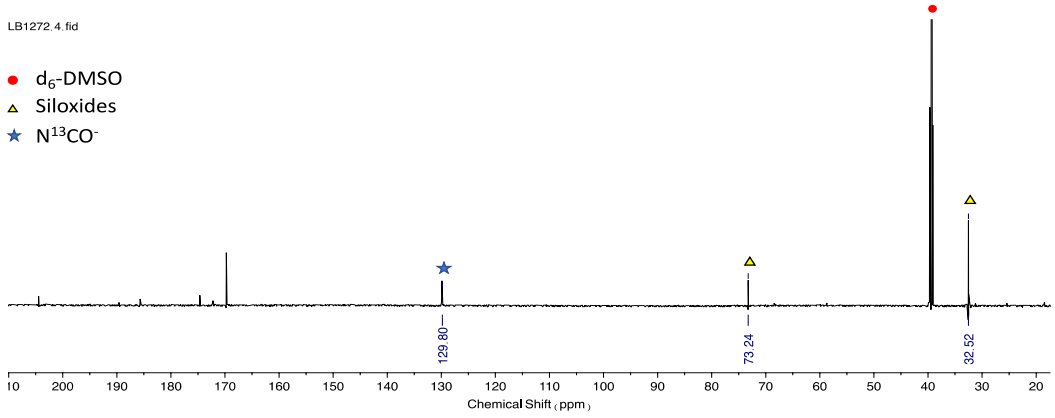


Figure S20. ^{1}H NMR spectra (400 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 10 equiv of ^{13}CO before and b) immediately after addition.

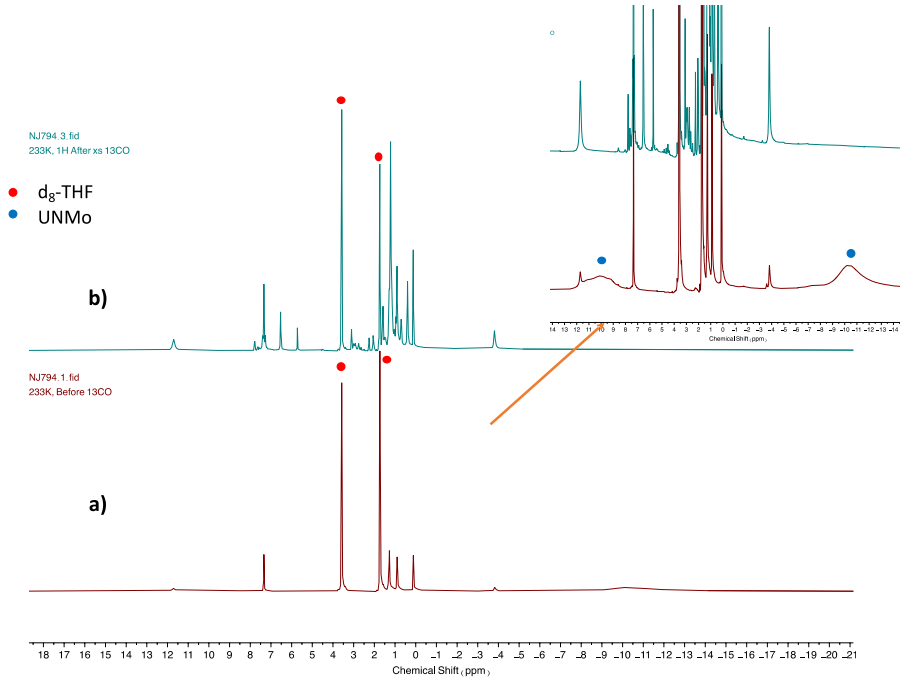


Figure S21. ^{31}P{^{1}H} NMR (162 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 10 equiv of ^{13}CO a) before and b) immediately after addition.

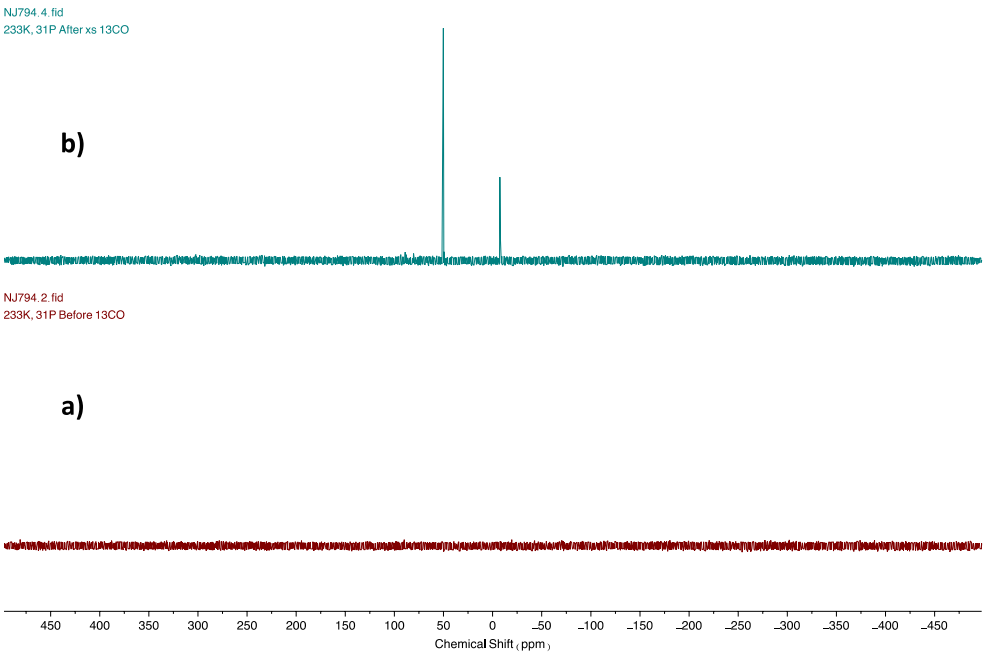


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, d_8-thf, 233K) of the reaction mixture of complex **1** with 10 equiv. of ^{13}CO immediately after addition.

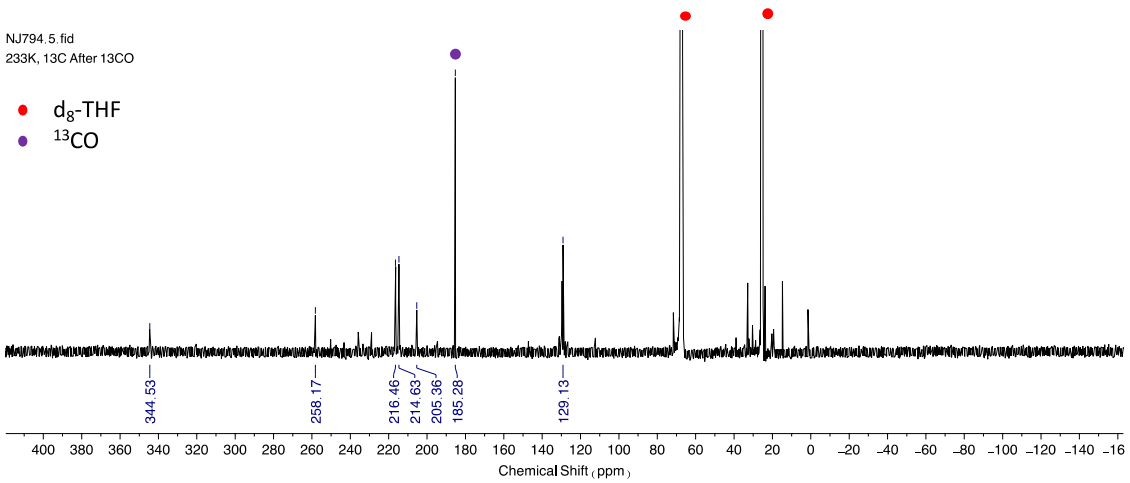


Figure S23. ^{1}H NMR spectra (400 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 10 equiv of ^{13}CO a) 24 hs after at -40°C and b) 24 hs after warmed up to 25°C.

