

ELECTRONIC SUPPORTING INFORMATION

Cation assisted binding and cleavage of dinitrogen by uranium complexes

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Experimental Procedures

General Considerations Unless otherwise noted, all manipulations were carried out at ambient temperature under an inert argon 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. ¹H and ¹³C NMR spectra were recorded on a Bruker 400 MHz or 600 Hz spectrometers. NMR chemical shifts are reported in ppm with solvent as internal reference. High-pressure experiments were performed in sapphire NMR tube (length 13 cm, internal diameter 0.80 cm), which was built in-house according to a literature protocol.¹

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

EPR. EPR experiments were recorded with a Bruker Elexsys E500 spectrometer working at 9.4 GHz frequency with an Oxford ESR900 cryostat for 4-300K operations. The solution state spectra were recorded inside J-Young EPR tubes. The solid-state measurements were performed with solid samples inside J-Young EPR tubes

Magnetic Measurements. Magnetic measurements in solid state were performed using a QuantumDesign MPMS-5T superconducting quantum interference device (SQUID) magnetometer in a temperature range 2–250 K. The crushed crystalline sample was enclosed in an evacuated and flame-sealed quartz capsule and placed inside a plastic straw. Samples were restrained in an NVM immersion oil matrix to prevent sample torquing during measurements. Diamagnetic corrections were applied to the data using Pascal's constants.

The magnetic moment per uranium of complex **M₂-2** and **Cs₄-(N)₂** was calculated at all temperatures using the formula:

$$\mu_{eff} = \sqrt{\frac{8\chi_{corr}T}{2}}$$

where $\chi_{corr} = \chi_{meas} - \chi_d$, χ_d was calculated using Pascal's constants.²

Electrochemical Methods. Cyclic voltammetry data were carried out at room temperature in an argon-filled glovebox described above. Data were collected using a Biologic SP-300 potentiostat connected to a personal computer. All samples were saturated in complex with 0.1 M [Bu₄N][BPh₄] supporting electrolyte in THF solution. The experiments were carried out with a platinum disk (d = 5 mm) working electrode, a platinum wire counter electrode, and an Ag/AgCl reference electrode. The experiments were repeated on independently synthesized samples to assess the reproducibility of the measurement. Potential calibration was performed at the end of each data collection cycle using the ferrocene/ferrocenium [(C₅H₅)₂Fe]⁺⁰ couple as an internal standard.

Starting materials Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Tris(*tert*-butoxy)silanol was purified by sublimation. The solvents were purchased from Aldrich or Cortecnet (deuterated solvents) in their anhydrous form, conditioned under argon and vacuum distilled from K/benzophenone (toluene, hexane, THF, *d*₈-THF, *d*₈-toluene).

*d*₆-DMSO was freeze-degassed and dried over 3 Å molecular sieves for several days. ¹³CO (93.13% ¹³C) 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^{IV}(OSi(O^tBu)₃)₃]₂(μ-O)] (**1**)³, [K₂{U^{III}(OSi(O^tBu)₃)₃]₂(μ-O)] (**K₂-2**)³ and [K₂{U^V(OSi(O^tBu)₃)₃]₂(μ-O)(μ-N₂)] (**K₂-N₂**)³, CsC₈,⁴ RbC₈,⁴ were prepared according to the published procedures.

Caution: Depleted uranium (primary isotope ²³⁸U) is a weak α-emitter (4.197 MeV) with a half-life of 4.47×10⁹ 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.

Syntheses

Synthesis [Cs₂{U^{III}(OSi(O^tBu)₃)₃]₂(μ-O)], Cs₂-2. A cold (-80°C) teal solution of **1** (89.5 mg, 0.0479 mmol, 1 equiv.) in THF (6.0 mL) was added to a bronze cold (-80°C) suspension of CsC₈ (54.8 mg, 0.239 mmol, 5 equiv.) in THF (0.4 mL).

The reaction mixture was stirred at -80°C for 30 min. The resultant suspension was filtered through cold (-80°C) glassware to remove the excess reducing agent and graphite, obtaining a dark red solution. Volatiles were removed under vacuum and the resultant dark red solid was dissolved in cold (-40°C) toluene (1.0 mL). The resultant solution was left standing at -40°C for 3 days affording dark red crystals of **Cs₂-2** (79.2 mg, 70% yield). Anal. Calcd for $[\text{Cs}_2\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})\}(\text{Toluene})_1]$ $\text{Cs}_2\text{C}_{79}\text{H}_{170}\text{O}_{25}\text{U}_2\text{Si}_6$: C: 39.04%; H: 7.05 %; N: 0.00%. Found: C: 38.77%; H: 7.19%; N: 0.00%.

^1H NMR (400 MHz, d_8 -THF, 233 K): $\delta = -0.58$ ppm (br, CH_3 terminal siloxide) (Figure S1)

^1H NMR (400 MHz, d_8 -THF, 298 K): $\delta = 0.18$ ppm (s, CH_3 terminal siloxide) (Figure S2)

^1H NMR (400 MHz, d_8 -toluene, 233 K): $\delta = -0.08$ ppm (s, CH_3 terminal siloxide) (Figure S3)

^1H NMR (400 MHz, d_8 -toluene, 298 K): $\delta = 0.38$ ppm (s, CH_3 terminal siloxide) (Figure S4)

Cs₂-2 is stable at 25°C in a toluene solution over the course of 17 days (Figure S5) and is still the major species in a THF solution at 25°C over the course of 24 hs (80% of starting material is still present in solution), but decomposes completely over the course of 6 days (Figure S6). Complex **Cs₂-2** is stable in a THF solution at -40°C for the course of 21 days, showing only small signs of decomposition (84% of complex still remains) (Figure S7). The same reduction performed at -40°C yielded **Cs₂-2** in lower yields.

Synthesis $[\text{Rb}_2\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})\}]$, **Rb₂-2.** A cold (-80°C) teal solution of **1** (113.5 mg, 0.0548 mmol, 1 equiv.) in THF (7.5 mL) was added to a bronze cold (-80°C) suspension of RbC_8 (49.7 mg, 0.274 mmol, 5 equiv.) in THF (0.5 mL). The reaction mixture was stirred at -80°C for 30 min. The resultant suspension was filtered through cold (-80°C) glassware to remove the excess reducing agent and graphite. Volatiles were removed under vacuum and the resultant dark red solid was dissolved in cold (-40°C) toluene (1.0 mL). The resultant solution was left standing at -40°C for 2 days affording dark red crystals of **Rb₂-2** in 60% yield (73.8 mg). Anal. Calcd for $[\text{Rb}_2\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})\}]$ $\text{Rb}_2\text{C}_{72}\text{H}_{162}\text{O}_{25}\text{U}_2\text{Si}_6$: C: 38.55%; H: 7.28 %; N: 0.00%. Found: C: 38.68%; H: 7.16%; N: 0.00%.

The use of less equivalents of RbC_8 leads to incomplete reduction and concomitant formation of $[\text{Rb}\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}]$ (Figure S62)

^1H NMR (400 MHz, d_8 -toluene, 233 K): $\delta = -0.27$ ppm (s, CH_3 terminal siloxide) (Figure S8)

^1H NMR (400 MHz, d_8 -toluene, 298 K): $\delta = 0.29$ ppm (s, CH_3 terminal siloxide) (Figure S9)

^1H NMR (400 MHz, d_8 -THF, 233 K): $\delta = -0.87$ ppm (s, CH_3 terminal siloxide) (Figure S10)

^1H NMR (400 MHz, d_8 -THF, 298 K): $\delta = 0.06$ ppm (s, CH_3 terminal siloxide) (Figure S11)

Rb₂-2 is still the major species in a THF solution at 25°C after 24 hs (60% of starting material is still present in solution) but decomposes completely over the course of 6 days (Figure S12). **Rb₂-2** is still the major species (62% of starting material is still present in solution) in a THF solution at -40°C after 14 days (Figure S13). **Rb₂-2** is still the major species in a toluene solution after 24 hs (70% of starting material is still present in solution) but decomposes completely over the course of 5 days into $[\text{Rb}_2\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})_2\}]$, complex **Rb₂-4** (-1.57 ppm) and other unidentified species. (Figure S14) A few yellow-green crystals of $[\text{Rb}_2\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})_2\}]$, **Rb₂-4** (Figure S59) were grown from a saturated toluene solution over the course of 2 days at -40°C .

Comparison of the ^1H NMR spectra in toluene solution of **M₂-2** at -40°C (Figure S15) shows a single sharp resonance for all of them, showing that these complexes show the same fluxional behaviour in solution even at low temperatures.

Synthesis $[\text{Na}\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}]$, **Na-3.** A cold (-40°C) teal solution of **1** (34.9 mg, 0.0168 mmol, 1 equiv.) in THF (2.0 mL) was added to cold Na^0 mirror. The reaction was kept at -40°C for 15 hs. The resultant red-orange solution was filtered through cold glassware (-80°C) yielding a red-orange solution which was evaporated at -80°C (0.4 mL). The ^1H NMR spectrum of the reaction mixture at -40°C (Figure S16) shows the presence of 4 broad resonances at $\delta = 14.58$ ppm, 9.99 ppm, 0.41 ppm and -3.78 ppm. The solution was left standing at -40°C for 2 days affording dark red crystals of **Na-3** (Figure S58) (11.3 mg, 0.0054 mmol, 30% yield). Anal. Calcd for $[\text{Na}\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_3\}]$ $\text{NaC}_{72}\text{H}_{162}\text{O}_{25}\text{U}_2$: C: 41.27%; H: 7.79 %; N: 0.00%. Found: C: 40.91%; H: 7.74%; N: 0.00%.

Synthesis $[\text{Rb}_2\{\text{U}^{\text{V}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})(\mu\text{-N}_2)\}]$, **Rb₂-N₂.** A cold (-40°C) dark red solution of **Rb₂-2** in toluene (1.5 ml) prepared by reduction of **1** (128.5 mg, 0.0620 mmol, 1 equiv.) in an Ar glovebox was transferred in a reaction tube and connected to a Schlenk line. The solution was degassed by two cycles of freeze-pump-thawing and N_2 (1 atm) was added to the reaction mixture which changed colour to dark brown over the course of 5 minutes.

The solution was left standing at -40°C under a N_2 atmosphere for 2 days yielding dark brown crystals suitable for X-ray diffraction of the complex $[\text{Rb}_2\{\text{U}(\text{OSi}(\text{O}^t\text{Bu})_3)_2(\mu\text{-O})(\mu\text{-N}_2)\}]$, **Rb₂-N₂** in 53% yield (75.0 mg, 0.0330 mmol). Due to the reversible binding of N_2 of the complex (Figures S19 and S20), **Rb₂-N₂** has to be recovered under a gentle N_2 flux.

The conversion of **Rb₂-2** into **Rb₂-N₂** is higher (82%), as determined by ¹H NMR studies, using trimethylsilyl ether as internal standard.

Anal. Calcd for [Rb₂{U(OSi(O^tBu)₃)₃}₂(μ-O)(μ-N₂)] C₇₂H₁₆₂N₂O₂₅U₂Rb₂Si₆: C: 38.07%; H: 7.19 %; N: 1.23%. Found: C: 37.84%; H: 6.82%; N: 0.92%.

¹H NMR (400 MHz, d₈-toluene, 233 K): δ = -3.54 ppm (s, br, CH₃ terminal siloxide) (Figure S17)

Comparison of the ¹H NMR spectrum in toluene solution at -40°C (Figure S44) shows that **Rb₂-N₂** shows the same fluxional behaviour in solution as **K₂-N₂** even at low temperatures.

¹H NMR (400 MHz, d₈-toluene, 298 K): δ = -2.27 ppm (s, CH₃ terminal siloxide) (Figure S18)

Drying the solid under vacuum for 1 h at -80°C leads to the complete loss of the bound N₂ and the reformation of **Rb₂-2** (Figure S19). In toluene solution at -40°C, the same process occurs over the course of 14 days after removing the headspace (Figure S20). The loss of N₂ under vacuum renders further characterization of the complex very difficult.

Low-temperature (6-30 K) X-band EPR measurements carried out in isolated complex **Rb₂-N₂** revealed the presence of two signals in a 10.2 mM frozen solution at g=3.37 and g=1.15.

Reaction of in situ prepared complex Rb₂-2 with H₂. A cold (-80°C) teal solution of complex **1** (10.4 mg, 0.00502 mmol, 1 equiv.) in THF (0.5 mL) was added to a cold (-80°C) bronze suspension of RbC₈ (4.4 mg, 0.0240 mmol, 5 equiv.) in THF (0.1 mL). The suspension was stirred at -80 °C for 30 min. The reaction mixture was then filtered on cold (-80°C) glassware. All the volatiles were removed under vacuum at -80 °C and cold d₈-toluene (0.4 mL) added to afford a dark red solution of **Rb₂-2**. The ¹H NMR spectrum of the solution at 25°C confirmed the presence of **Rb₂-2** as a pure species, together with traces of THF and the complex was reacted without further purification. The reaction tube was transferred to a Schlenk line and degassed by 3 freeze-pump-thaw cycles. Hydrogen gas (1 atm) was added into the tube and the reaction mixture was left stirring at room temperature. The reaction mixture turned from dark red to light orange within 30 min. The ¹H NMR spectrum at 25°C after 24 hs shows the presence one main resonance at δ= -1.71 ppm, the signals of remaining THF together with other smaller resonances. (Figure S21, top)

Reaction of in situ prepared complex Rb₂-N₂ with H₂. A cold (-80°C) teal solution of complex **1** (10.3 mg, 0.00497 mmol, 1 equiv.) in THF (0.5 mL) was added to a cold (-80°C) bronze suspension of RbC₈ (4.5 mg, 0.0248 mmol, 5 equiv.) in THF (0.1 mL). The suspension was stirred at -80 °C for 30 min. The reaction mixture was then filtered on cold (-80°C) glassware. All the volatiles were removed under vacuum at -80 °C and cold toluene (0.4 mL) added to afford a dark red solution of **Rb₂-2**. The reaction tube was transferred to a Schlenk line and degassed by 3 freeze-pump-thaw cycles. N₂ (1 atm) was added into the tube and the reaction mixture was left stirring at room temperature for 5 min. The ¹H NMR spectrum of the solution in d₈-tol (0.4 mL) confirmed the presence of **Rb₂-N₂** as a pure species, together with traces of THF and the complex was reacted without further purification. The reaction tube was transferred to a Schlenk line and Hydrogen gas (1 atm) was added on the frozen solution and the reaction mixture was left stirring at room temperature. The reaction mixture turned from dark red to light orange within 30 min. The ¹H NMR spectrum at 25°C after 24 hs shows the presence one main resonance at δ= -1.71 ppm, the signals of remaining THF together with other smaller resonances. (Figure S21, bottom)

Synthesis [Cs₃{U^V(OSi(O^tBu)₃)₃}₂(μ-N)₂{U^V(OSi(O^tBu)₃)₂(κ-O)}][CsOSi(O^tBu)₃], Cs₄-(N)₂. A cold (-40°C) bronze suspension of CsC₈ (23.5 mg, 0.103 mmol, 2 equiv.) in toluene (1.5 mL) was added to a cold (-40°C) stirring dark red solution of **Cs₂-2** (120.0 mg, 0.0513 mmol, 1 equiv.) in toluene (2.0 mL) under a N₂ atmosphere. The reaction mixture was left to react under stirring for 15 hs at -40°C. Afterwards it was filtered, yielding a dark yellow solution. The ¹H NMR spectrum at 25°C (Figure S22) and at -40°C (Figure S23) of the solution shows the presence of the signals of **Cs₄-(N)₂**, and CsOSi(O^tBu)₃. The solution was concentrated until 0.4 mL and left standing at -40°C for 2 days, affording golden crystals of complex **Cs₄-(N)₂** (50.0% yield, 67.3 mg, 0.0253 mmol).

Anal. Calcd for [Cs₃{U^V(OSi(O^tBu)₃)₃}₂(μ-N)₂{U^V(OSi(O^tBu)₃)₂(κ-O)}][CsOSi(O^tBu)₃]•(Toluene)_{1.2} Cs₄C_{80.4}H_{71.62}O₂₅N₂U₂: C: 35.21%; H: 6.31 %; N: 1.02%. Found: C: 35.48%; H: 6.35%; N: 1.04%.

¹H NMR (400 MHz, d₈-toluene, 298 K): δ = 17.08 ppm (br), 9.90 ppm (s), -3.97 ppm (s), -10.21 ppm (br) (Figure S24)

¹H NMR (400 MHz, d₈-tol, 233 K): δ = 13.22 ppm (s), -4.58 ppm (br), -14.11 ppm (br) (Figure S25)

The stability of complex **Cs₄-(N)₂** at -40 °C and at 25°C was investigated by ¹H NMR spectroscopy. Complex **Cs₄-(N)₂** converts cleanly into another species with resonances at δ= 10.69 ppm (s). and -11.54 (s, br) in 12 hs at 25°C (Figure S26).

Complex **Cs₄-(N)₂** converts very slowly (75% still present after 2 weeks) at -40° C (Figure S27). This compares well with the analogous species reported recently ⁵

Reduction of Cs₂-2 with 2 equiv. of CsC₈ under Ar atmosphere. A cold (-40°C) bronze suspension of CsC₈ (2.1 mg, 0.0092 mmol, 2 equiv.) in d₈-tol (0.5 mL) was added to a cold (-40°C) stirring dark red solution of **Cs₂-2** (10.1 mg, 0.00432 mmol, 1 equiv.) in d₈-tol (0.5 mL) under an Ar atmosphere. The reaction mixture was stirred for 24 hs at -40°C. Afterwards it was filtered, yielding a red solution. The ¹H NMR spectrum at 25°C of the solution shows the presence of the signals of **Cs₂-2** (Figure S28).

Addition of HCl to the reaction mixture obtained after reacting complex Cs₂-2 with 2 equiv. of CsC₈ at -40°C under a N₂ atmosphere. A cold (-40°C) bronze suspension of CsC₈ (3.0 mg, 0.0131 mmol, 2 equiv.) in d₈-tol (0.4 mL) was added to a cold (-40°C) stirring dark red solution of **Cs₂-2** (14.2 mg, 0.00607 mmol, 1 equiv.) in d₈-tol (0.5 mL) under a N₂ atmosphere. The reaction mixture stirred for 24 hs at -40°C. Afterwards it was filtered, yielding a dark yellow-brown solution. Volatiles were removed under vacuum and 1.0 mL of a cold (-80°C) 2 M HCl solution in Et₂O was added, yielding a yellow solution and a white precipitate. After 1 hour, volatiles were removed under vacuum. The resulting solid was dissolved in d₆-DMSO and dimethylsulfone was added as an internal standard for the quantitative NH₄Cl detection. NH₄Cl is formed in 83% yield (1.66 equiv., 100% conversion corresponding to 2 equiv. of NH₄Cl) (Figure S29)

Reaction of complex Cs₄-(N)₂ with excess HCl. 1 mL of a cold (-80°C) 2 M solution of HCl in Et₂O was added to solid complex **Cs₄-(N)₂** (7.0 mg, 0.0026 mmol, 1 equiv.). The solution immediately turned yellow and a white precipitate formed. After 1 hour, volatiles were removed under vacuum. The resulting solid was dissolved in d₆-DMSO and dimethylsulfone was added as an internal standard for the quantitative NH₄Cl detection. NH₄Cl is formed in 100% yield (2 equiv. of NH₄Cl). (Figure S30)

Dissolution of complex Cs₄-(N)₂ in THF at -40°C. A yellow-brown solution of **Cs₄-(N)₂** (7.2 mg, 0.0027 mmol, 1 equiv.) in cold (-40°C) was prepared and analyzed by ¹H NMR spectroscopy at -40°C (Figure S31, bottom). All volatiles were removed under vacuum at -80°C and the solid was further dried for 2 hs to complete removal of the toluene. Afterwards it was dissolved in cold (-40°C) d₈-THF (0.4 mL), yielding a yellow solution. The ¹H NMR of the solution shows two resonances at δ= 13.85 ppm and -0.25 ppm, assigned to complex **Cs₄-(N)₂**, together with a resonance at δ= 1.33 ppm assigned to CsO(Si(O^tBu)₃) salt (Figure S32). All volatiles were removed under vacuum at -80°C and the solid was further dried for 2 hs at -80°C. The mixture was dissolved in d₈-tol (0.5 mL) and analyzed by ¹H NMR spectroscopy at -40°C and 25°C. The ¹H NMR spectrum at -40°C (Figure S32, top) shows the presence of **Cs₄-(N)₂**, but with an increase in the formation of CsO(Si(O^tBu)₃). The ¹H NMR spectrum in toluene solution at 25°C (Figure S33) after THF shows the signals assigned to complex **Cs₄-(N)₂** in the same ratio which was observed for the crystals immediately dissolved in toluene, together with the presence of other unknown signals and CsO(Si(O^tBu)₃).

Reaction of complex Rb₂-N₂ with 2 equiv. of RbC₈. A cold (-40°C) bronze suspension of RbC₈ (4.3 mg, 0.0237 mmol, 2 equiv.) in toluene (0.4 mL) was added to a cold (-40°C) stirring dark brown solution of **Rb₂-N₂** (25.5 mg, 0.0112 mmol, 1 equiv.) in toluene (0.5 mL) under a N₂ atmosphere. The reaction mixture was left to react under stirring for 24 hs at -40°C. Afterwards it was filtered, yielding a dark yellow solution. The ¹H NMR spectrum at 25°C of the solution shows four main resonances at δ= 10.37 ppm, 1.45 ppm (RbOSi(O^tBu)₃), -1.57 ppm ([Rb₂{U^{IV}(OSi(O^tBu)₃)₃]₂(μ-O)₂]) and -4.31 ppm. (Figure S34). A similar set of signals at δ= 11.08 ppm and -4.06 ppm in a 1:2 ratio was also observed for the previously reported **K₄-(N)₂**.

Comparison of the reduction of **K₂-N₂**, **Rb₂-N₂** and **Cs₂-2** with 2 equiv. of MC₈ (M = K, Rb and Cs, respectively) at 233 K under a N₂ atmosphere for 24 hs (Figure S35) shows that the formation of the bis-nitride species is cleaner for K and Rb, with the latter having some bis-oxo species as impurity from side reactions.

Reaction of complex Rb₂-2 with 2 equiv. of RbC₈ under N₂. A cold (-40°C) bronze suspension of RbC₈ (3.8 mg, 0.021 mmol, 2 equiv.) in toluene (0.6 mL) was added to a cold (-40°C) stirring dark red solution of **Rb₂-2** (22.0 mg, 0.00981 mmol, 1 equiv.) in toluene (1.2 mL) under a N₂ atmosphere. The reaction mixture was left to react under stirring for 24 hs at -40°C. Afterwards it was filtered, yielding a dark yellow-brown solution. The ¹H NMR spectrum at -40°C (Figure S36) of the solution shows two sharp resonances δ= 14.06 ppm, 1.45 ppm (RbOSi(O^tBu)₃) and three broad resonances at δ= 23.56 ppm, -6.42 ppm, and -15.32 ppm. The ¹H NMR spectrum at 25°C (Figure S37) of the solution shows two main sharp resonances δ= 10.47 ppm, -4.38 ppm and two broad resonances at δ= 17.08 ppm and -10.51 ppm. Comparison with the ¹H NMR spectrum for the putative bis-nitride obtained for the 2-electron reduction of **K₂-N₂** and

the reduction of the analogue **Cs₂-2** suggest that in this case a similar species is obtained upon reduction under N₂ in similar conditions (Figure S38-39).

Addition of HCl to the reaction mixture obtained after reacting complex Rb₂-2 with 2 equiv. of RbC₈ at -40°C under a N₂ atmosphere. A cold (-40°C) bronze suspension of RbC₈ (3.2 mg, 0.018 mmol, 2 equiv.) in toluene (0.5 mL) was added to a cold (-40°C) stirring dark red solution of Rb₂-2 (19.8 mg, 0.00869 mmol, 1 equiv.) in toluene (0.5 mL) under an Ar atmosphere. The reaction mixture stirred for 24 hs at -40°C. Volatiles were removed under vacuum and 1.0 mL of a cold (-80°C) 2 M HCl solution in Et₂O was added, yielding a yellow solution and a white precipitate. After 1 hour, volatiles were removed under vacuum. The resulting solid was dissolved in *d*₆-DMSO and dimethylsulfone was added as an internal standard for the quantitative NH₄Cl detection. NH₄Cl is formed in 85% yield (1.7 equiv., 100% conversion corresponding to 2 equiv. of NH₄Cl) (Figure S40)

Reaction of complex Cs₂-2 with higher pressure of N₂ at 25°C. A dark red solution of complex **Cs₂-2** (17.0 mg, 0.0073 mmol, 1 equiv.) in *d*₈-toluene (2.5 mL) was transferred into sapphire NMR tube inside the glovebox. Once the tube had been sealed by means of the titanium alloy valve, it was removed from the glovebox, transported inside a safety shield, and pressurized with 99.9999% N₂ (Carbagas) with increasing pressures (1-100 bar) at 25°C. The ¹H NMR spectra of the reaction mixture showed that no reaction occurs (Figure S41).

Reaction of complex Cs₂-2 with higher pressure of N₂ at -40°C. A dark red solution of complex **Cs₂-2** (14.3 mg, 0.00612 mmol, 1 equiv.) in *d*₈-toluene (2.5 mL) was transferred into sapphire NMR tube inside the glovebox. Once the tube had been sealed by means of the titanium alloy valve, it was removed from the glovebox, transported inside a safety shield, and pressurized with 99.9999% N₂ (Carbagas) with increasing pressures (1-100 bar) at -40°C. The ¹H NMR spectra at -40°C of the reaction mixture showed the partial to total consumption of the starting material and the formation of a new broad resonance at δ = -3.97 ppm (Figure S42).

Reaction of complex Cs₂-2 with 50 bar of N₂ at -40°C removal of headspace. A dark red solution of complex **Cs₂-2** (15.4 mg, 0.00659 mmol, 1 equiv.) in *d*₈-toluene (2.5 mL) was transferred into sapphire NMR tube inside the glovebox. Once the tube had been sealed by means of the titanium alloy valve, it was removed from the glovebox, transported inside a safety shield, and pressurized with 99.9999% N₂ (Carbagas) with 50 bar at -40°C. The ¹H NMR spectra at -40°C of the reaction mixture showed the partial consumption of the starting material and the formation of a new broad resonance at δ = -3.97 ppm. Afterwards, the excess pressure was removed at -40°C and the evolution of its ¹H NMR spectrum at -40°C was followed. Over the course of 16 hs, most of the starting material is reformed (70%). (Figure S43).

Comparison of the ¹H NMR spectrum of the toluene solution of **Cs₂-2** after addition of 100 bar of N₂ at -40°C with the spectra of **K₂-N₂** and **Rb₂-N₂** shows that they all exhibit the same fluxional behaviour in solution at -40°C (Figure S44)

Reaction of complex Cs₄-(N)₂ with 5 equiv. of ¹³CO. A yellow-brown solution of complex **Cs₄-(N)₂** (8.5 mg, 0.0032 mmol, 1 equiv.) in *d*₈-toluene (0.6 mL) was transferred in a J-Young adapted NMR tube and connected to a Schlenk line. The solution was degassed by three cycles of freeze-pump-thawing and ¹³CO (0.016 mmol, 5 equiv.) was added to the reaction mixture at -40°C which changed colour to pale yellow over the course of 5 minutes. The ¹H NMR spectrum of the reaction mixture at -40°C immediately after (Figure S45, top) shows the disappearance of the starting material and the presence of three broad resonances at δ = 30.21 ppm, -3.30 ppm and -14.69 ppm, together with CsO(Si(O^tBu)₃). The ¹³C NMR spectrum of the reaction mixture at -40°C (Figure S46) showed one resonance attributable to U-bound ¹³C species, at δ = -1.40 ppm, the presence of ¹³CO (184.5 ppm) and two signals at δ = 70.30 ppm and 32.37 ppm assigned to the siloxide ligands. The reaction was left under stirring at -40°C for 24 hs, after which white powder came down. The ¹H NMR spectrum of the reaction mixture at -40°C after 24 hs (Figure S47, top) shows the presence of the same three broad signals but the disappearance of CsO(Si(O^tBu)₃). The ¹H NMR spectrum of the reaction mixture at 25°C after 24 hs (Figure S48) shows the one resonance at δ = -1.40 ppm, assigned to [Cs₂{U^{IV}(OSi(O^tBu)₃)₃]₂(μ-O)₂] (91% conversion), similarly to what has been reported recently by its K analogue.⁵ Volatiles were removed under vacuum and 0.5 mL of D₂O (pD=13) were added to the resultant light-yellow solid together with few drops of *d*₆-DMSO as a reference. Quantitative ¹³C NMR spectroscopy revealed the formation of N¹³CO⁻ and ¹³CN⁻ in a 1:1 ratio (Figure S49) and in 100% yield (measured using ¹³C-labelled sodium acetate as internal standard). A few yellow-green crystals of [Cs₂{U^{IV}(OSi(O^tBu)₃)₃]₂(μ-O)₂, complex **Cs₂-4** (Figure S60) were grown from a saturated toluene solution (0.2 mL) over the course of 2 days at -40°C after addition of ¹³CO and filtering the white powder.

Reduction of [U(OSi(O^tBu)₃)₃]₂(μ-O), complex 1 under N₂ with 4 equiv. of CsC₈ in toluene at -40°C. A cold (-40°C) bronze suspension of CsC₈ (7.0 mg, 0.031 mmol, 4 eq) in toluene (0.5 mL) was added to a cold solution (-40°C) of

complex **1** (15.6 mg, 0.00753 mmol, 1 eq) in toluene (1.0 mL) under N₂ atmosphere. The mixture was allowed to react at -40°C for 24 hs and its ¹H NMR spectrum was followed over time. The ¹H NMR spectrum of the reaction mixture shows the presence of the signals of CsOSi(O^tBu)₃ and complex **Cs₄-(N)₂** together with unknown species with a chemical shift of -0.77 ppm (Figure S50 and S51).

Reduction of Cs₂-2 with 2 equiv. of CsC₈ under N₂ atmosphere in THF. A cold (-40°C) bronze suspension of CsC₈ (3.3 mg, 0.014 mmol, 2 equiv.) in d₈-THF (0.2 mL) was added to a cold (-40°C) stirring dark red solution of **Cs₂-2** (15.9 mg, 0.00680 mmol, 1 equiv.) in d₈-THF (0.7 mL) under a N₂ atmosphere. The reaction mixture was left to react under stirring for 20 hs at -40°C, and its evolution was followed by ¹H NMR studies. The ¹H NMR spectrum of the reaction mixture at -40°C shows the slow consumption of the starting material over the course of 20 hs, with the concomitant formation of CsO(Si(O^tBu)₃) salt. (Figure S52). Afterwards it was filtered, yielding an orange solution. The ¹H NMR spectrum at 25°C of the solution in toluene shows the presence of the signals of **Cs₄-(N)₂**, the CsO(Si(O^tBu)₃) salt and the decomposition from the first one at δ= 10.49 ppm (s) (Figure S53).

Reduction of [U(OSi(O^tBu)₃)₃]₂(μ-O)], complex **1 with 4 equiv. of CsC₈ in toluene at -40°C under Ar.** A cold (-40°C) bronze suspension of CsC₈ (7.2 mg, 0.031 mmol, 4 eq) in d₈-toluene (0.2 mL) was added to a cold dark red solution (-40°C) of complex **1** (16.0 mg, 0.00772 mmol, 1 eq) in d₈-toluene (0.4 mL) under Ar atmosphere. The reaction mixture was left to react under stirring for 20 hs at -40°C, and its evolution was followed by ¹H NMR studies. The ¹H NMR spectrum of the reaction mixture at -40°C shows the consumption of the starting material over the course of 3 hs, with the concomitant formation of **Cs₂-2**. The reaction does not evolve further over the course of 48 hs (Figure S54).

Addition of 2.2.2-cryptand to K₂-2 in THF. A cold (-80°C) teal solution of complex **1** (9.7 mg, 0.00468 mmol, 1 equiv.) in THF (0.8 mL) was added to a cold (-80°C) bronze suspension of KC₈ (3.2 mg, 0.0237 mmol, 5 equiv.) in THF (0.1 mL). The suspension was stirred at -80 °C for 30 min. The reaction mixture was then filtered on cold (-80°C) glassware. All the volatiles were removed under vacuum at -80 °C and cold d₈-THF (0.4 mL) added to afford a dark red solution of **K₂-2**. The ¹H NMR spectrum of the solution at -40°C (Figure S55, bottom) confirmed the presence of **K₂-2** as a pure species with a resonance at δ= -0.52 ppm (s). A cold (-40°C) colorless solution of 2.2.2-cryptand (1.8 mg, 0.00478 mmol, 1 equiv.) in d₈-THF (0.2 mL) was added and left to react for 20 min. The ¹H NMR of the reaction mixture at -40°C (Figure S56, middle) shows the shift of the resonance assigned to the siloxides, and the apparition of the resonances for 2.2.2-cryptand. A cold (-40°C) colorless solution of 2.2.2-cryptand (1.8 mg, 0.00478 mmol, 1 equiv.) in in d₈-THF (0.2 mL) was added and left to react for 20 min. The ¹H NMR of the reaction mixture at -40°C (Figure S55, top) shows the shift of the resonance assigned to the siloxides.