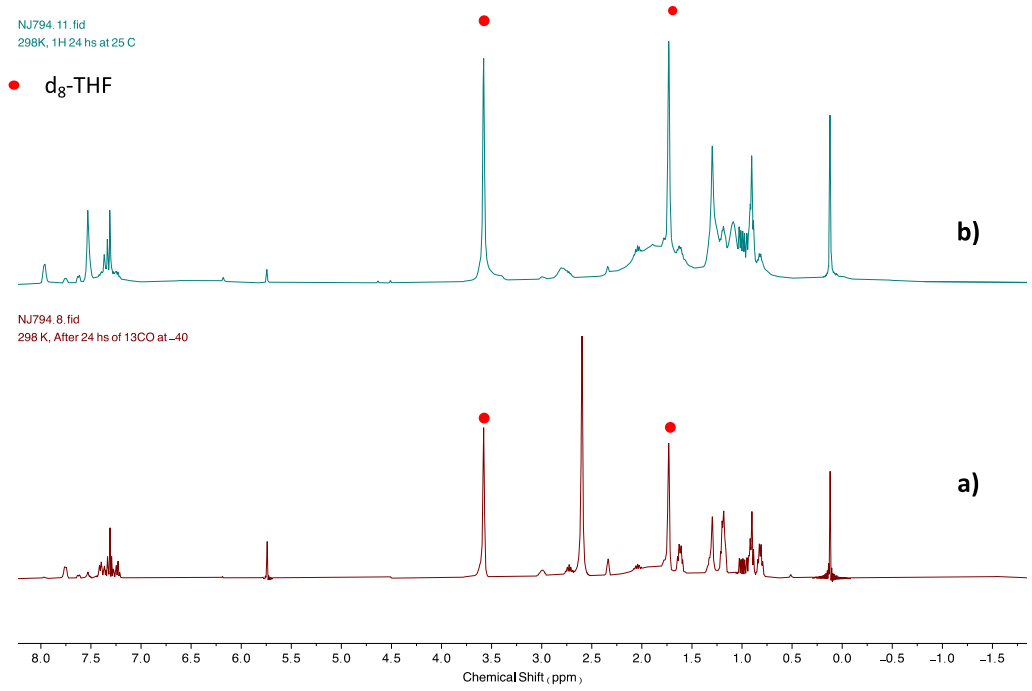


Figure S24. $^{31}P\{^{1}H\}$ NMR (162 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 10 equiv of ^{13}CO a) 24 hs after at -40°C and b) 24 hs after warmed up to 25°C.

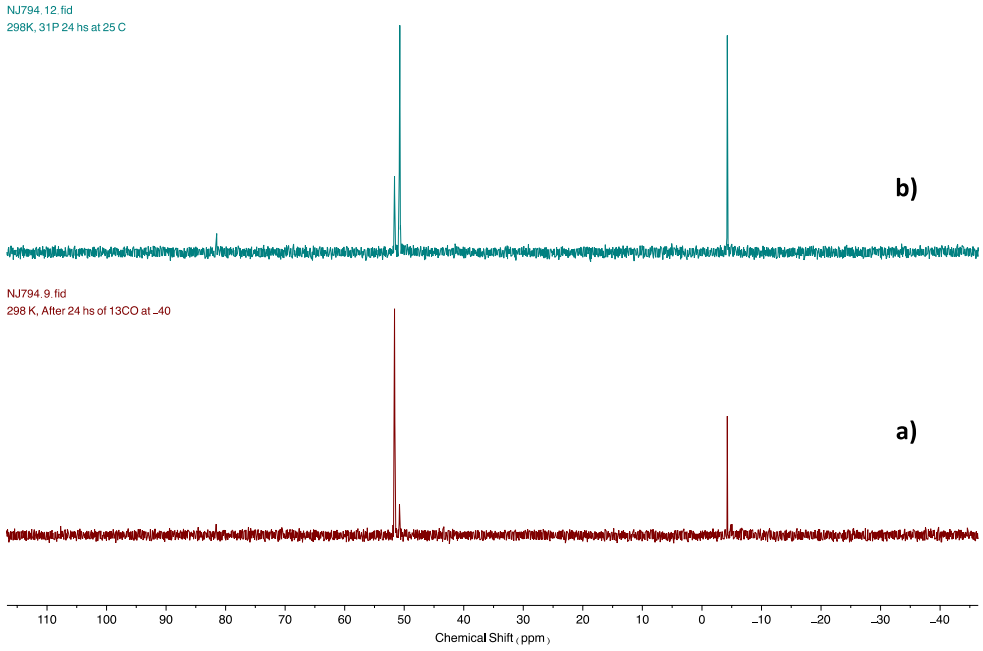


Figure S25. $^{13}C\{^{1}H\}$ NMR (100 MHz, d_8-thf, 298K) of the reaction mixture of complex **1** with 10 equiv of ^{13}CO a) 24 hs after at -40°C and b) 24 hs after warmed up to 25°C.

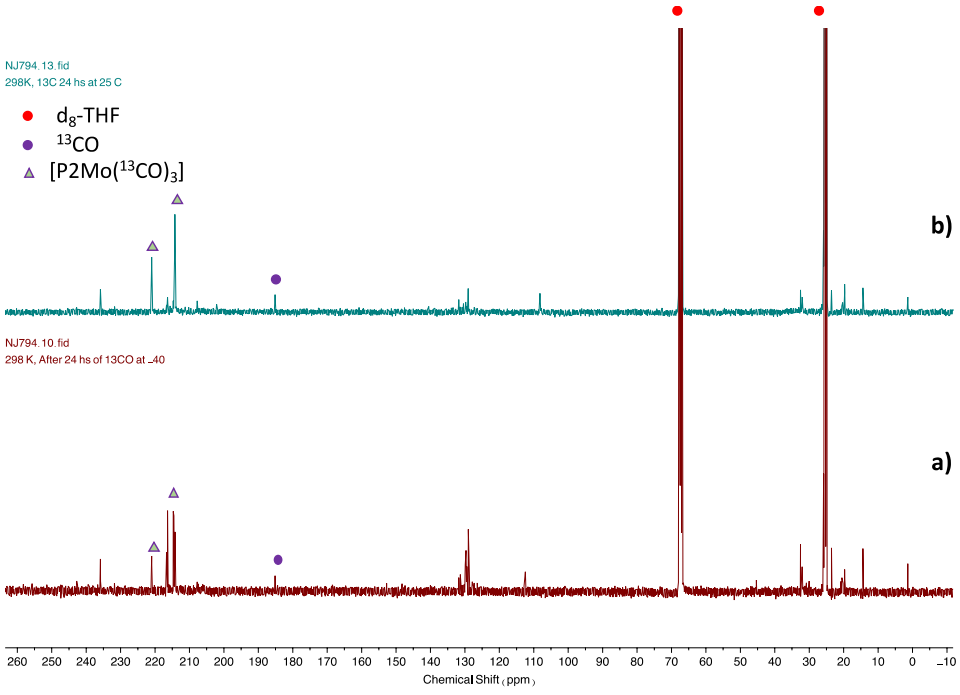


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, D_2O, 298K) of the hydrolysis with pD=13 D_2O of the reaction mixture between complex **1** and 10 equiv of ^{13}CO.

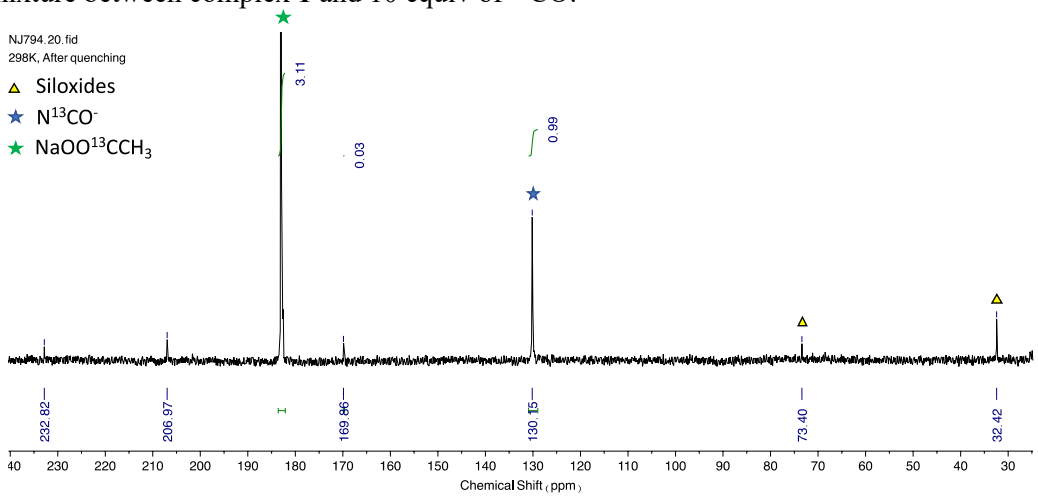
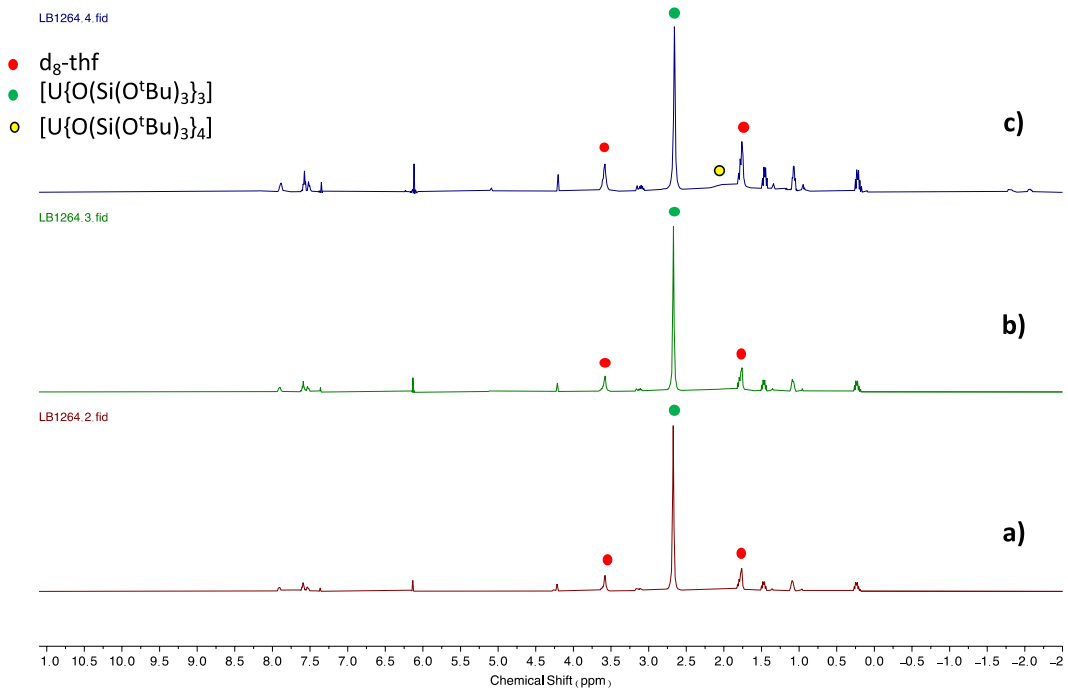