NMR Spectra

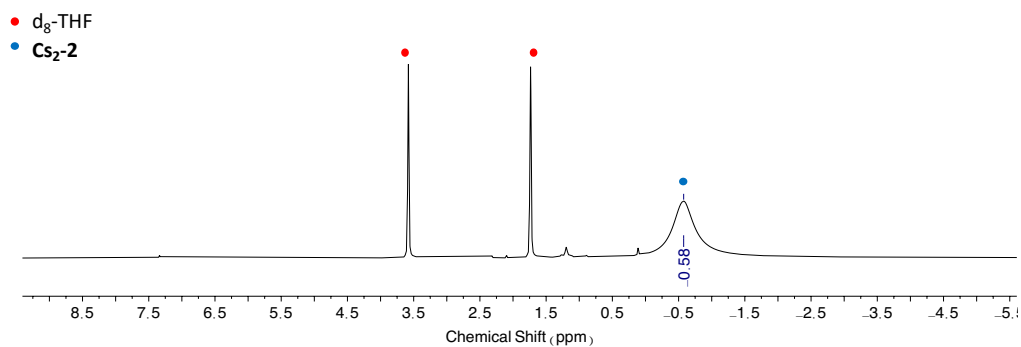


Figure S1: ^1H NMR spectrum (400 MHz, $d_8\text{-THF}$, 233 K) of $[\text{Cs}_2\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}_2(\mu\text{-O})]$, $\text{Cs}_2\text{-2}$

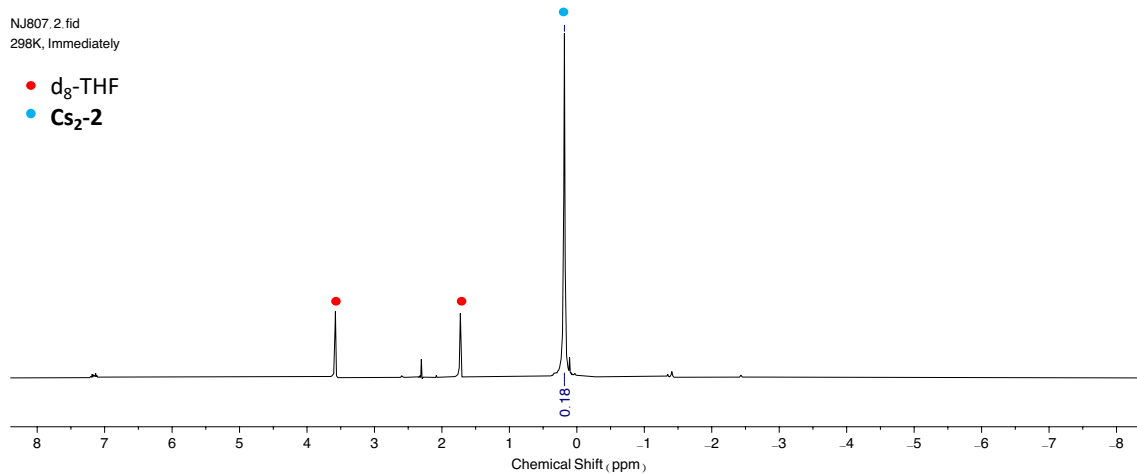


Figure S2: ^1H NMR spectrum (400 MHz, $d_8\text{-THF}$, 298 K) of $\text{Cs}_2\text{-2}$

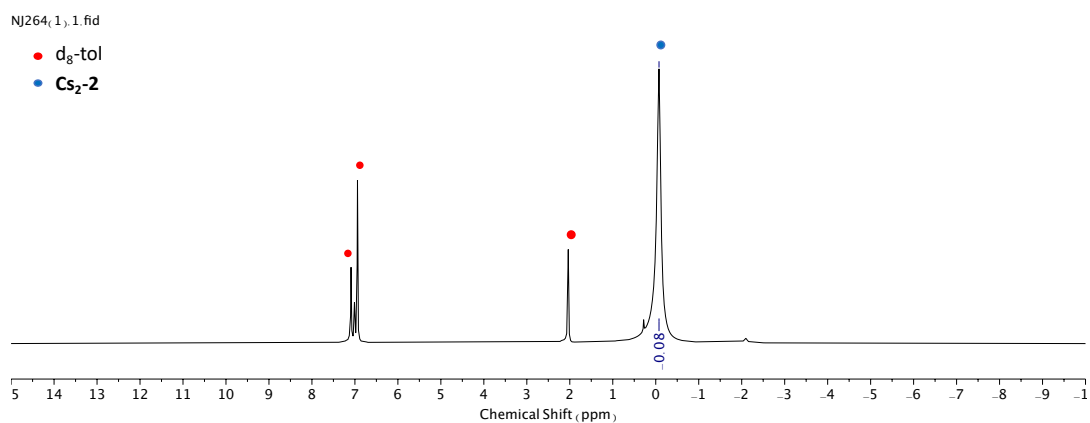


Figure S3: ^1H NMR spectrum (400 MHz, $d_8\text{-toluene}$, 233 K) of $\text{Cs}_2\text{-2}$

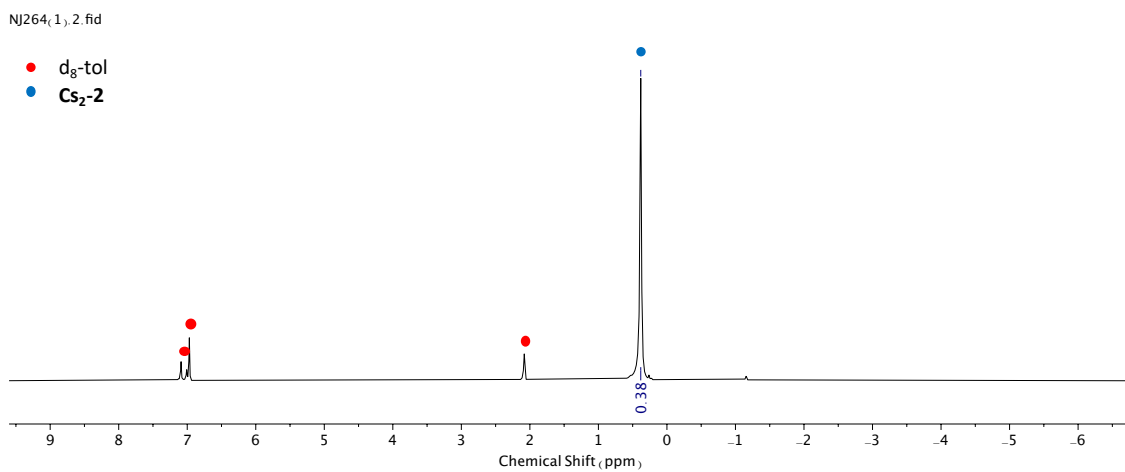


Figure S4: ¹H NMR spectrum (400 MHz, d₈-toluene, 298 K) of Cs₂-2

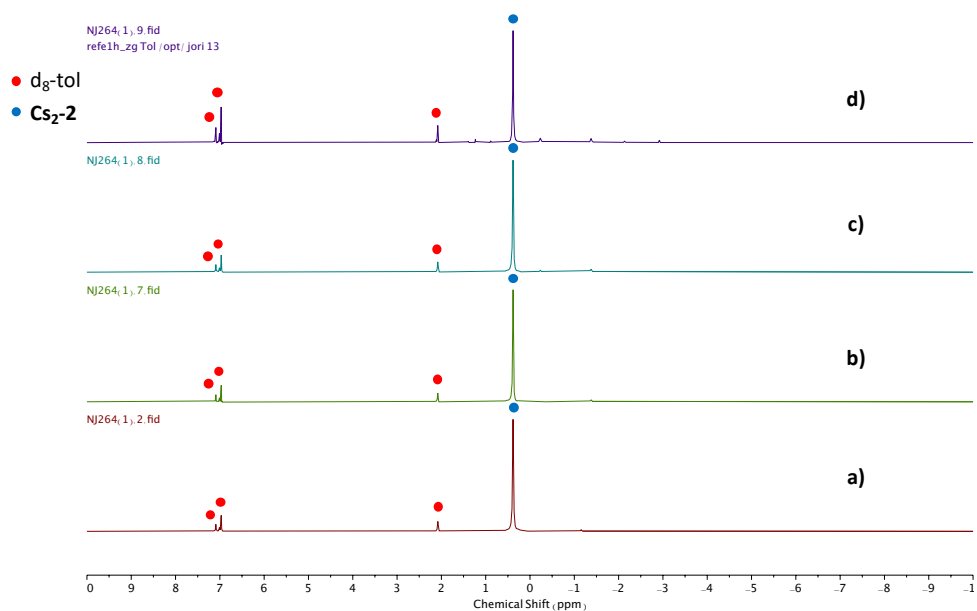


Figure S5: ¹H NMR spectrum (400MHz, d₈-toluene, 298 K) evolution at 298 K of Cs₂-2 in toluene a) immediately, b) 1 day after, c) 6 days after and d) 17 days after.

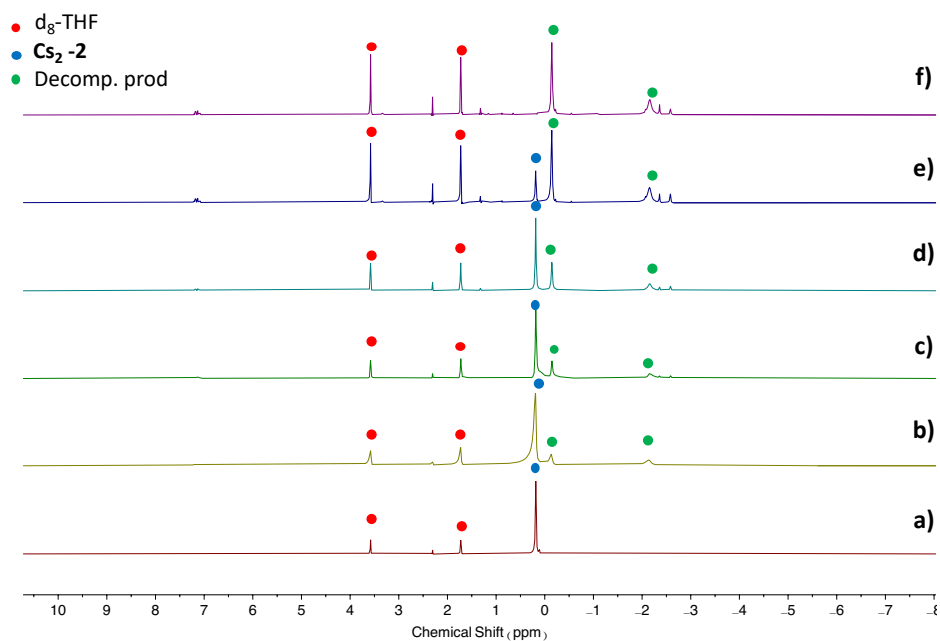


Figure S6: ^1H NMR spectrum (400MHz, $\text{d}_8\text{-THF}$, 298 K) evolution at 298 K of $\text{Cs}_2\text{-2}$ in THF a) immediately, b) 1 day after, c) 2 days after d) 3 days after e) 4 days after and f) 6 days after.

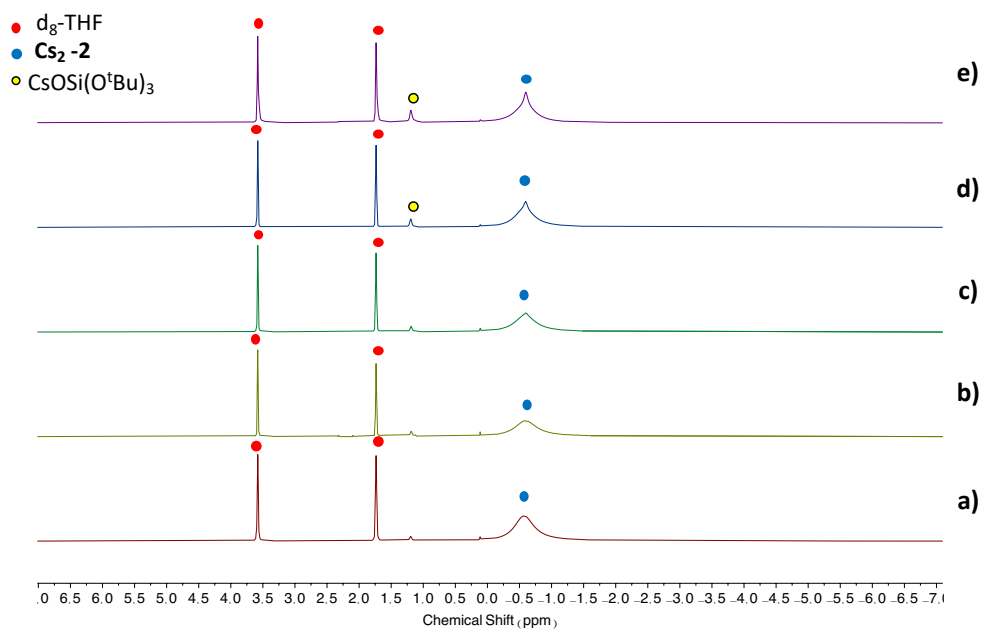


Figure S7: ^1H NMR spectrum (400MHz, $\text{d}_8\text{-THF}$, 298 K) evolution at 233 K of $\text{Cs}_2\text{-2}$ in THF a) immediately, b) 3 days after, c) 6 days after d) 14 days after and e) 21 days after.

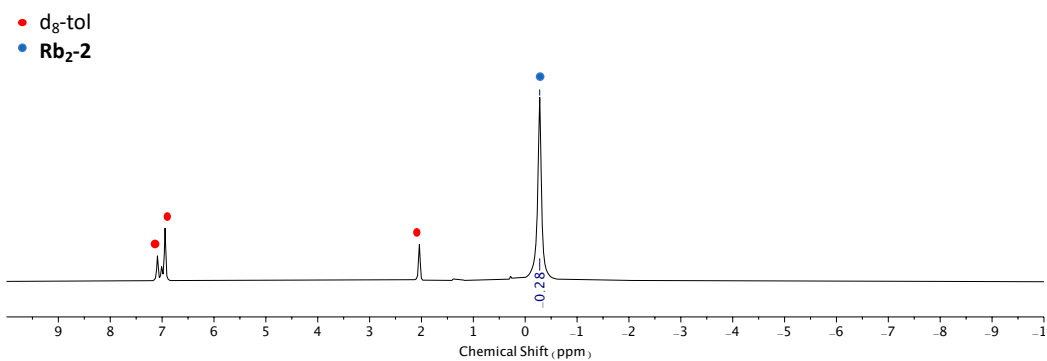


Figure S8: ¹H NMR spectrum (400 MHz, d₈-toluene, 233 K) of [Rb₂{U^{III}(OSi(O^tBu))₃}₂(μ-O)] **Rb₂-2**

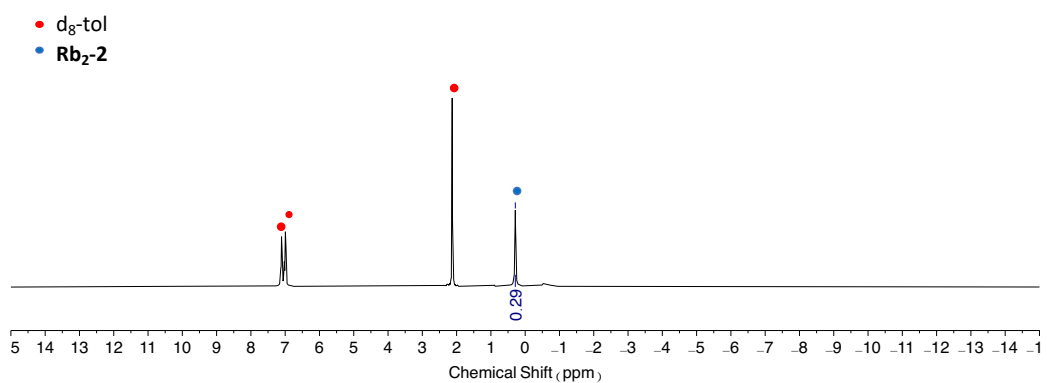


Figure S9: ¹H NMR spectrum (400 MHz, d₈-toluene, 298 K) of **Rb₂-2**

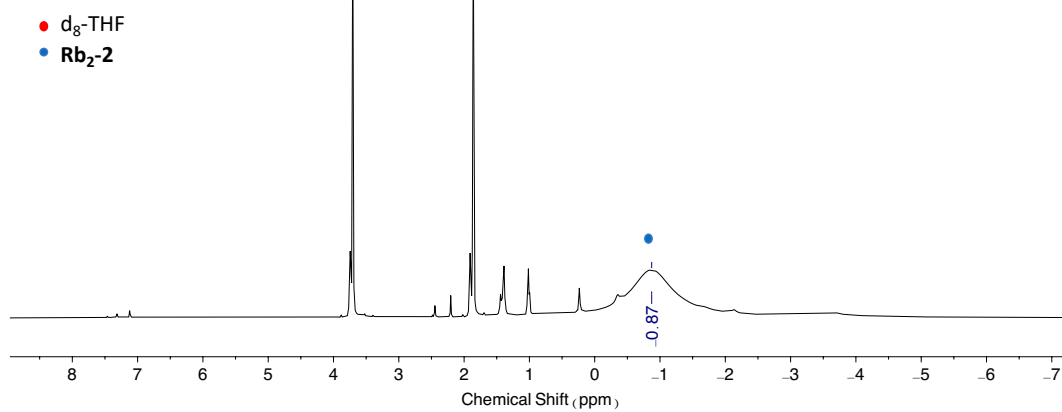


Figure S10: ¹H NMR spectrum (400 MHz, d₈-THF, 233 K) of **Rb₂-2**

NJ85.1.fid
refe1h_zg THF / opt / jori 55

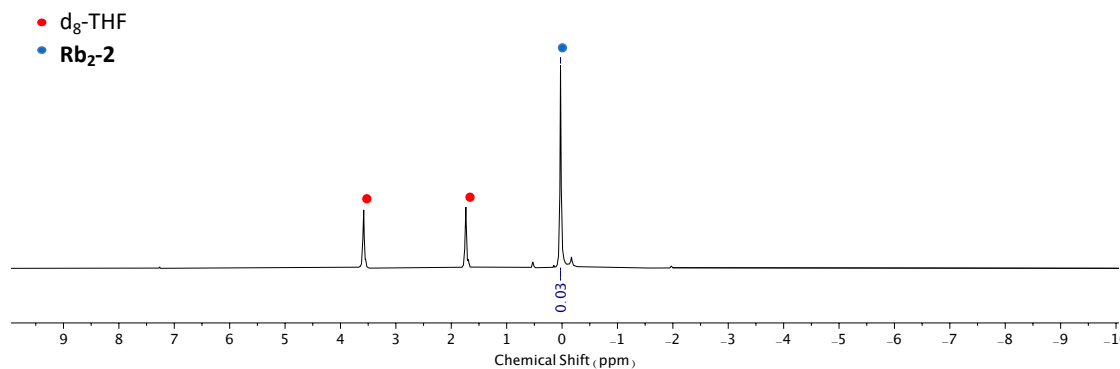


Figure S11: ^1H NMR spectrum (400 MHz, d_8 -THF, 298 K) of $\text{Rb}_2\text{-2}$

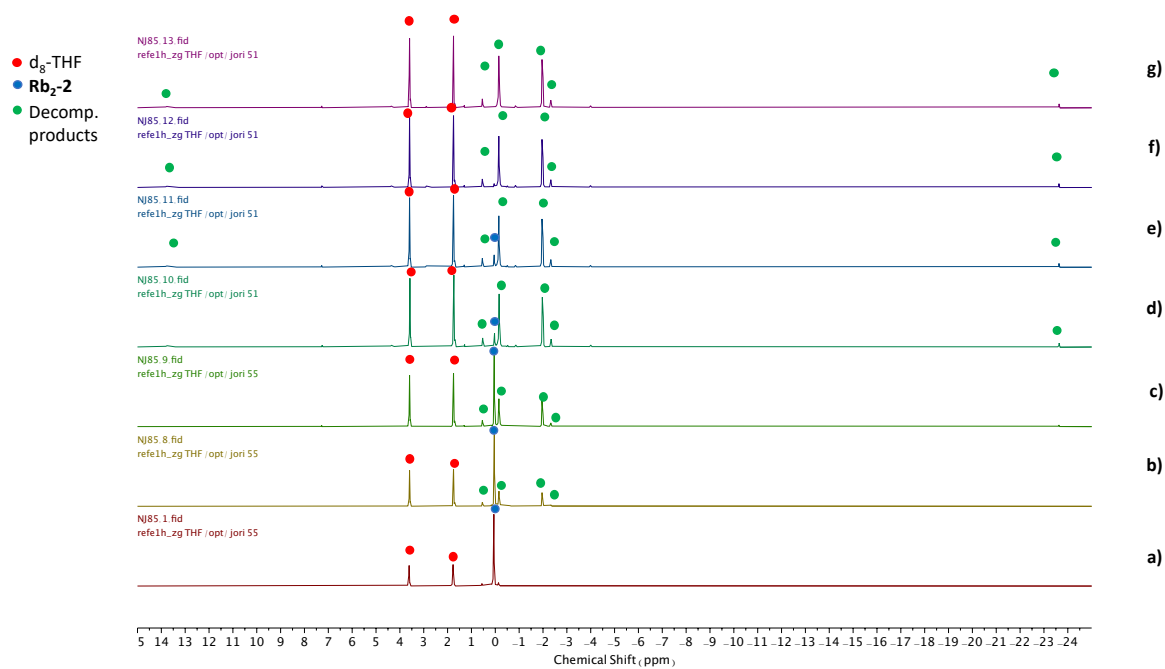


Figure S12: ^1H NMR spectrum (400MHz, d_8 -THF, 298 K) evolution at 298 K of $\text{Rb}_2\text{-2}$ in THF a) immediately, b) 1 day after, c) 2 days after d) 4 days after e) 5 days after, f) 6 days after and g) 7 days after.

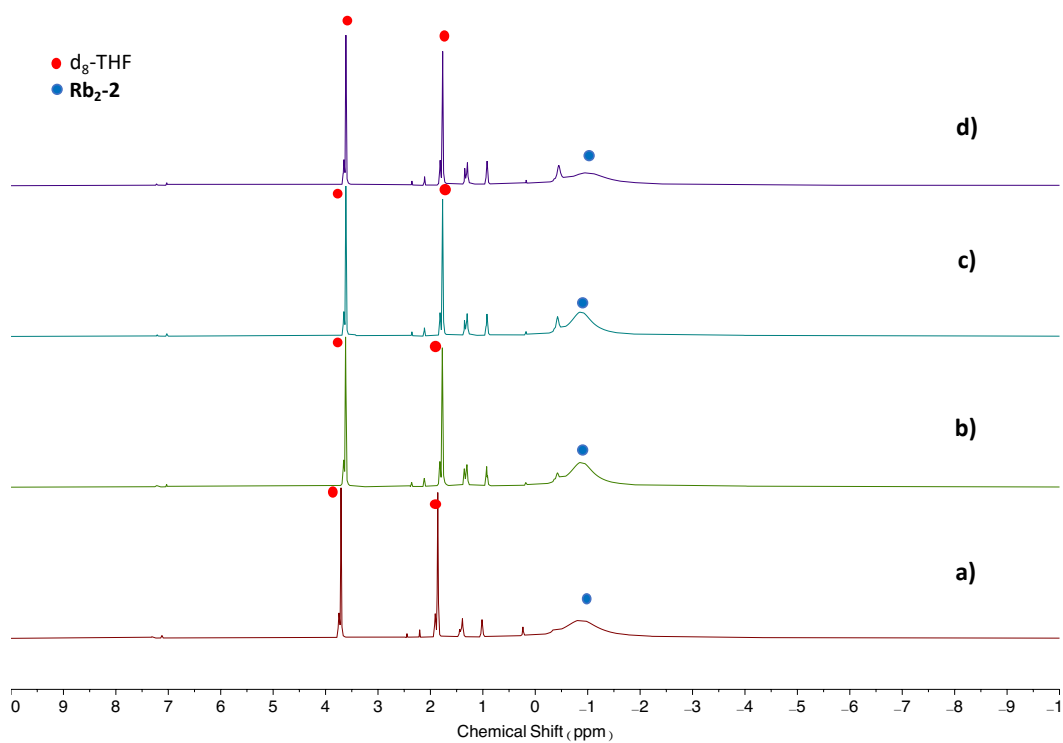


Figure S13: ^1H NMR spectrum (400MHz, $\text{d}_8\text{-THF}$, 233 K) evolution at 233 K of $\text{Rb}_2\text{-2}$ in THF a) immediately, b) 2 days after, c) 6 days after d) 14 days after.

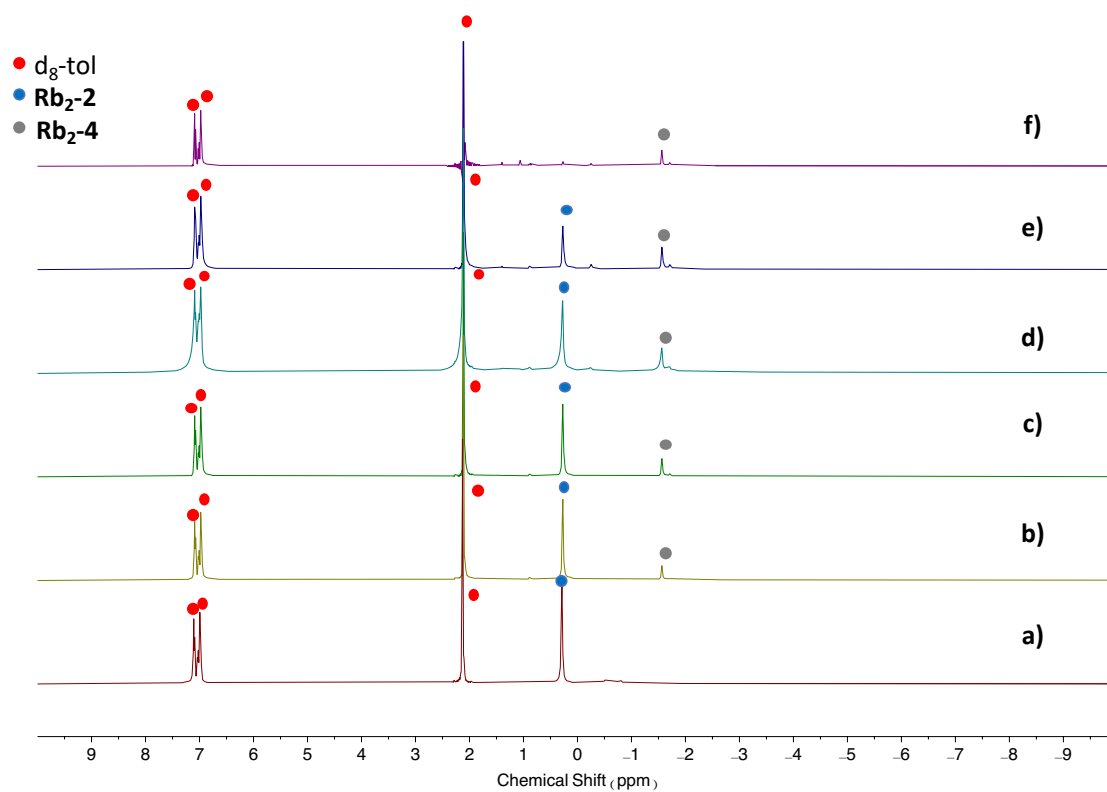


Figure S14: ^1H NMR spectrum (400MHz, $\text{d}_8\text{-toluene}$, 298 K) evolution at 298 K of $\text{Rb}_2\text{-2}$ in toluene a) immediately, b) 6 hs after, c) 12 hs after d) 1 day after e) 2 days after, and f) 5 days after.

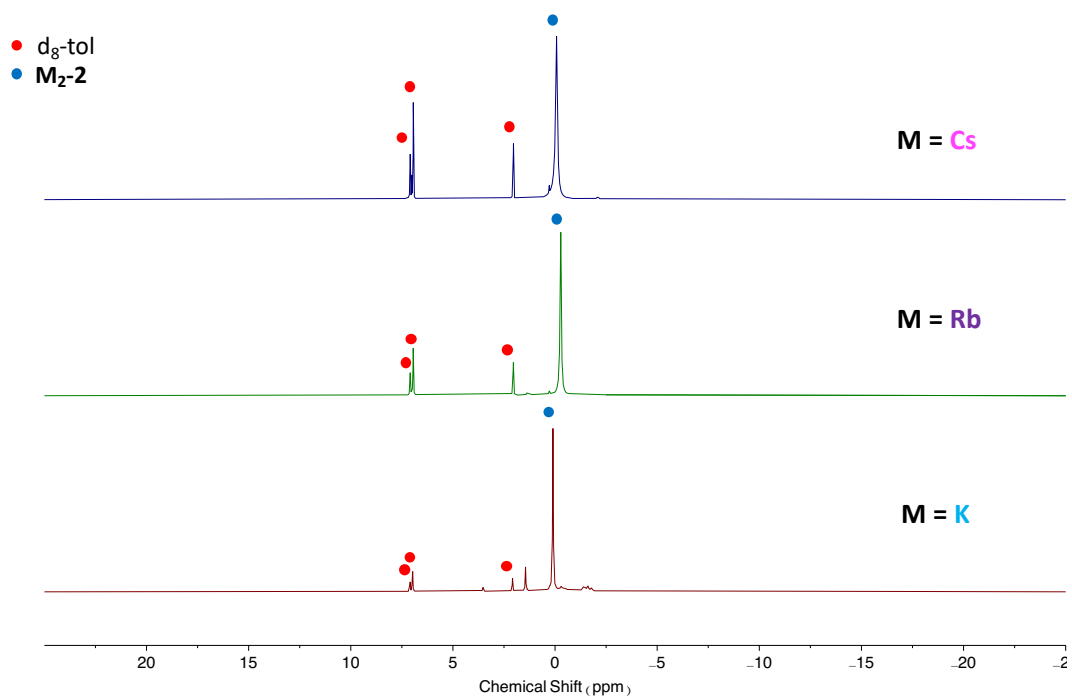


Figure S15: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison of $\text{M}_2\text{-2}$ in toluene solution at -40°C . $\text{M} = \text{K}$ (bottom), Rb (middle) and Cs (top)

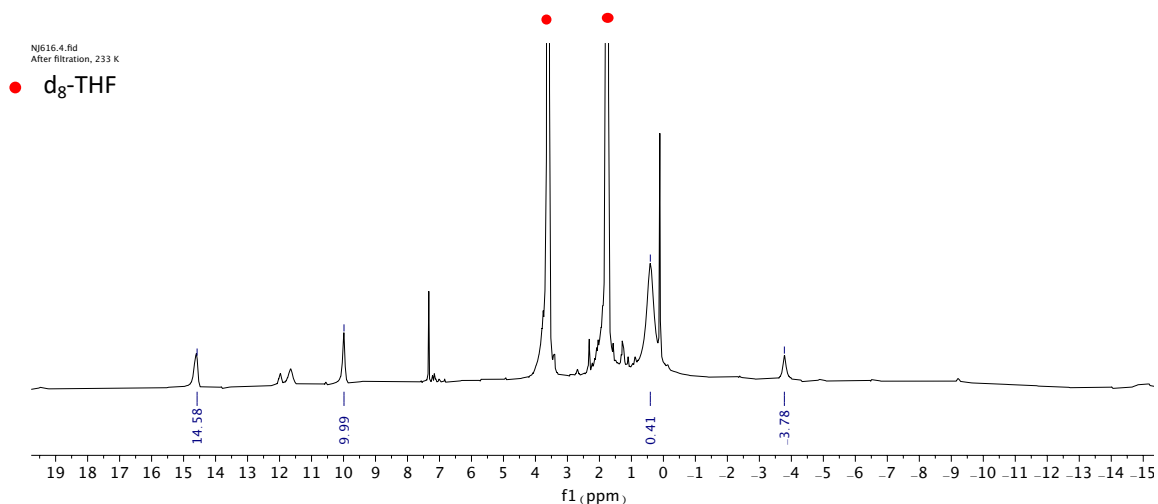


Figure S16: ^1H NMR spectrum (400 MHz, d_8 -THF, 233 K) of the reaction mixture of **1** with excess Na^0 mirror after 24 h at -40°C

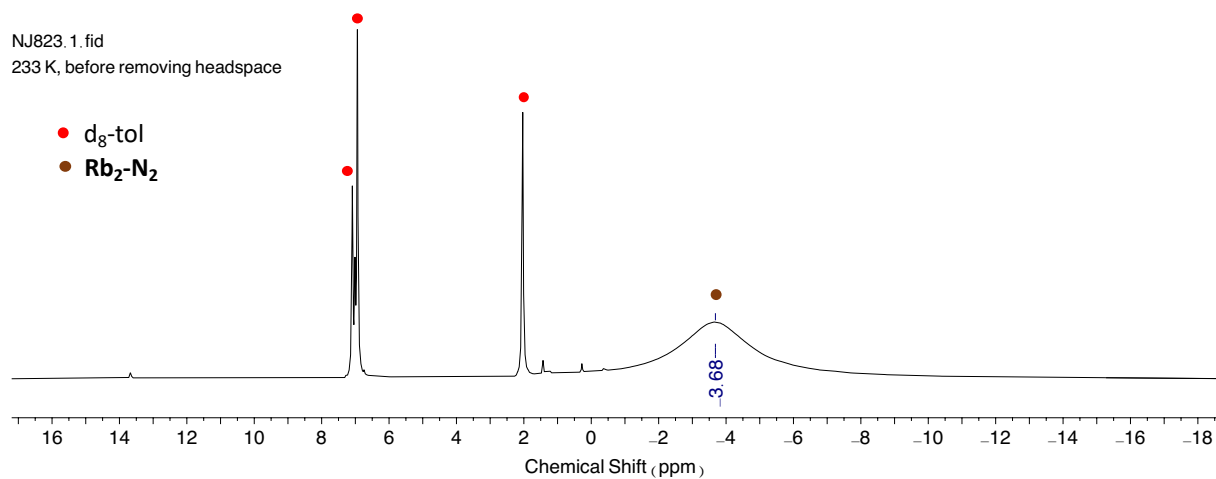


Figure S17: ^1H NMR spectrum (400 MHz, 233 K, d_8 -toluene) of $\text{Rb}_2\text{-N}_2$