Figure S27. ^{1}H NMR spectra (400 MHz, d_8-thf, 298K) of the evolution of the reaction mixture of 2 equiv. of $[Cl(N)Mo^{IV}P2]$ with 1 equiv. of $[U(OSi(O^tBu)_3)_3]_2$ at room temperature, a) immediately after addition, b) 6 hs after addition, c) 24 hs after addition at -40°C.



XRD data

A translucent dark black irregular-shaped crystal with dimensions 0.40 × 0.23 × 0.19 mm^3 was mounted and its diffraction data were collected using a SuperNova diffractometer operating at T = 140.00(10) K. Data were measured using ω scans using Cu K α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro.[4] The maximum resolution that was achieved was Θ = 76.009° (0.79 Å).
The unit cell was refined using CrysAlisPro [4] on 38652 reflections, 78% of the observed reflections. Data reduction, scaling and absorption corrections were performed using CrysAlisPro.[4] The final completeness is 99.80 % out to 76.009° in Θ. A gaussian absorption correction was performed using CrysAlisPro.[4] The numerical absorption correction was based on gaussian integration over a multifaceted crystal model. The empirical absorption correction was obtained using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The absorption coefficient μ of this crystal is 7.873 mm^{-1} at this wavelength (λ = 1.54184Å) and the minimum and maximum transmissions are 0.194 and 0.880. The structure was solved and the space group P-1 (# 2) determined by the ShelXT [5] structure solution program using dual methods and refined by full matrix least squares minimisation on F^2 using version 2018/3 of ShelXL. [6]All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. CCDC deposition number: 2126561.

Table S1: Crystallographic parameters for complex 1

Compound	1
Formula	$C_{72}H_{135}MoNNaO_{12}P_2Si_3U$
Crystal size [mm]	0.40×0.23×0.19
Crystal system	triclinic
Space group	P-1
V [Å^3]	4186.49(16)
a [Å]	13.6525(2)
b [Å]	16.4788(4)
c [Å]	19.2469(4)
α [°]	81.3024(19)
β [°]	79.5672(16)
γ [°]	82.5868(18)
Z	2
Absorption coefficient [mm^{-1}]	7.873
F(000)	1774.0
T(K)	140.00(10)
Total no. reflections	49516
Unique reflexions [R_{int}]	17241
Final R_1 [I>2 σ(I)]	0.0268
Largest diff. peak and hole [eA^{-3}]	1.724 and -2.013
GOOF	1.070

EPR data

CW EPR spectroscopy. The solution state spectra were recorded from an 8.6 mM solution of complex **1** in THF inside J-Young EPR tubes. The solid state measurements were performed with solid samples of complex **1** inside J-Young EPR tubes or in sealed quartz tubes. X-band CW EPR spectra were acquired on a Bruker Elexsys E500 spectrometer working at 9.4 GHz frequency and on a Bruker (Billerica, MA) EMX spectrometer using a Bruker ER 4116DM Dual Mode resonator coupled to the TE-102 perpendicular mode (MW B_1 perpendicular to the applied magnetic field B_0). Acquisition parameters: MW frequency = 9.638 GHz; temperature = 5 K; MW power = 5.5 mW; modulation amplitude = 0.8 mT; conversion time = 10.10 ms. Temperature control was achieved using liquid helium and an Oxford Instruments (Oxford, UK) ESR-900 cryogen flow cryostat and an ITC-503 temperature controller

Pulse EPR spectroscopy. All pulse EPR experiments were aquired using a Bruker (Billerica, MA) ELEXSYS E580 pulse EPR spectrometer. All data was acquired using a Bruker MD-4 resonator. Temperature control was achieved using an ER 4118HV-CF5-L Flexline Cryogen-Free VT cryostat manufactured by ColdEdge (Allentown, PA) equipped with an Oxford Instruments Mercury ITC.

X-band HYSCORE spectra[8] were acquired using the 4-pulse sequence ($\pi/2 - \tau - \pi/2 - t_1 - \pi - t_2 - \pi/2 -$ echo), where τ is a fixed delay, while t_1 and t_2 are independently incremented by Δt_1 and Δt_2, respectively. The time domain data was baseline-corrected (third-order polynomial) to eliminate the exponential decay in the echo intensity, apodized with a Hamming window function, zero-filled to eight-fold points, and fast Fourier-transformed to yield the 2-dimensional frequency domain.

In general, the ENDOR spectrum for a given nucleus with spin I= ½ (^{1}H, ^{31}P) coupled to the S = ½ electron spin exhibits a doublet at frequencies

$$\nu_{\pm} = \left|\frac{A}{2} \pm \nu_N\right|$$

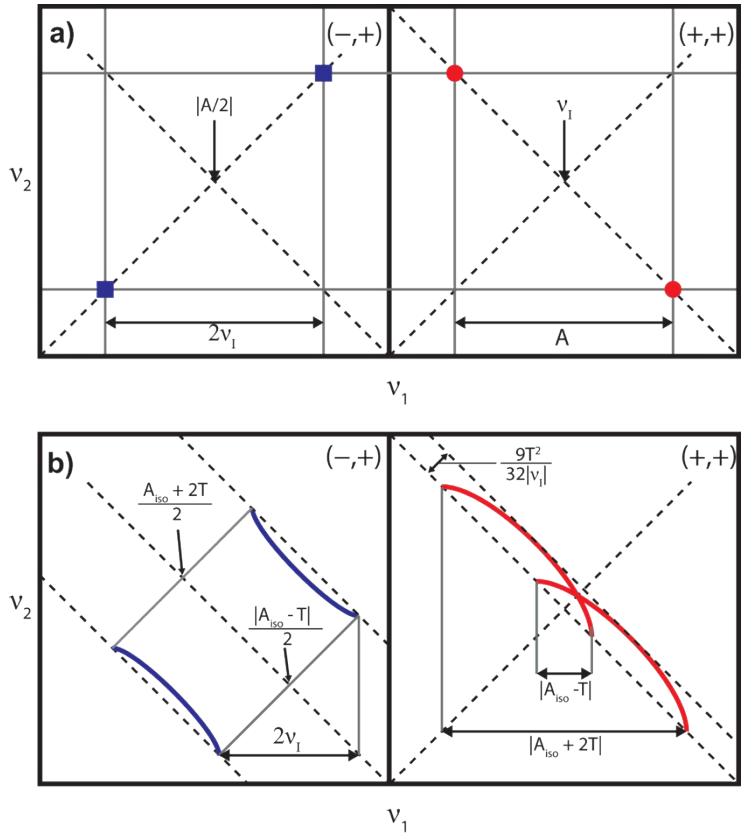
Where ν_N is the nuclear Larmor frequency and A is the hyperfine coupling. For nuclei with $I \geq 1$ (14N, 2H), an additonal splitting of the $\nu_{\pm}$ manifolds is produced by the nuclear quadrupole interaction (P)

$$\nu_{\pm,m_I} = \left|\nu_N \pm \frac{3P(2m_I - 1)}{2}\right|$$

In HYSCORE spectra, these signals manifest as cross-peaks or ridges in the 2-D frequency spectrum which are generally symmetric about the diagonal of a given quadrant. This technique allows hyperfine levels corresponding to the same electron-nuclear submanifold to be differentiated, as well as separating features from hyperfine couplings in the weak-coupling regime ($|A| < 2|\nu_I|$) in the (+,+) quadrant from those in the strong coupling regime ($|A| > 2|\nu_I|$) in the (−,+) quadrant. The (−,−) and (+,−) quadrants of these frequency spectra are symmetric to the (+,+) and (−,+) quadrants, thus only two of the quadrants are typically displayed in literature.