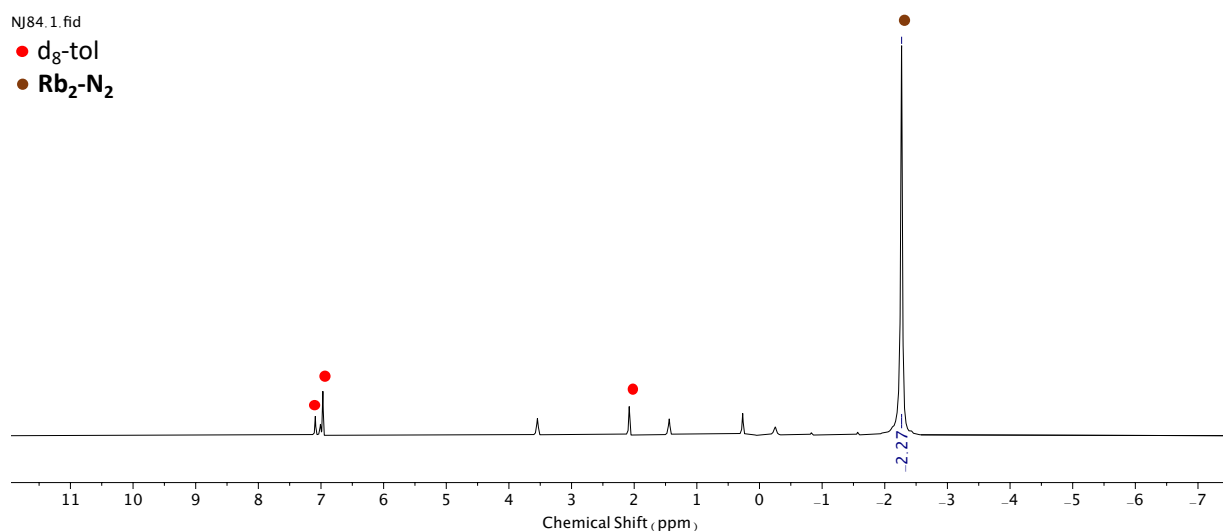


Figure S18: ¹H NMR spectrum (400 MHz, 298 K, d₈-toluene) of Rb₂-N₂

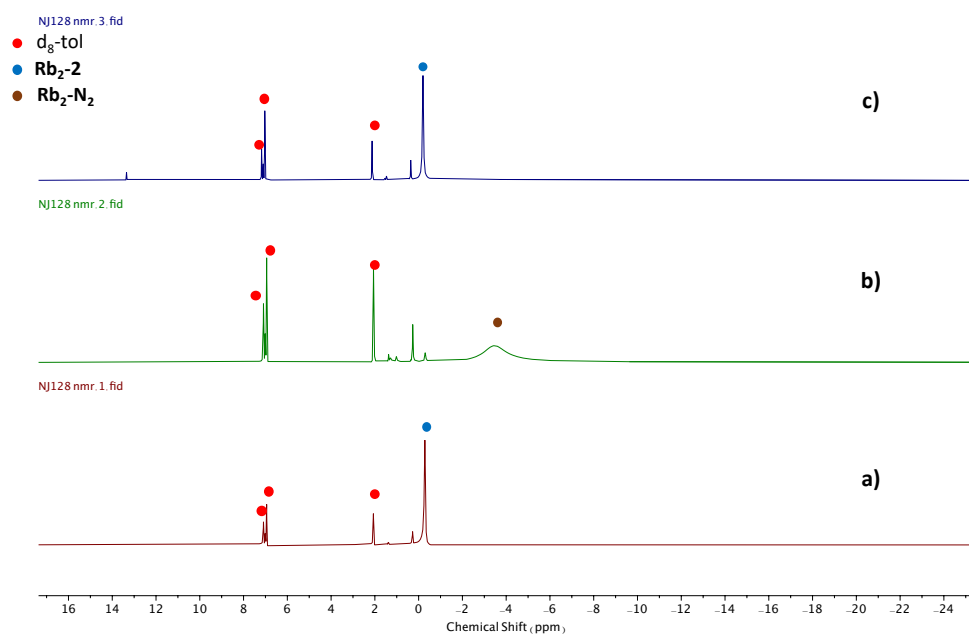


Figure S19: ¹H NMR spectra (400 MHz, d₈-toluene, 233 K) comparison of the reaction mixture of Rb₂-2 a) before, b) after addition of 1 atm N₂ and c) after removing all the volatiles and leaving the resulting solid under vacuum at -80°C for 1 h (top)

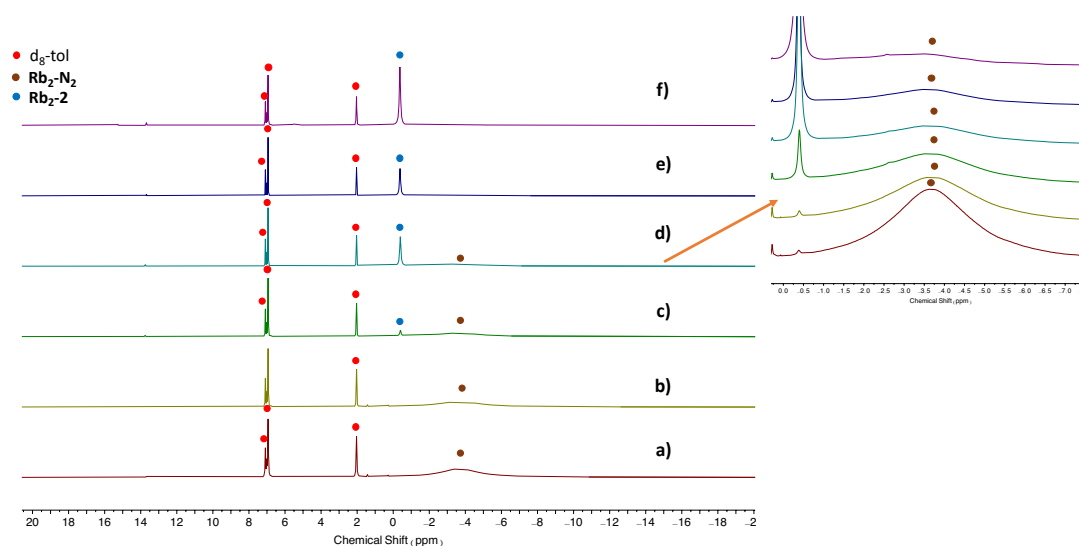


Figure S20: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison of the reaction mixture of $\text{Rb}_2\text{-N}_2$ a) before, b) immediately after, c) 1 day after, d) 4 days after, e) 7 days after and f) 15 days after removing the headspace in the Ar glovebox

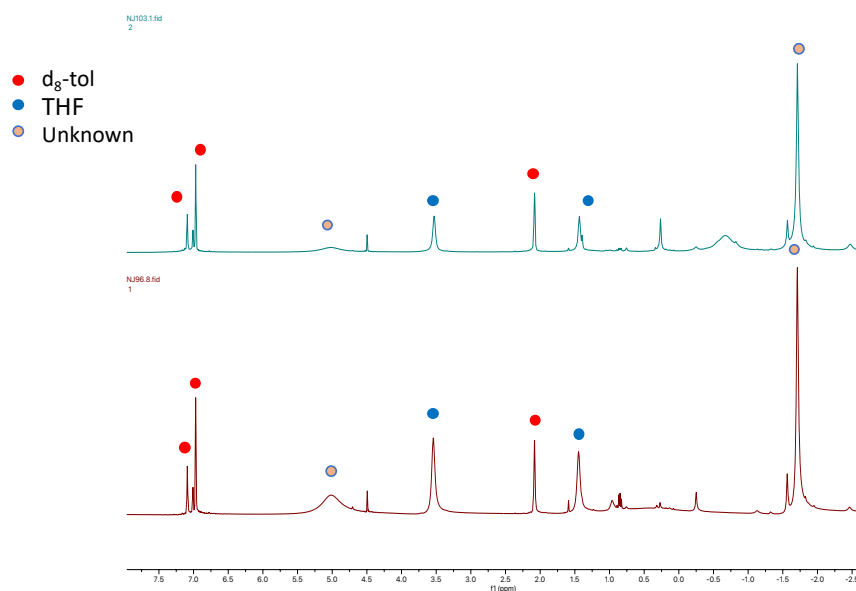


Figure S21: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison of the reaction mixture of in situ generated $\text{Rb}_2\text{-2}$ 24 hs after addition 1 atm H_2 (top) and 24 hs after addition of H_2 to in situ generated $\text{Rb}_2\text{-N}_2$ (bottom)

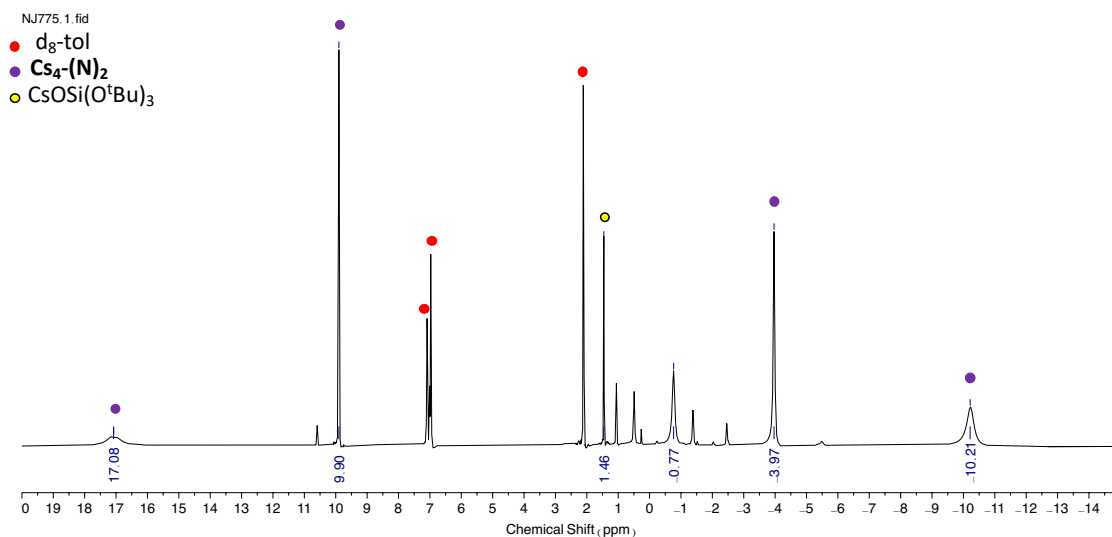


Figure S22: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture obtained after addition of 2 equiv. of CsC_8 to complex Cs_2-2 after 24 hs at 233 K under a N_2 atmosphere.

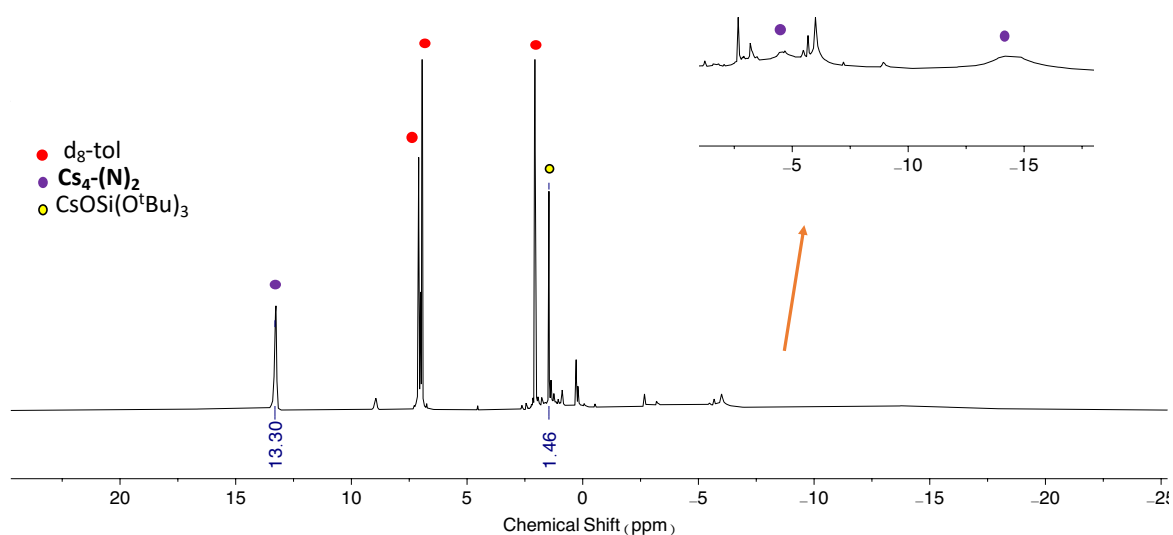


Figure S23: 1H NMR spectrum (400 MHz, d_8 -toluene, 233 K) of the reaction mixture obtained after addition of 2 equiv. of CsC_8 to complex Cs_2-2 after 24 hs at 233 K under a N_2 atmosphere.

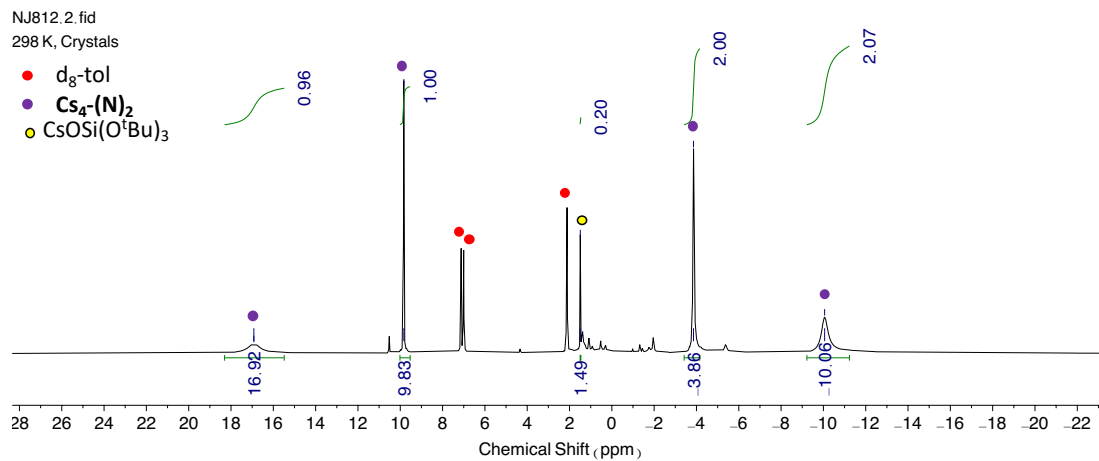


Figure S24: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of crystals of $Cs_4(N)_2$

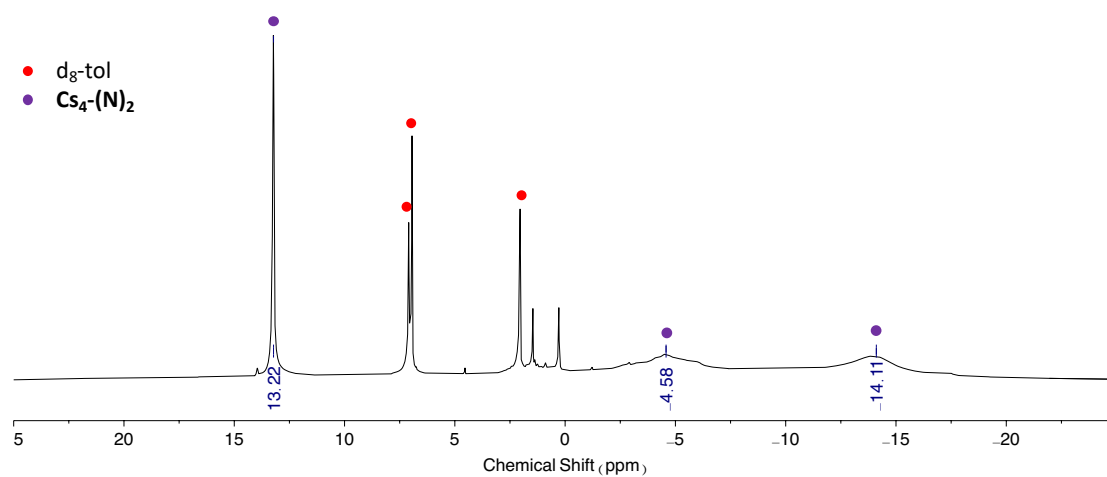


Figure S25: 1H NMR spectrum (400 MHz, d_8 -toluene, 233 K) of crystals of $Cs_4-(N)_2$