For systems with appreciable hyperfine anisotropy in frozen solutions or solids, HYSCORE spectra typically do not exhibit sharp cross peaks, but show ridges that represent the sum of cross peaks from selected orientations within the excitation bandwidth of the MW pulses at the magnetic field position at which the spectrum is collected. The length and curvature of these correlation ridges can allow for the separation and estimation of the magnitude of the isotropic and dipolar components of the hyperfine tensor (Figure S28).

Figure S28. a) HYSCORE powder patterns for an $S = ½$, $I = ½$ spin system with an isotropic hyperfine tensor A. b) HYSCORE powder patterns for an $S = ½$, $I = ½$ spin system with an axial hyperfine tensor that contains isotropic (a_{iso}) and dipolar (T) contributions. Blue correlation ridges represent the strong coupling case; red correlation ridges represent the weak coupling case.



For I = 1 nuclei such as ^{14}N, the nuclear quadrupole interaction will further split the hyperfine correlation ridges parallel to the diagonal of the quadradrant by 3P.

Figure S29. X-band EPR spectrum of frozen 8.4 mM solution complex **1** in THF at 10K.

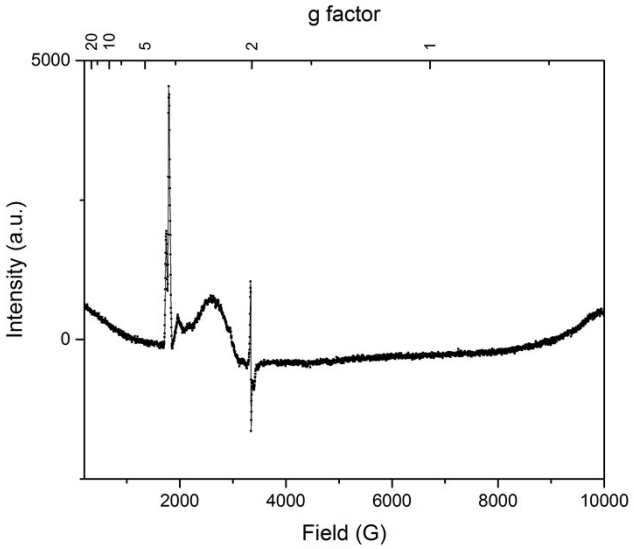


Figure S30. (Top) X-band CW-EPR spectrum of pure powder of **1**. Acquisition parameters: MW frequency = 9.638 GHz; temperature = 5 K; MW power = 5.5 mW; modulation amplitude = 0.8 mT; conversion time = 10.10 ms. (A signal centred at $g = 1.99$ is sometimes observed which is due to degradation products.

(**Bottom) X**-band electron spin-echo (ESE) detected EPR spectrum of pure powder of **1** (top trace), with same spectrum treated with pseudomodulation (bottom trace) to generate the "CW-like" 1st derivative using an amplitude of 20 mT. Acquisition parameters: MW frequency = 9.387 GHz; temperature = 6 K; π pulse length = 16 ns; τ = 200 ns; shot rep time (srt) = 500 μs.

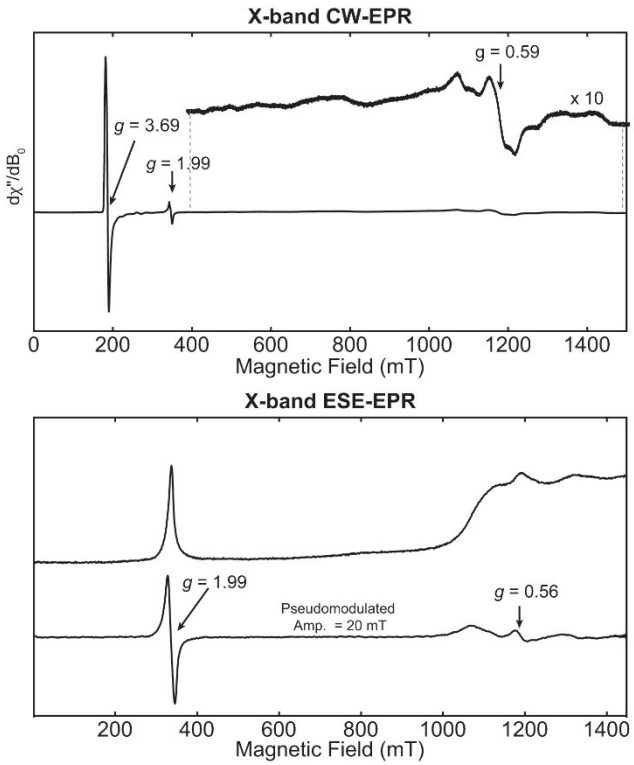


Figure S31. X-band HYSCORE spectra of pure powder of **1** acquired at 1000 mT (g = 0.671), 1060 mT (g = 0.633), 1200 mT (g = 0.559), 1440 mT (g = 0.466). Acquisition parameters: MW frequency = 9.387 GHz; temperature = 6 K; τ = 100 ns, $t_1 = t_2$ = 100 ns; $\Delta t_1 = \Delta t_2$ = 16 ns; shot repetition time (srt) = 500 µs.

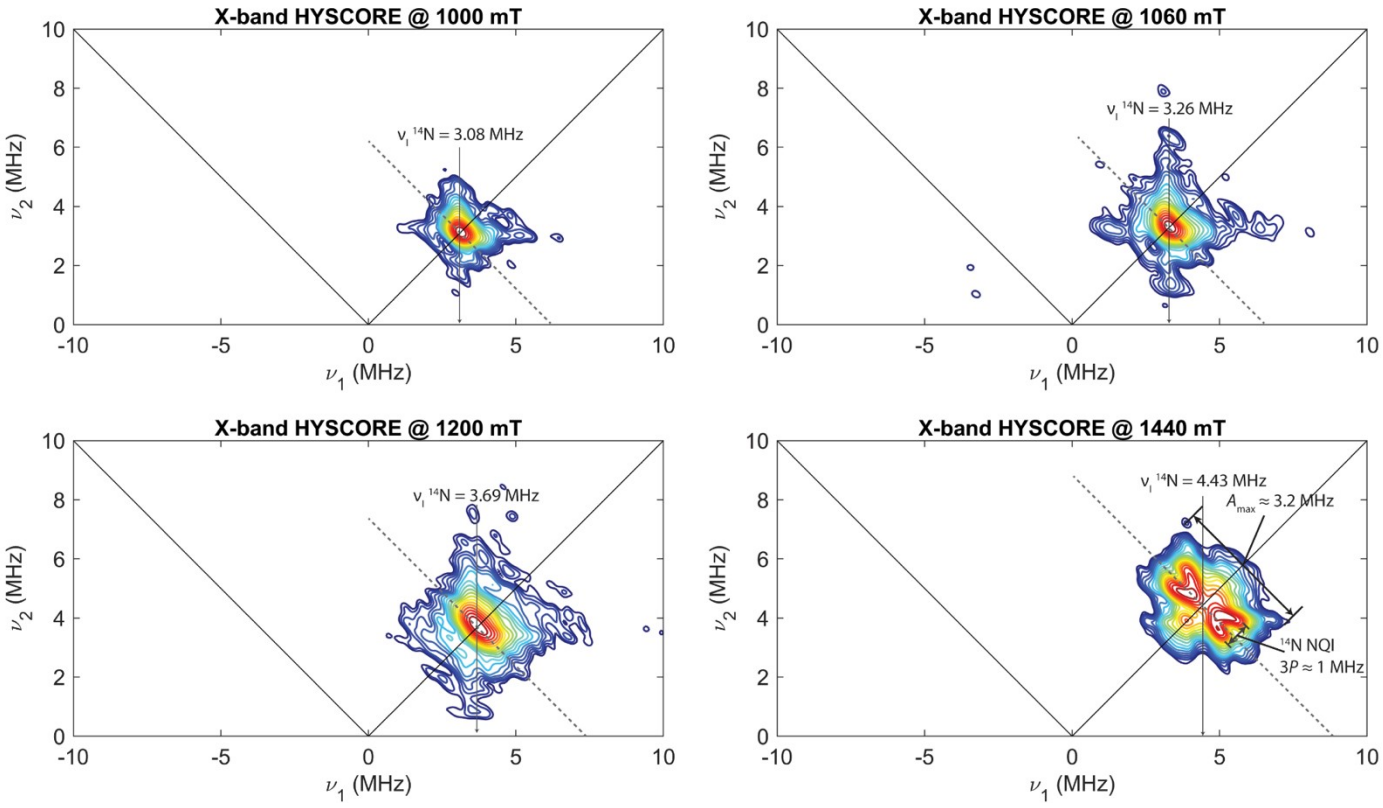
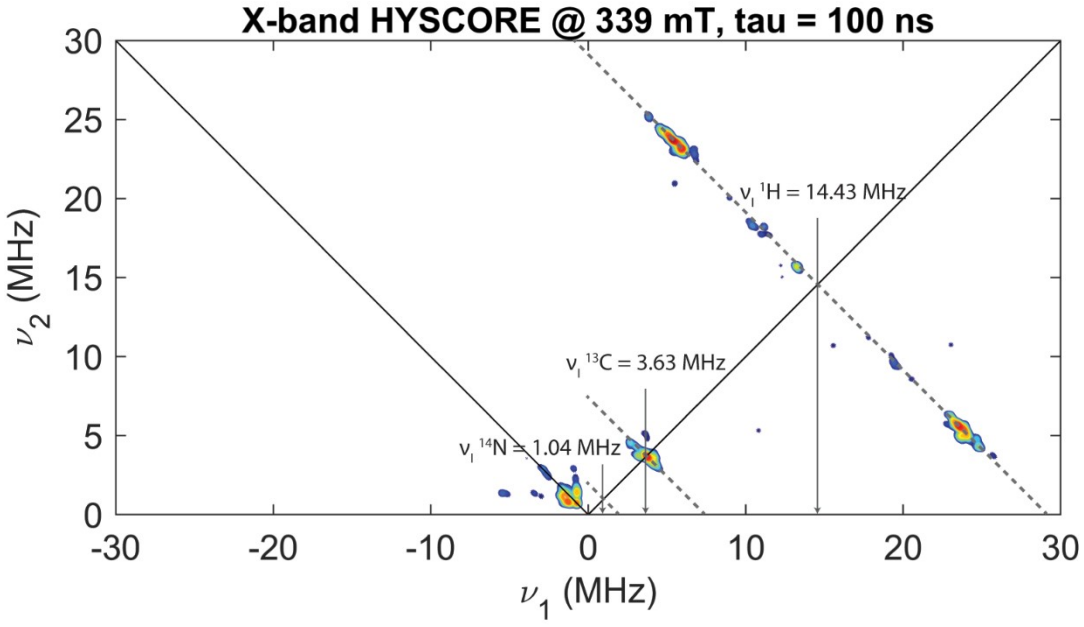


Figure S32. X-band HYSCORE spectrum of pure powder of **1** acquired at 339 mT (g = 1.98), a magnetic field corresponding to the narrow signal associated with degradation product(s) of **1**. Acquisition parameters: MW frequency = 9.387 GHz; temperature = 6 K; τ = 100 ns, $t_1 = t_2$ = 100 ns; $\Delta t_1 = \Delta t_2$ = 16 ns; shot repetition time (srt) = 500 μs.



Computational details

The optimization of three different spin states (S=2, 4 and 6) for complex **1** were carried out by employing unrestricted-DFT hybrid functional (B3PW91) [7] along with small core relativistic effective core potential Stuggart basis set for uranium, molybdenum, phosphorus, and silicon atoms with additional polarization functions for phosphorus and silicon atoms.[9] Pople basis sets (6-31^{++}G** basis set for sodium and 6-31G** for carbon, nitrogen, oxygen, hydrogen atoms) were employed for the rest of the atoms.[10] Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs. [11] NBO analysis was done in two main steps. The first one defines the Natural Localized Molecular Orbital (NLMO) which are the bonds and the lone pairs. These NLMO are thus used in a second step as possible donor (when occupied) and potential acceptor (when empty) to look for the presence of donor-acceptor bonds in the complex. The donor-acceptor interactions are accounted for at the second order perturbation level by computing an interaction energy ($\propto \frac{S^2}{\Delta\epsilon}$).

Bonding orbitals between uranium and nitrogen from NBO analysis for ground state spin (2s+1=2)

(0.98344) BD (1) U 1 - N 21
(33.62%) 0.5798* U 1 s(0.01%)p23.29(0.32%)d99.99(28.73%) f99.99(70.90%)g 3.10(0.04%)
(66.38%) 0.8147* N 21 s(13.91%)p 6.17(85.78%)d 0.02(0.31%)
(0.96717) BD (2) U 1 - N 21
(28.06%) 0.5297* U 1 s(0.00%)p 1.00(0.87%)d34.46(30.14%) f78.84(68.95%)g 0.04(0.03%)
(71.94%) 0.8482* N 21 s(0.00%)p 1.00(99.77%)d 0.00(0.23%)
(0.83262) BD (3) U 1 - N 21
(20.20%) 0.4495* U 1 s(0.17%)p 8.84(1.54%)d99.99(43.36%) f99.99(54.88%)g 0.24(0.04%)
(79.80%) 0.8933* N 21 s(7.47%)p12.37(92.36%)d 0.02(0.17%)

Table ST1: Computed Wiberg bond index for UNMo core (2s+1=2)

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
U1	0.0000	U1	0.5243
Mo2	0.5243	Mo2	0.0000
N21	2.2633	N21	0.7308

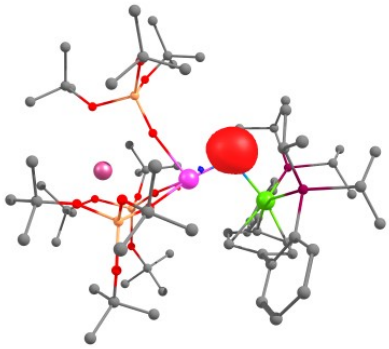
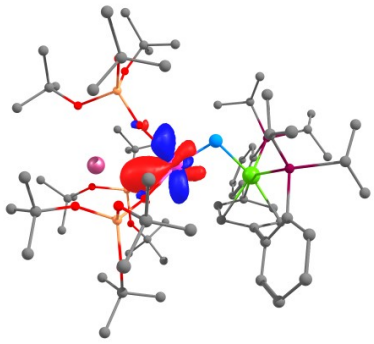
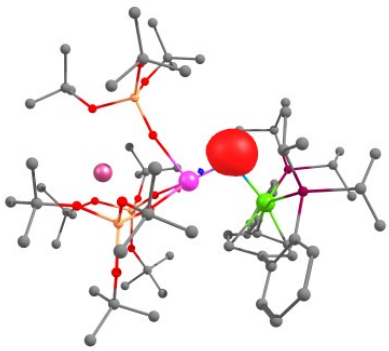
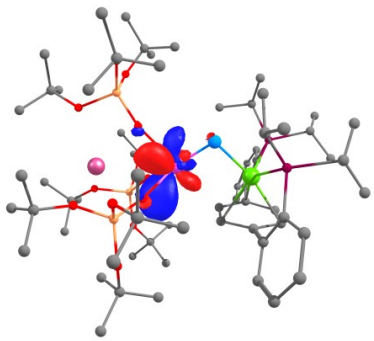
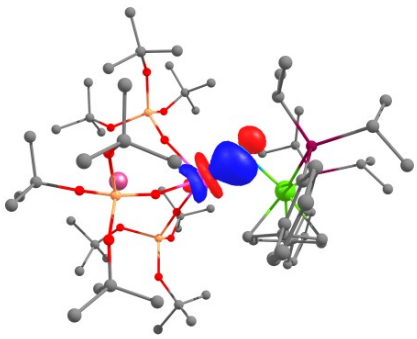
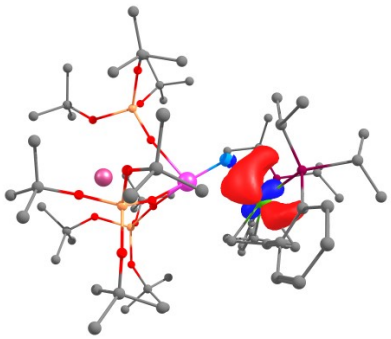
Table ST2: Computed spin densities for UNMo core

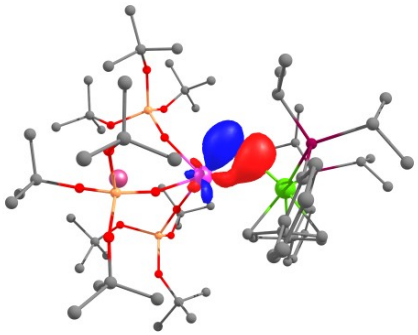
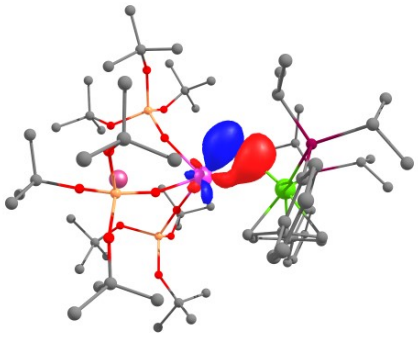
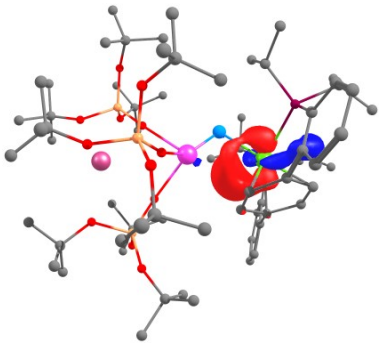
Atom Label	Spin density		
	2s+1=2	2s+1=4	2s+1=6
U1	1.24	2.35	3.28
Mo2	-0.05	0.72	0.70
N21	-0.13	0.02	0.49

Table ST3: Energetics of different spin states computed for UNMo complex

Spin states	ΔH (kcal/mol)
2s+1=2	0.0
2s+1=4	6.32
2s+1=6	23.07

Table ST4: DFT computed NBO second order perturbation analysis for 2s+1=2 spin state. For sake of clarity only the alpha part is reported since the beta part is similar. The value between bracket before the donor or acceptor unit indicates the electron occupancy.