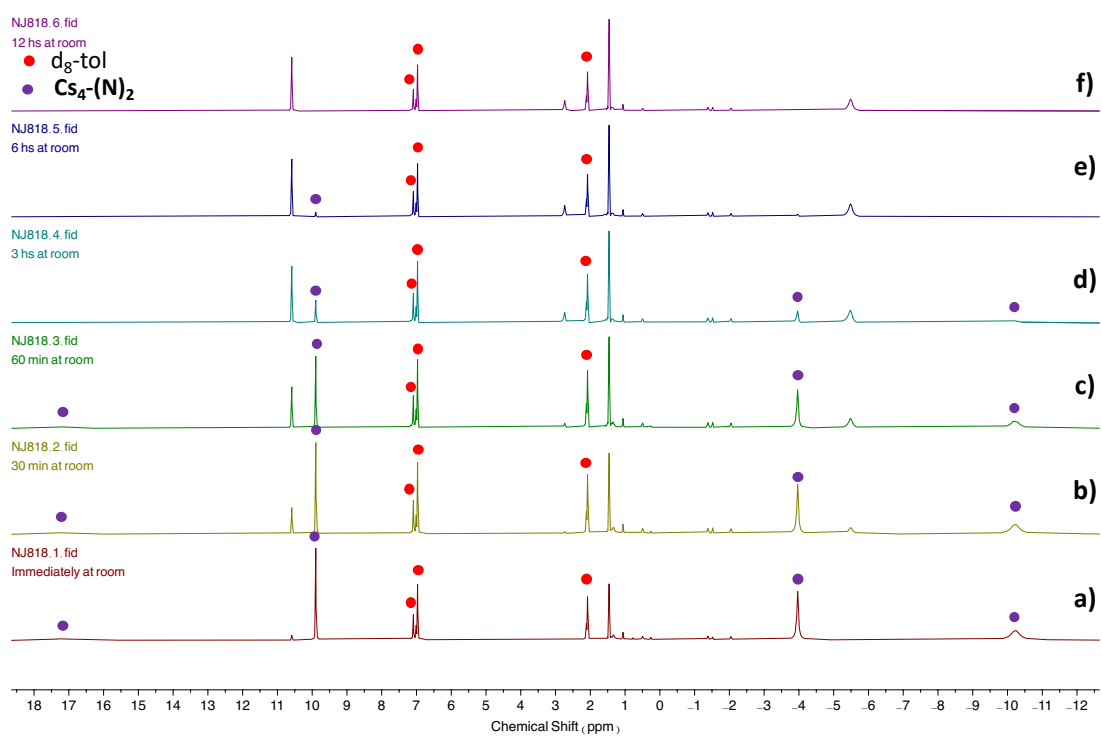


Figure S26: 1H NMR spectrum (400MHz, d_8 -toluene, 298 K) evolution at 298 K of $Cs_4-(N)_2$ in toluene a) immediately, b) 30 min after, c) 1h after d) 3 hs after e) 6 hs after and f) 12 hs after.

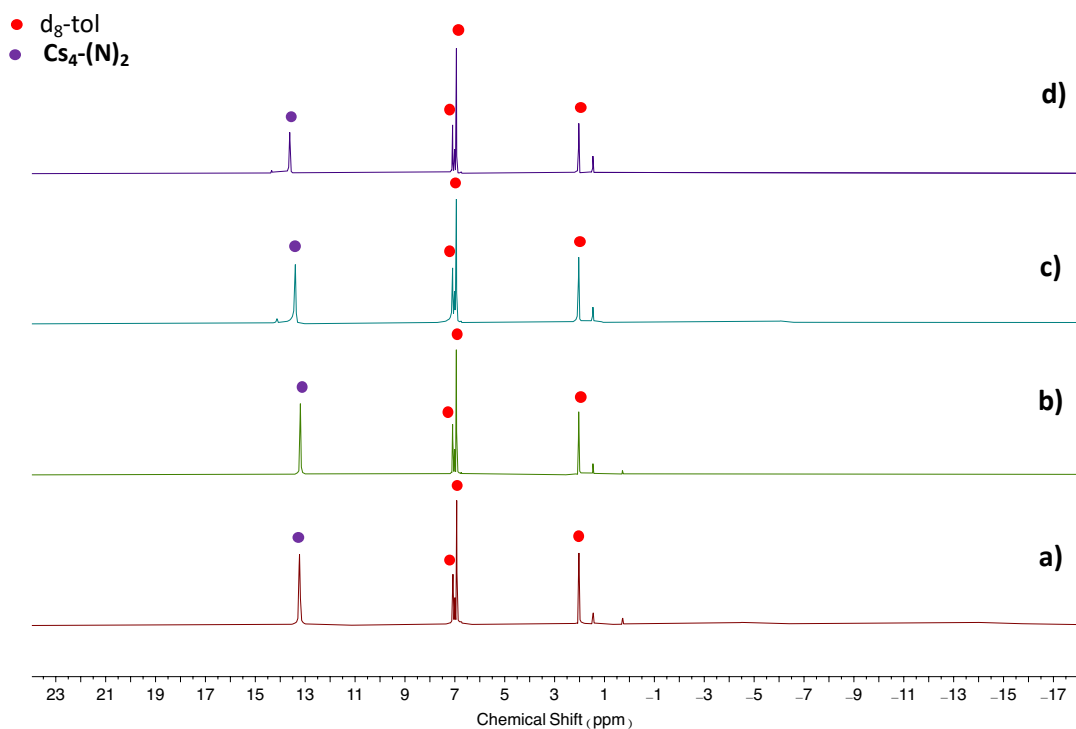


Figure S27: ^1H NMR spectrum (400MHz, d_8 -toluene, 233 K) evolution at 233 K of $\text{Cs}_4\text{-(N)}_2$ in toluene a) immediately, b) 3 days after, c) 10 days after and d) 14 days after.

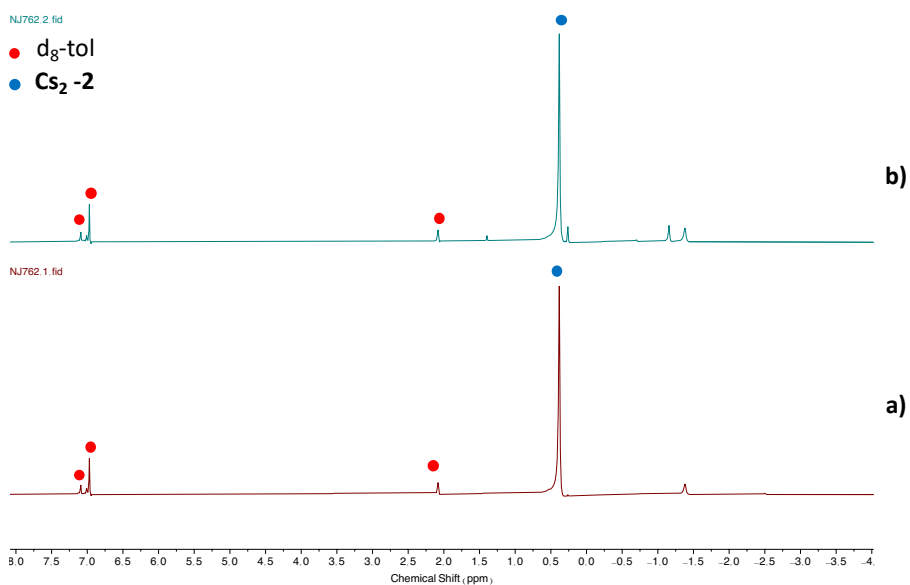


Figure S28: ^1H NMR spectra (400 MHz, d_8 -toluene, 298 K) comparison. of the reaction mixture of complex $\text{Cs}_2\text{-2}$ a) before and b) 15 hs after addition of 2 equiv. of CsC_8 at 233 K under an Ar atmosphere.

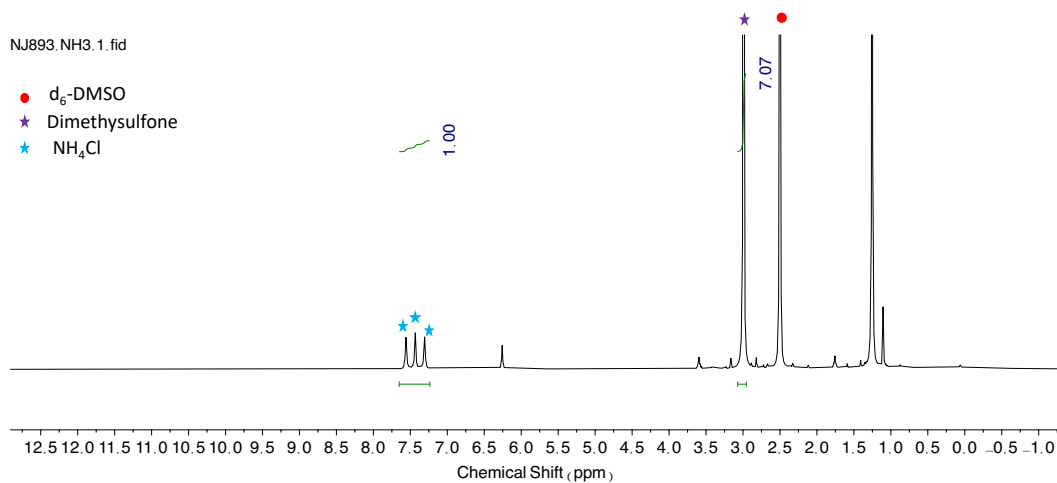


Figure S29: ^1H NMR spectrum (400 MHz, d_6 -DMSO, 298 K) of the residue after evaporation of the reaction mixture resulting from the reaction of complex **Cs₂-2** with 2 equiv. of CsC_8 at 233 K for 24 hs under N_2 atmosphere, after addition of excess 2M HCl (Et_2O).

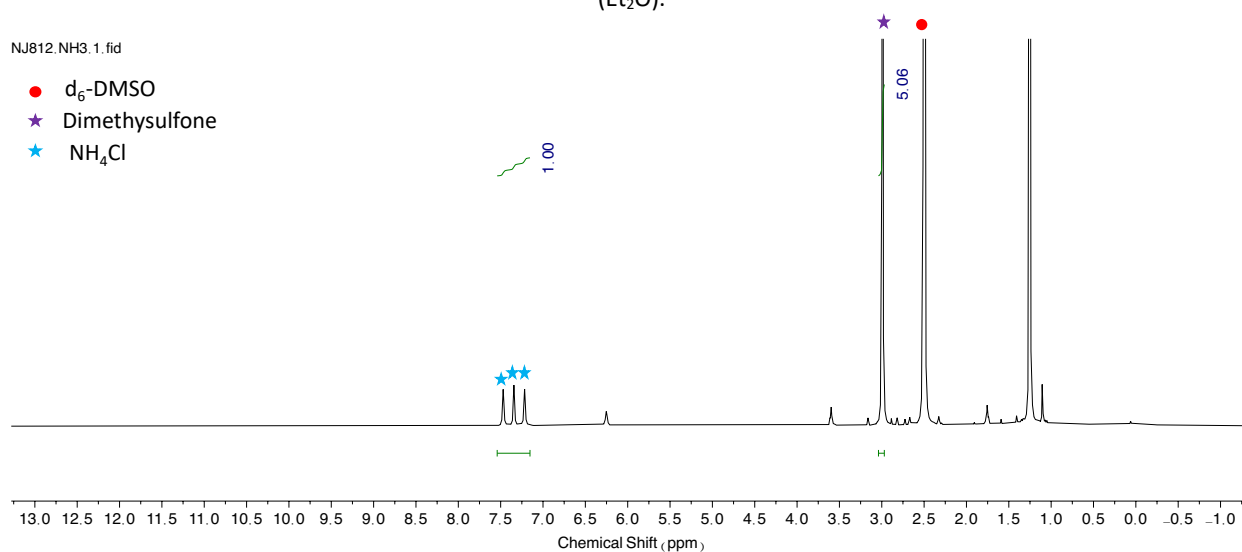


Figure S30: ^1H NMR spectrum (400 MHz, d_6 -DMSO, 298 K) of the residue after evaporation of the solution obtained from the addition of excess 2M HCl (Et_2O) to isolated complex **Cs₄-(N)₂**.

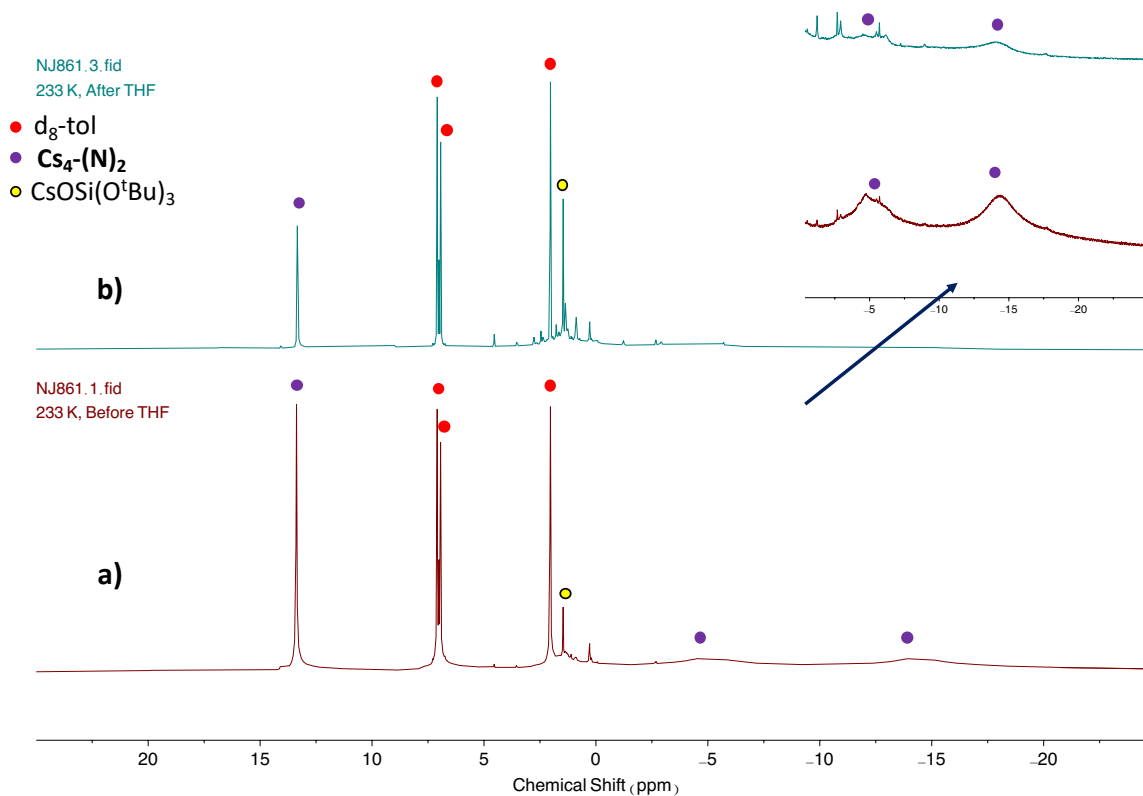


Figure S31: 1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison of the crystals of $Cs_4-(N)_2$ a) before and b) after dissolution in d_8 -THF at $-40^\circ C$.