Donor NBO	Acceptor NBO	E(2) kcal/mol
(0.84547) LP (1) N 21 s(78.62%)p 0.27(21.34%)d 0.00(0.04%) 	(0.12375) LP*(1) U 1 s(0.33%)p 0.60(0.20%)d99.99(57.42%) f99.99(42.03%)g 0.02(0.01%) 	12.65
(0.84547) LP (1) N 21 s(78.62%)p 0.27(21.34%)d 0.00(0.04%) 	(0.08514) LP*(5) U 1 s(0.18%)p12.19(2.21%)d99.99(63.71%) f99.99(33.90%)g 0.04(0.01%) 	7.38
(0.98344) BD (1) U 1 - N 21 (33.62%) 0.5798* U 1 s(0.01%)p23.29(0.32%)d99.99(28.73%)f99.99(70.90%)g 3.10(0.04%) (66.38%) 0.8147* N 21 s(13.91%)p 6.17(85.78%)d 0.02(0.31%) 	(0.22822) LP*(2)Mo 2 s(37.59%)p 0.69(25.92%)d 0.97(36.49%) 	6.54

(0.83262) BD (3) U 1 - N 21 (20.20%) 0.4495* U 1 s(0.17%)p 8.84(1.54%)d99.99(43.36%)f99.99(54.88%)g 0.24(0.04%) (79.80%) 0.8933* N 21 s(7.47%)p12.37(92.36%)d 0.02(0.17%) 	(0.22822) LP*(2)Mo 2 s(37.59%)p 0.69(25.92%)d 0.97(36.49%) 	40.58
(0.83262) BD (3) U 1 - N 21 (20.20%) 0.4495* U 1 s(0.17%)p 8.84(1.54%)d99.99(43.36%)f99.99(54.88%)g 0.24(0.04%) (79.80%) 0.8933* N 21 s(7.47%)p12.37(92.36%)d 0.02(0.17%) 	(0.16714) LP*(3)Mo 2 s(11.48%)p 6.04(69.36%)d 1.67(19.16%) 	19.71
(0.84547) LP (1) N 21 s(78.62%)p 0.27(21.34%)d 0.00(0.04%) 	(0.22822) LP*(2)Mo 2 s(37.59%)p 0.69(25.92%)d 0.97(36.49%) 	34.94
(0.84547) LP (1) N 21 s(78.62%)p 0.27(21.34%)d 0.00(0.04%)	(0.16714) LP*(3)Mo 2 s(11.48%)p 6.04(69.36%)d 1.67(19.16%)	21.63

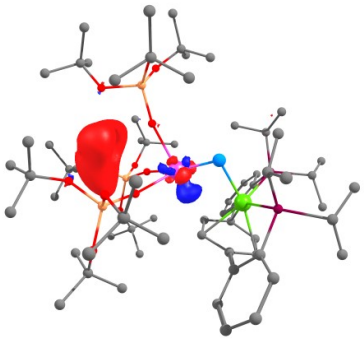
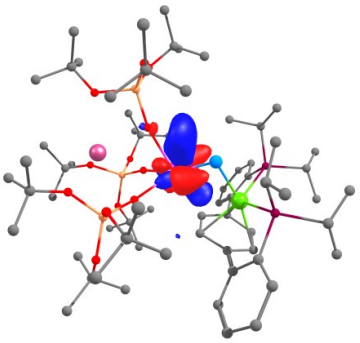
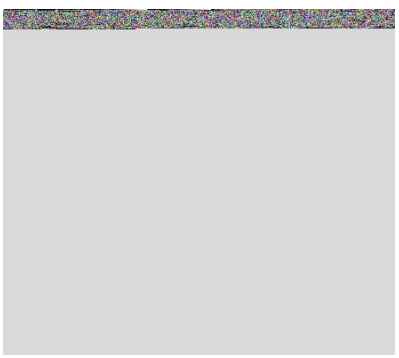
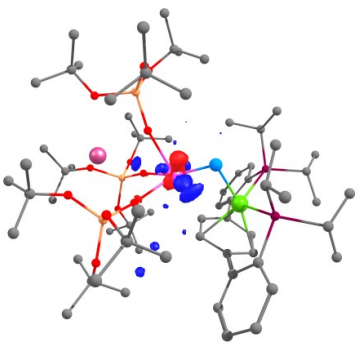
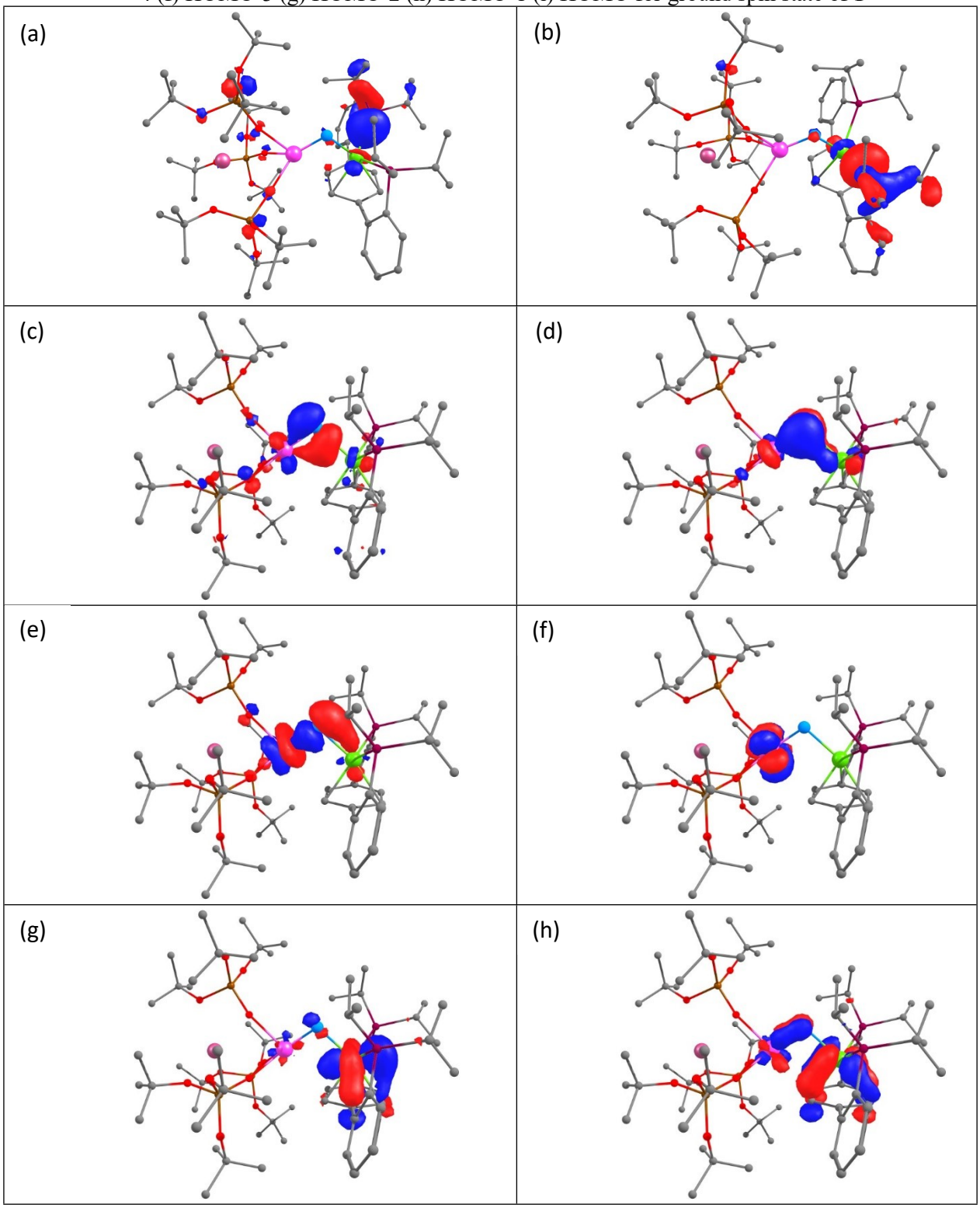
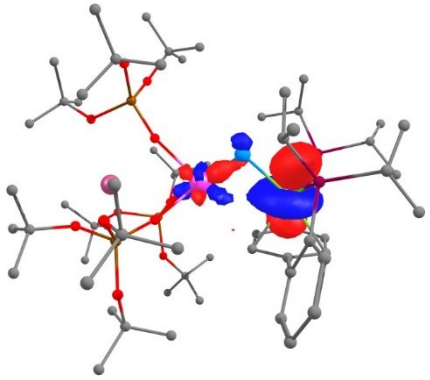
		