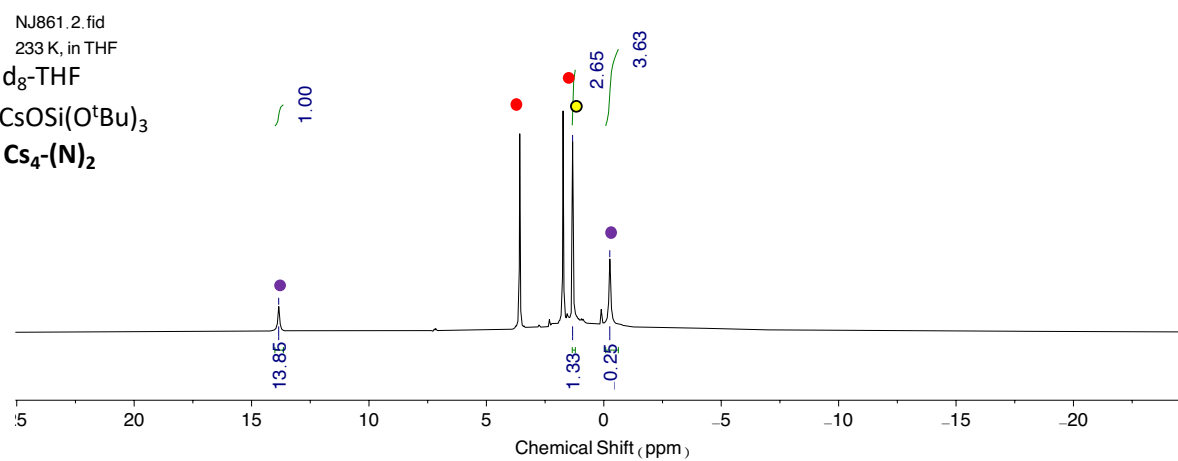


Figure S32: 1H NMR spectrum (400 MHz, d_8 -THF, 233 K) of crystals of $Cs_4-(N)_2$

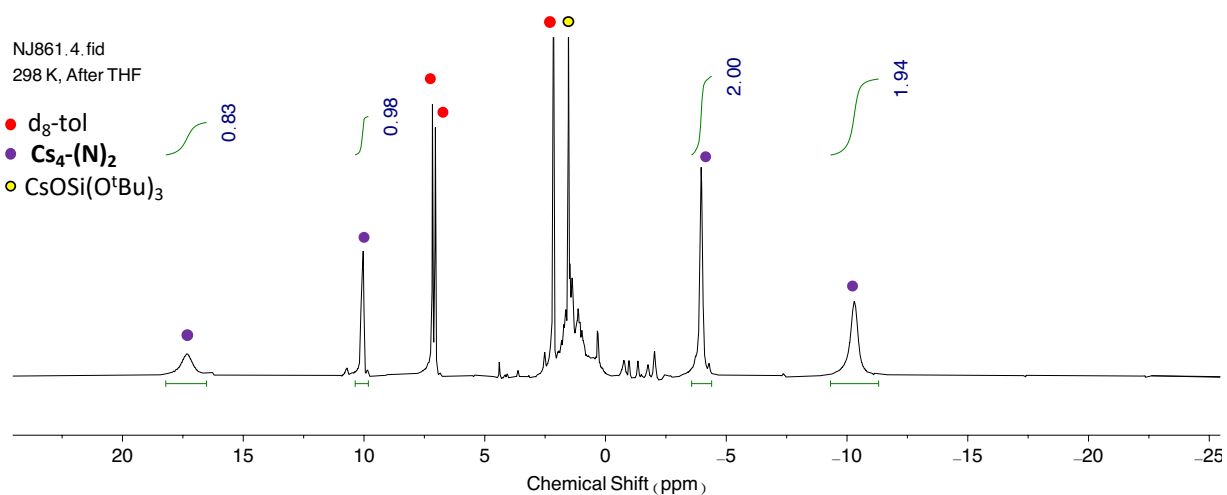


Figure S33: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of crystals of $Cs_4(N)_2$ after dissolution in THF at $-40^\circ C$.

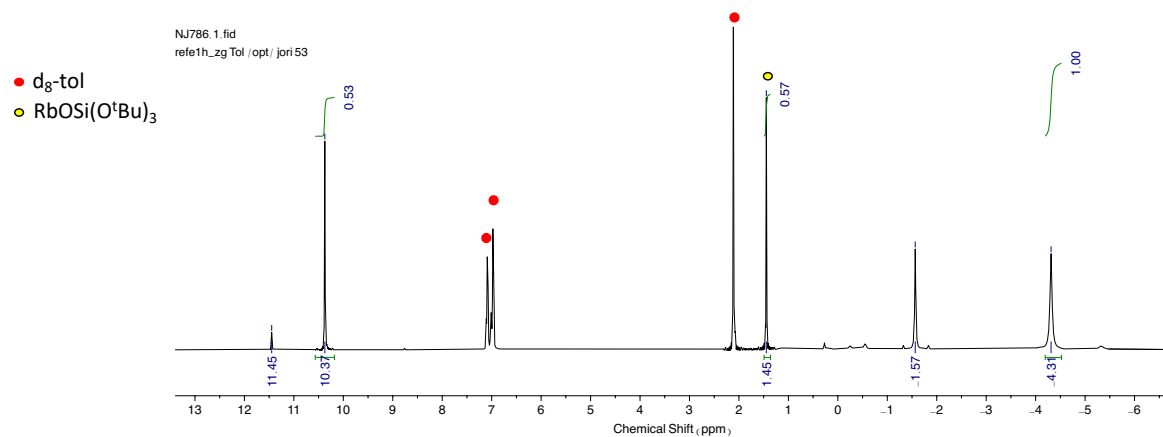


Figure S34: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture obtained after addition of 2 equiv. of RbC_8 to complex Rb_2-N_2 after 24 hs at 233 K under a N_2 atmosphere.

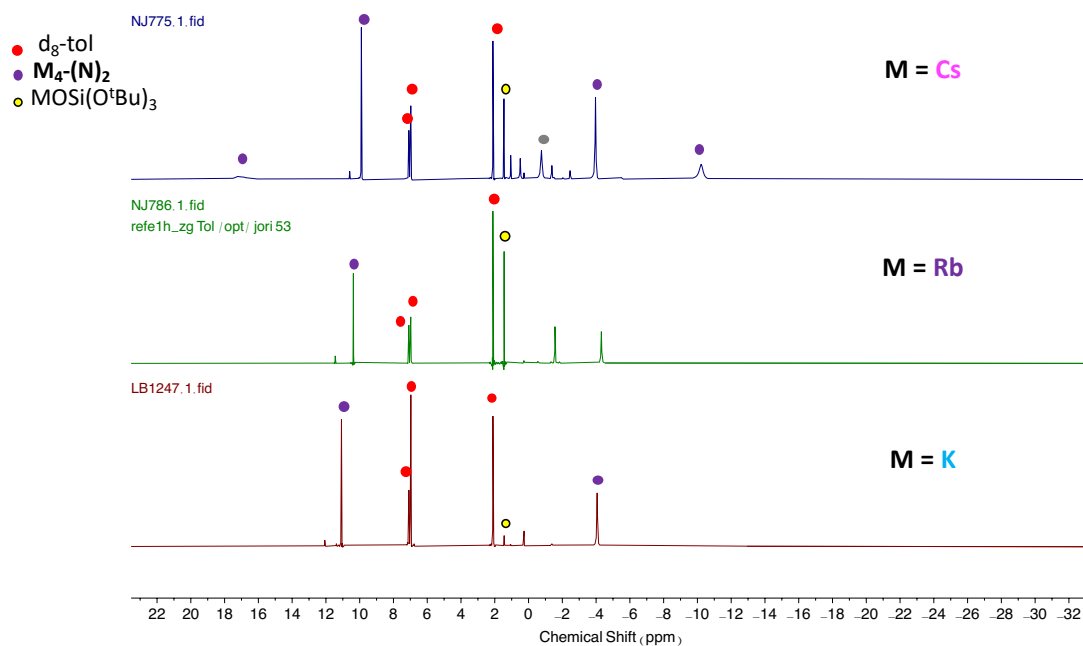


Figure S35: 1H NMR spectra (400 MHz, d_8 -toluene, 298 K) comparison of the reaction mixture obtained after addition of 2 equiv. of MC_8 to complex K_2-N_2 (bottom, redrawn from ⁵), Rb_2-N_2 (middle) and Cs_2-2 (top) after 24 hs at 233 K under a N_2 atmosphere.

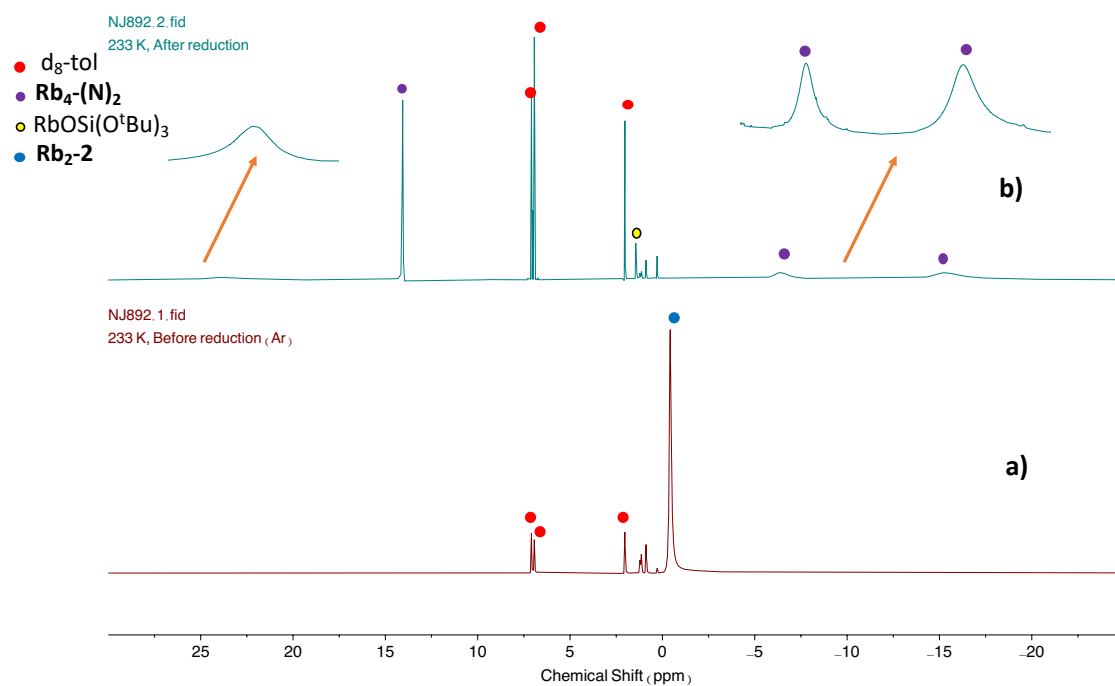


Figure S36: 1H NMR spectrum (400 MHz, d_8 -toluene, 233 K) of the reaction mixture of complex Rb_2-2 a) before (under Ar) and b) 24 hs after addition of 2 equiv. of RbC_8 at 233 K under a N_2 atmosphere.

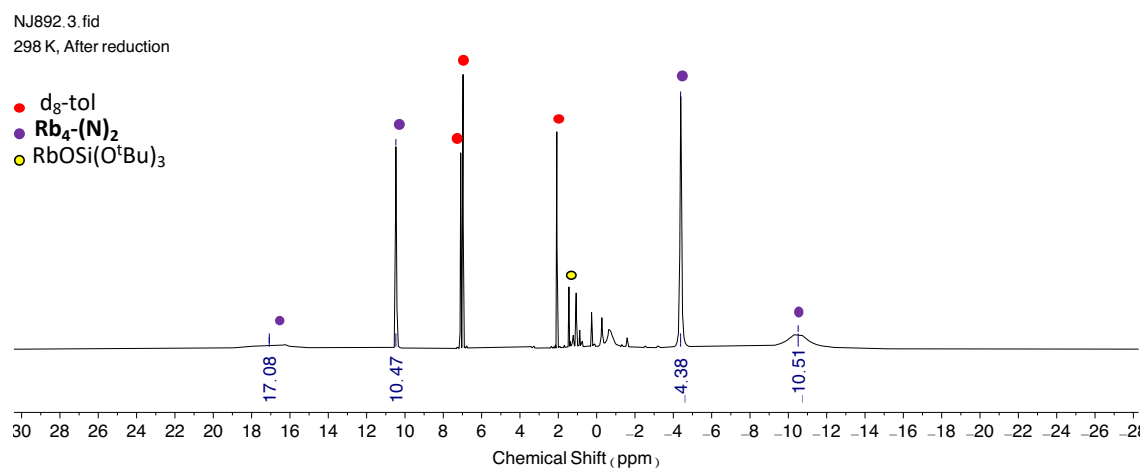


Figure S37: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture obtained after addition of 2 equiv. of RbC_8 to complex Rb_2-2 after 24 hs at 233 K under a N_2 atmosphere.

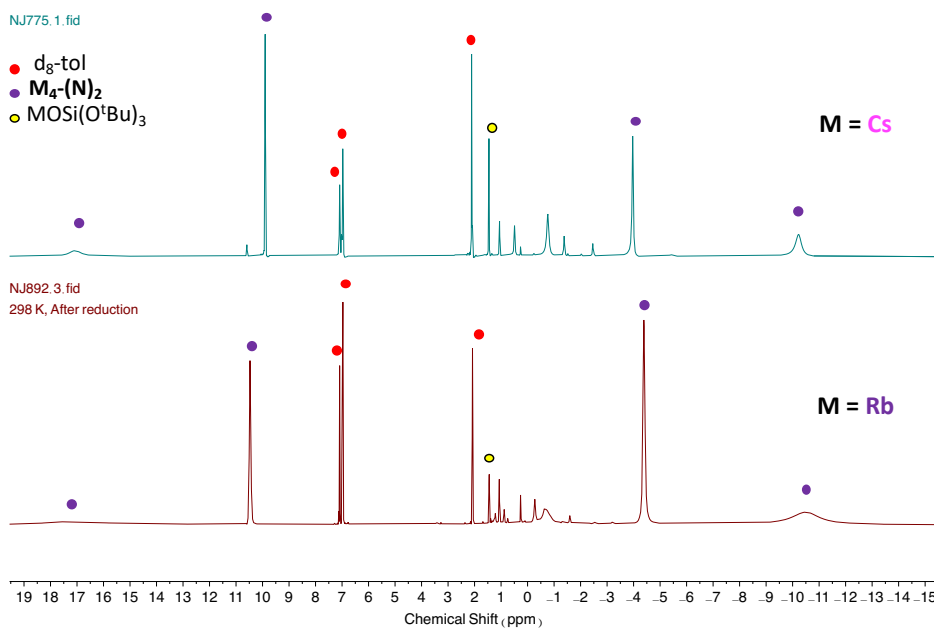


Figure S38: ^1H NMR spectra (400 MHz, d_8 -toluene, 298 K) comparison of the reaction mixture obtained after addition of 2 equiv. of MC_8 to complex $\text{Rb}_2\text{-2}$ (bottom) and $\text{Cs}_2\text{-2}$ (top) after 24 hs at 233 K under a N_2 atmosphere.

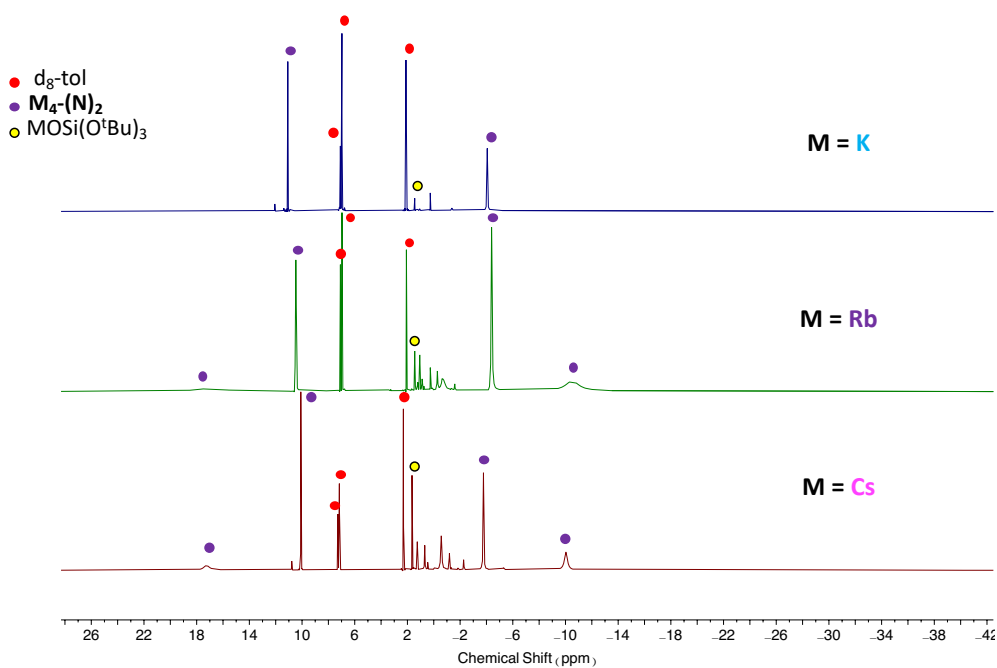


Figure S39: ^1H NMR spectra (400 MHz, d_8 -toluene, 298 K) comparison of the reaction mixture obtained after addition of 2 equiv. of MC_8 to complex $\text{K}_2\text{-N}_2$ (top redrawn from ⁵), $\text{Rb}_2\text{-2}$ (middle) and $\text{Cs}_2\text{-2}$ (bottom) after 24 hs at 233 K under a N_2 atmosphere.