(0.16714) LP*(3)Mo 2 s(11.48%)p 6.04(69.36%)d 1.67(19.16%) 	(0.05464) LP*(6) U 1 s(2.17%)p37.80(81.86%)d 3.67(7.94%)f 3.71(8.03%)g 0.00(0.01%) 	38.92
(0.16714) LP*(3)Mo 2 s(11.48%)p 6.04(69.36%)d 1.67(19.16%) 	(0.03593) LP*(8) U 1 s(6.22%)p 3.53(21.95%)d 3.35(20.81%)f 8.20(50.99%)g 0.01(0.04%) 	28.11
(0.16714) LP*(3)Mo 2 s(11.48%)p 6.04(69.36%)d 1.67(19.16%) 	(0.03280) LP*(9) U 1 s(79.76%)p 0.05(3.68%)d 0.05(4.26%)f 0.15(12.29%)g 0.00(0.00%) 	10.00

Figure S33: DFT computed MO's (a) HOMO-13 (b) HOMO-12 (c) HOMO-10 (d) HOMO-5 (e) HOMO-4 (f) HOMO-3 (g) HOMO-2 (h) HOMO-1 (i) HOMO for ground spin state of **1**



(i)



DFT optimized geometry of different spin states for 1
Doublet

U	13.373014000	7.508402000	14.309249000
Mo	14.054513000	10.438451000	15.203738000
P	12.592982000	11.984486000	13.784119000
P	16.535300000	10.911015000	14.833859000
Si	14.303842000	4.508047000	16.563289000
Si	9.766138000	6.142340000	14.379542000
Si	13.946501000	5.195736000	11.273678000
Na	12.416378000	4.304268000	13.901776000
O	14.066600000	5.744646000	15.517618000
O	15.896142000	4.116063000	16.845905000
O	13.599295000	4.678158000	18.058553000
O	13.466498000	3.210826000	15.844509000
O	11.302513000	6.667215000	14.581467000
O	8.967692000	6.754345000	13.051812000
O	9.944509000	4.482477000	14.043751000
O	8.741265000	6.423176000	15.664034000
O	13.469778000	6.064380000	12.570414000
O	15.588432000	4.968788000	11.109708000
O	13.447491000	5.742550000	9.779228000
O	13.307797000	3.656540000	11.634079000
N	14.034595000	9.038130000	13.553368000
C	17.050721000	4.105051000	15.989713000
C	16.714584000	3.502333000	14.626778000
H	17.611707000	3.446856000	14.002180000
H	15.978534000	4.111516000	14.095068000
H	16.315750000	2.490069000	14.740189000
C	18.087316000	3.243378000	16.713350000
H	17.718333000	2.221419000	16.842380000
H	18.301919000	3.657246000	17.703196000
H	19.021940000	3.204453000	16.144677000
C	17.560763000	5.536078000	15.837322000
H	18.468780000	5.562408000	15.225888000
H	17.789831000	5.970614000	16.814646000
H	16.801564000	6.155307000	15.354793000
C	13.947434000	5.220079000	19.343564000
C	12.928516000	6.317529000	19.654959000
H	13.093422000	6.725839000	20.657696000
H	11.912959000	5.914501000	19.608838000
H	13.006713000	7.136817000	18.935291000
C	15.366469000	5.781992000	19.374497000
H	15.492546000	6.574963000	18.632574000
H	16.101564000	5.003000000	19.165366000
H	15.572231000	6.207756000	20.362515000
C	13.816455000	4.081552000	20.359115000
H	14.001812000	4.448372000	21.374069000
H	14.539128000	3.287965000	20.147526000
H	12.810334000	3.652593000	20.329245000
C	13.212692000	1.911152000	16.440533000
C	13.007934000	0.944624000	15.276340000
H	12.809732000	-0.066447000	15.646415000
H	13.897999000	0.910437000	14.641560000
H	12.151785000	1.248025000	14.667380000

C	11.942831000	2.000619000	17.285896000
H	11.101544000	2.332301000	16.671636000
H	12.079374000	2.719225000	18.095567000
H	11.694204000	1.022920000	17.712728000
C	14.388920000	1.432273000	17.291960000
H	14.158829000	0.445560000	17.707483000
H	14.583896000	2.115286000	18.120487000
H	15.300282000	1.350676000	16.695072000
C	8.186413000	7.952095000	12.883307000
C	6.751943000	7.678353000	13.340286000
H	6.315972000	6.857692000	12.761206000
H	6.126324000	8.565698000	13.195769000
H	6.737735000	7.408600000	14.398902000
C	8.215796000	8.256704000	11.385515000
H	9.241552000	8.439245000	11.053511000
H	7.614133000	9.143207000	11.160183000
H	7.813630000	7.413223000	10.815698000
C	8.793203000	9.106528000	13.672627000
H	8.779242000	8.895851000	14.744665000
H	8.231556000	10.030032000	13.505349000
H	9.828107000	9.280309000	13.366445000
C	8.922751000	3.579325000	13.540762000
C	8.842704000	3.718501000	12.021514000
H	8.544196000	4.732566000	11.750437000
H	8.116628000	3.008835000	11.610113000
H	9.817097000	3.513810000	11.570382000
C	9.379862000	2.171658000	13.917233000
H	10.343093000	1.939810000	13.453910000
H	8.656641000	1.428163000	13.566963000
H	9.476736000	2.070783000	15.002011000
C	7.558590000	3.855710000	14.171726000
H	7.592536000	3.724100000	15.255872000
H	6.821071000	3.154564000	13.767244000
H	7.219801000	4.870443000	13.956284000
C	8.783995000	6.175042000	17.077559000
C	7.330902000	5.955426000	17.507064000
H	6.724095000	6.829357000	17.251550000
H	7.267510000	5.795387000	18.588246000
H	6.903164000	5.084130000	17.003655000
C	9.631039000	4.947441000	17.403008000
H	9.242519000	4.060783000	16.895350000
H	9.618874000	4.753991000	18.480734000
H	10.671947000	5.093874000	17.101302000
C	9.345836000	7.413209000	17.773779000
H	10.391724000	7.569916000	17.501878000
H	9.290719000	7.304604000	18.862175000
H	8.774640000	8.299776000	17.484779000
C	16.586769000	5.644872000	10.322756000
C	17.913519000	5.373047000	11.033208000
H	17.891644000	5.777195000	12.048673000
H	18.746021000	5.833443000	10.490994000
H	18.097397000	4.295922000	11.096670000
C	16.312803000	7.146055000	10.249412000
H	15.390186000	7.339621000	9.698472000
H	17.134411000	7.657193000	9.736234000
H	16.213683000	7.573071000	11.249534000

C	16.607945000	5.040655000	8.917059000
H	16.810602000	3.965709000	8.962639000
H	17.391006000	5.508028000	8.310160000
H	15.646059000	5.199508000	8.422941000
C	12.243033000	6.372284000	9.317804000
C	11.014342000	5.715229000	9.938688000
H	11.004008000	4.643192000	9.722683000
H	10.097615000	6.154208000	9.532651000
H	10.997815000	5.856843000	11.022408000
C	12.238222000	6.184073000	7.799285000
H	13.139304000	6.621576000	7.358914000
H	11.364348000	6.668456000	7.351661000
H	12.213620000	5.120537000	7.543436000
C	12.299608000	7.857874000	9.668823000
H	12.382846000	7.994270000	10.750262000
H	11.400527000	8.374211000	9.315288000
H	13.169692000	8.326110000	9.199011000
C	13.589398000	2.404504000	10.962405000
C	14.913483000	1.847084000	11.486938000
H	15.130059000	0.874678000	11.031348000
H	14.866045000	1.715672000	12.571884000
H	15.728677000	2.537335000	11.262873000
C	13.643582000	2.579465000	9.444565000
H	14.444863000	3.259005000	9.150803000
H	12.699580000	2.977448000	9.063231000
H	13.824809000	1.609986000	8.968434000
C	12.440817000	1.462619000	11.319744000
H	12.588036000	0.483510000	10.852482000
H	11.485761000	1.867714000	10.972568000
H	12.386871000	1.310932000	12.401293000
C	12.259110000	10.705712000	16.483254000
C	12.623629000	9.322439000	16.530382000
H	11.859287000	8.563187000	16.352798000
C	13.983315000	8.945492000	16.889897000
H	14.263427000	7.896159000	16.984083000
C	14.937408000	9.970012000	17.195370000
C	14.516234000	11.336578000	17.261358000
H	15.231572000	12.096483000	17.549495000
C	13.202603000	11.701160000	16.904011000
H	12.907425000	12.743930000	16.912768000
C	10.970893000	11.243918000	15.968668000
C	9.804343000	11.173394000	16.738556000
H	9.825186000	10.620994000	17.673997000
C	8.646119000	11.836124000	16.338968000
H	7.746752000	11.774826000	16.946038000
C	8.658953000	12.607345000	15.178157000
H	7.770447000	13.155075000	14.874748000
C	9.817930000	12.683122000	14.406100000
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C	10.976593000	11.981288000	14.765652000
C	12.071262000	11.307171000	12.073970000
H	11.736302000	10.299206000	12.349207000
C	10.941407000	12.013319000	11.327252000
H	9.996440000	11.990703000	11.873606000
H	10.772228000	11.509896000	10.367065000
H	11.185007000	13.056900000	11.096253000

C	13.299163000	11.133385000	11.179073000
H	13.685044000	12.090222000	10.815702000
H	13.027993000	10.541572000	10.298001000
H	14.086218000	10.602569000	11.717556000
C	12.748022000	13.872406000	13.491883000
H	11.864386000	14.154526000	12.905289000
C	12.714158000	14.656770000	14.804029000
H	11.811807000	14.454907000	15.387011000
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C	14.001192000	14.234170000	12.695244000
H	14.897086000	13.836198000	13.181639000
H	14.107693000	15.324445000	12.635830000
H	13.977603000	13.850373000	11.673783000
C	16.395391000	9.736769000	17.387584000
C	16.886839000	9.138302000	18.552052000
H	16.183914000	8.813908000	19.313954000
C	18.257320000	8.970093000	18.743587000
H	18.625166000	8.496435000	19.649872000
C	19.150344000	9.415462000	17.771606000
H	20.220286000	9.282022000	17.908413000
C	18.669920000	10.031328000	16.616015000
H	19.380349000	10.352952000	15.860836000
C	17.295732000	10.204193000	16.406361000
C	17.617946000	10.066089000	13.521924000
H	18.653987000	10.357072000	13.732835000
C	17.517866000	8.549156000	13.634565000
H	17.831406000	8.197187000	14.619888000
H	18.163593000	8.073890000	12.886726000
H	16.487866000	8.224945000	13.458095000
C	17.242734000	10.554189000	12.123820000
H	16.202534000	10.303925000	11.900088000
H	17.877568000	10.069655000	11.372154000
H	17.367137000	11.635798000	12.008626000
C	17.229887000	12.698664000	14.721724000
H	16.834901000	13.012465000	13.746203000
C	16.625650000	13.611319000	15.785160000
H	15.536038000	13.538350000	15.803103000
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H	19.198527000	12.588236000	15.654975000
H	18.994276000	13.925358000	14.526043000
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Quartet

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P	12.488985000	12.205732000	13.679962000
P	16.433644000	10.863413000	14.787832000
Si	14.293618000	4.440034000	16.669791000
Si	9.787616000	6.086277000	14.388640000
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Na	12.460031000	4.291079000	13.893578000
O	14.113243000	5.716812000	15.677375000
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C	18.052208000	3.123738000	16.861745000
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C	17.615187000	5.528109000	16.291195000
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H	16.870934000	6.229508000	15.907634000
C	13.972304000	4.936799000	19.460989000
C	12.696449000	5.177520000	20.269907000
H	12.938090000	5.471849000	21.296518000
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H	12.099505000	5.971054000	19.811800000
C	14.801789000	6.217752000	19.397833000
H	14.208541000	7.037248000	18.983219000
H	15.689999000	6.074549000	18.777315000
H	15.128451000	6.510363000	20.401687000
C	14.787056000	3.802233000	20.086670000
H	15.096445000	4.067246000	21.103498000
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H	14.187307000	2.888194000	20.143774000
C	13.231288000	1.833087000	16.376100000
C	12.936544000	0.967324000	15.153712000
H	12.733391000	-0.065984000	15.452935000
H	13.788217000	0.965081000	14.467586000
H	12.053810000	1.336638000	14.623849000
C	12.010837000	1.868801000	17.296018000
H	11.139686000	2.250473000	16.756437000
H	12.196828000	2.522607000	18.149421000
H	11.776731000	0.861948000	17.658691000
C	14.443830000	1.263966000	17.112793000
H	14.222164000	0.245231000	17.448212000
H	14.701522000	1.863762000	17.986738000
H	15.316801000	1.226178000	16.456183000
C	8.276844000	8.023945000	13.008621000
C	6.835092000	7.848999000	13.491268000
H	6.320662000	7.092310000	12.889783000
H	6.280648000	8.789548000	13.402494000
H	6.824006000	7.532107000	14.536925000
C	8.299734000	8.388127000	11.524049000

H	9.330028000	8.505772000	11.176930000
H	7.763167000	9.325955000	11.346927000
H	7.823148000	7.600917000	10.931338000
C	8.995471000	9.090407000	13.830067000
H	8.972531000	8.836663000	14.893009000
H	8.513898000	10.065462000	13.709818000
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H	8.516419000	4.778153000	11.720526000
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C	9.268213000	2.150498000	13.841366000
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C	8.933225000	6.094702000	17.119751000
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H	7.007822000	7.032811000	17.459141000
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H	6.920746000	5.283075000	17.191964000
C	9.622953000	4.758715000	17.386513000
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H	9.668773000	4.563381000	18.462688000
H	10.648606000	4.765364000	17.008462000
C	9.728847000	7.232667000	17.757974000
H	10.760983000	7.219784000	17.400414000
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H	9.280874000	8.198808000	17.507206000
C	16.743292000	5.451097000	10.230703000
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H	18.087006000	5.557080000	11.929256000
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C	16.544805000	6.962903000	10.132221000
H	15.619461000	7.193774000	9.600962000
H	17.379882000	7.421315000	9.591336000
H	16.492857000	7.408630000	11.127480000
C	16.710773000	4.825207000	8.834614000
H	16.855102000	3.741712000	8.894232000
H	17.508029000	5.240014000	8.208229000
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C	12.405657000	6.458347000	9.405879000
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H	11.096784000	4.786565000	9.835080000
H	10.262437000	6.345236000	9.713838000
H	11.209712000	5.971088000	11.155423000
C	12.322805000	6.299985000	7.886001000
H	13.225356000	6.698370000	7.412507000
H	11.456634000	6.837620000	7.486766000
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C	12.552648000	7.933369000	9.777968000

H	12.681754000	8.055249000	10.857004000
H	11.667168000	8.497837000	9.465430000
H	13.425578000	8.365571000	9.278648000
C	13.591791000	2.397167000	10.928861000
C	14.894315000	1.762321000	11.419505000
H	15.048868000	0.784914000	10.949610000
H	14.862320000	1.621433000	12.503949000
H	15.740741000	2.410673000	11.186400000
C	13.625564000	2.591408000	9.412706000
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H	13.743093000	1.620576000	8.919527000
C	12.400408000	1.512913000	11.292843000
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H	11.464021000	1.973970000	10.965394000
H	12.353604000	1.349748000	12.372623000
C	12.131268000	11.001372000	16.427351000
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H	11.685368000	8.888959000	16.298435000
C	13.792190000	9.186284000	16.894009000
H	14.021889000	8.140196000	17.087760000
C	14.780981000	10.200359000	17.179534000
C	14.404908000	11.575053000	17.222458000
H	15.154718000	12.315031000	17.472382000
C	13.125058000	11.986459000	16.790200000
H	12.864112000	13.036910000	16.766774000
C	10.859836000	11.549424000	15.888366000
C	9.679163000	11.494550000	16.638012000
H	9.680161000	10.954900000	17.581326000
C	8.530210000	12.151378000	16.204139000
H	7.619340000	12.100350000	16.794512000
C	8.564228000	12.899925000	15.028825000
H	7.681343000	13.440439000	14.697964000
C	9.735350000	12.955571000	14.273509000
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C	11.970350000	11.453608000	12.010957000
H	11.834180000	10.409920000	12.319322000
C	10.701806000	11.970433000	11.339538000
H	9.808915000	11.801540000	11.944358000
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H	19.355314000	12.149814000	14.634773000

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