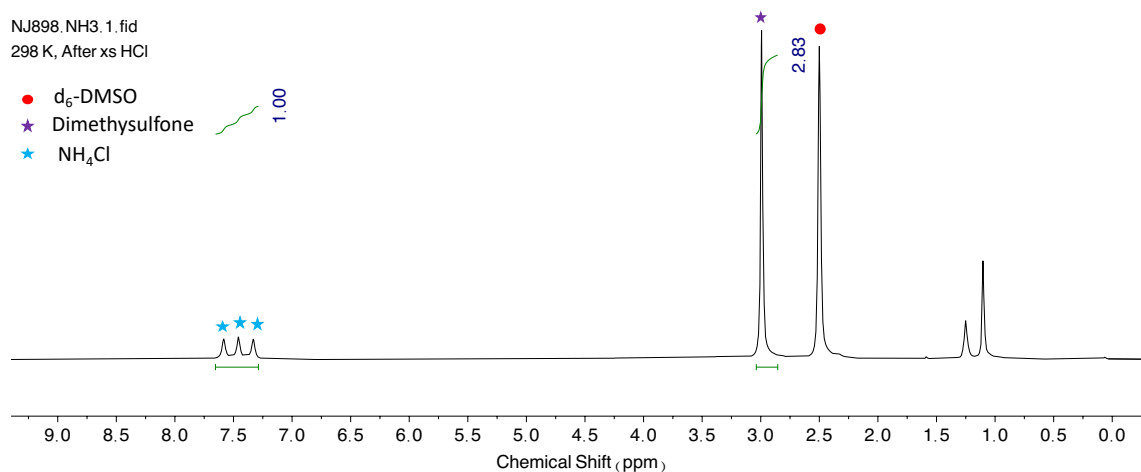


Figure S40: 1H NMR spectrum (400 MHz, d_6 -DMSO, 298 K) of the residue after evaporation of the reaction mixture resulting from the reaction of complex **Rb₂-2** with 2 equiv. of RbC_8 at 233 K for 24 hs under N_2 atmosphere, after addition of excess 2M HCl (Et_2O).

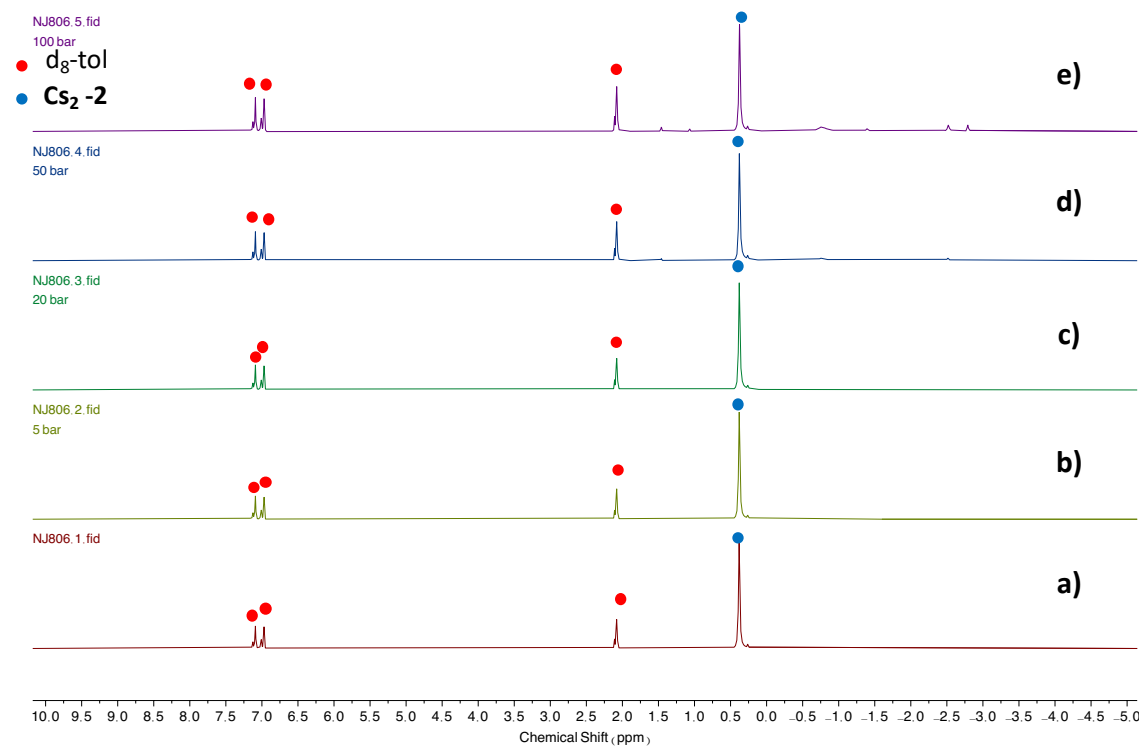


Figure S41: 1H NMR spectra (400 MHz, d_8 -toluene, 298 K) comparison. of the reaction mixture of complex **Cs₂-2** a) before and after addition of b) 5 bar, c) 10 bar, d) 20 bar, d) 50 bar and e) 100 bar of N_2 at 298 K.

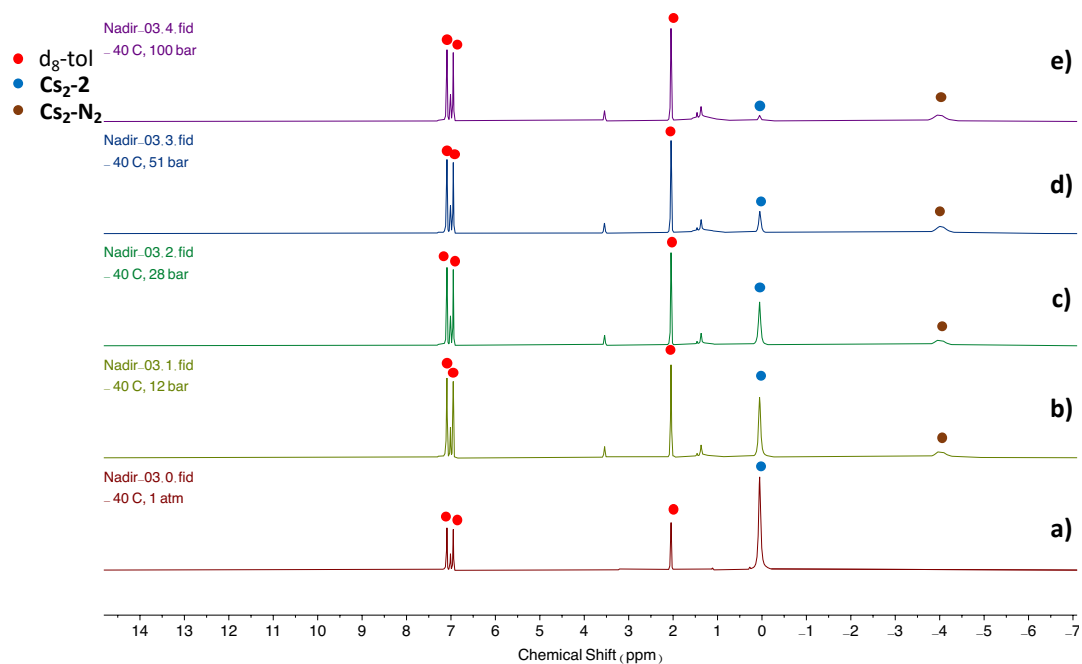


Figure S42: 1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison. of the reaction mixture of complex Cs_2-2 a) before and after addition of b) 12 bar, c) 28 bar, d) 51 bar and e) 100 bar of N_2 at 233 K.

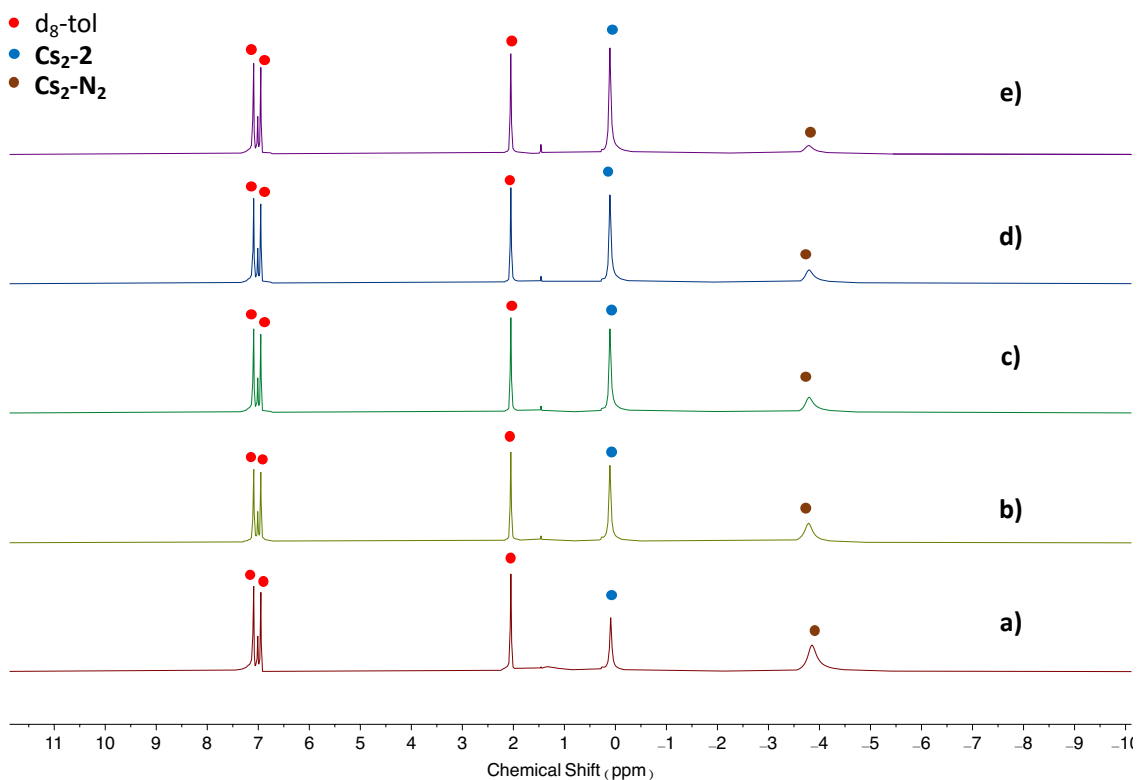


Figure S43: 1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison. of the reaction mixture of complex Cs_2-2 a) immediately after b) 1h after c) 2 hs after, d) 3 hs after, d) 16 hs removal of high pressure N_2 and evolution at 233K.

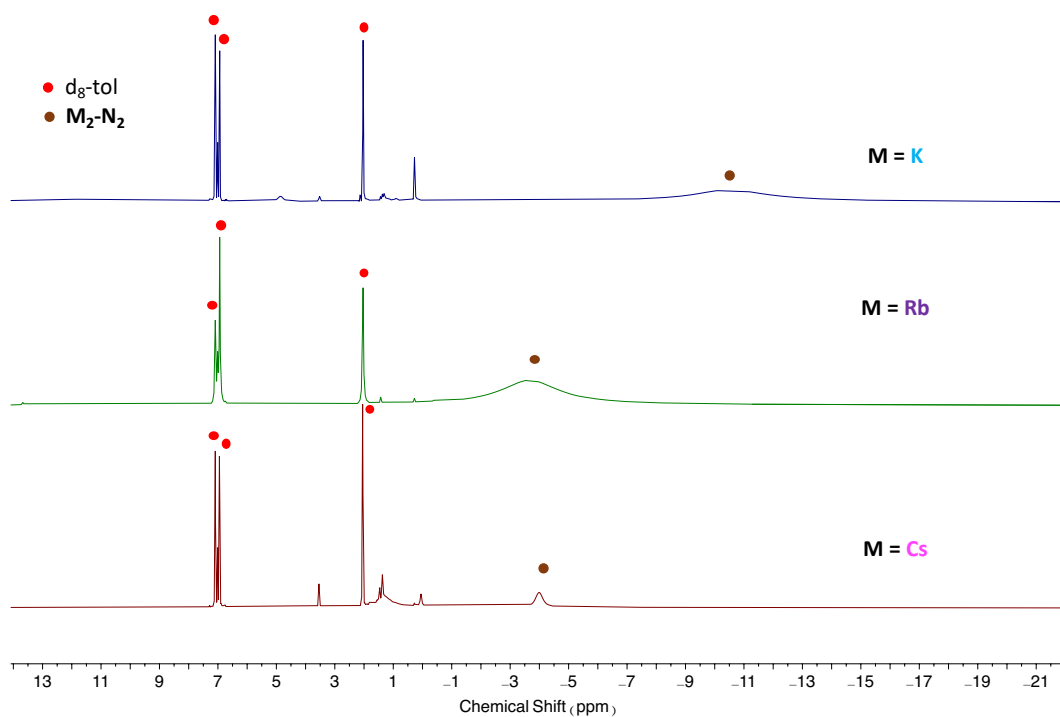


Figure S44: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) comparison of $\text{M}_2\text{-N}_2$ in toluene solution at -40°C . M = Cs (bottom), Rb (middle) and K (top)

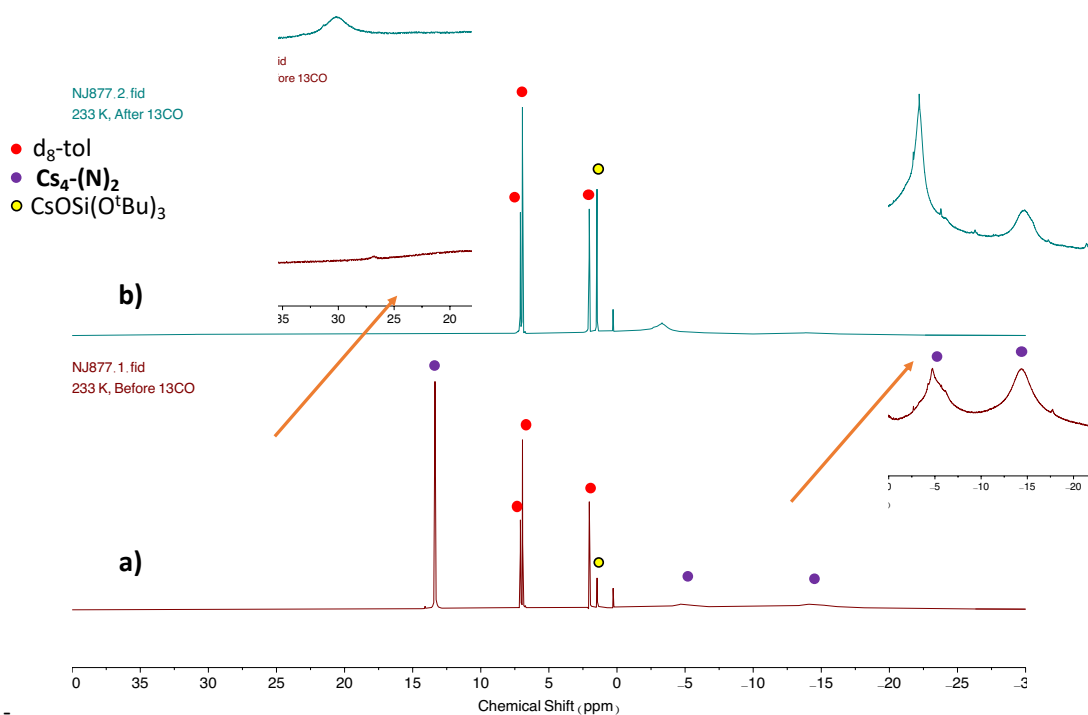


Figure S45: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) evolution of the reaction mixture of complex $\text{Cs}_4\text{-(N)}_2$ a) before and b) immediately after addition of 5 equiv. of ^{13}CO at 233 K.

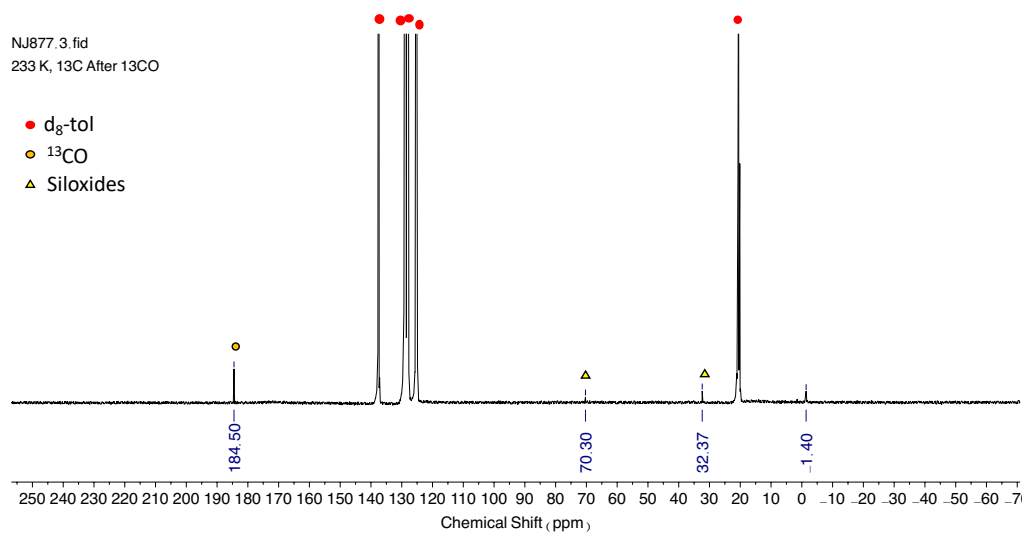


Figure S46: ^{13}C $\{^1\text{H}\}$ NMR spectrum (100 MHz, d_8 -toluene, 233 K) of the reaction mixture of complex $\text{Cs}_4\text{-(N)}_2$ immediately after addition of 5 equiv. of ^{13}CO at 233 K.

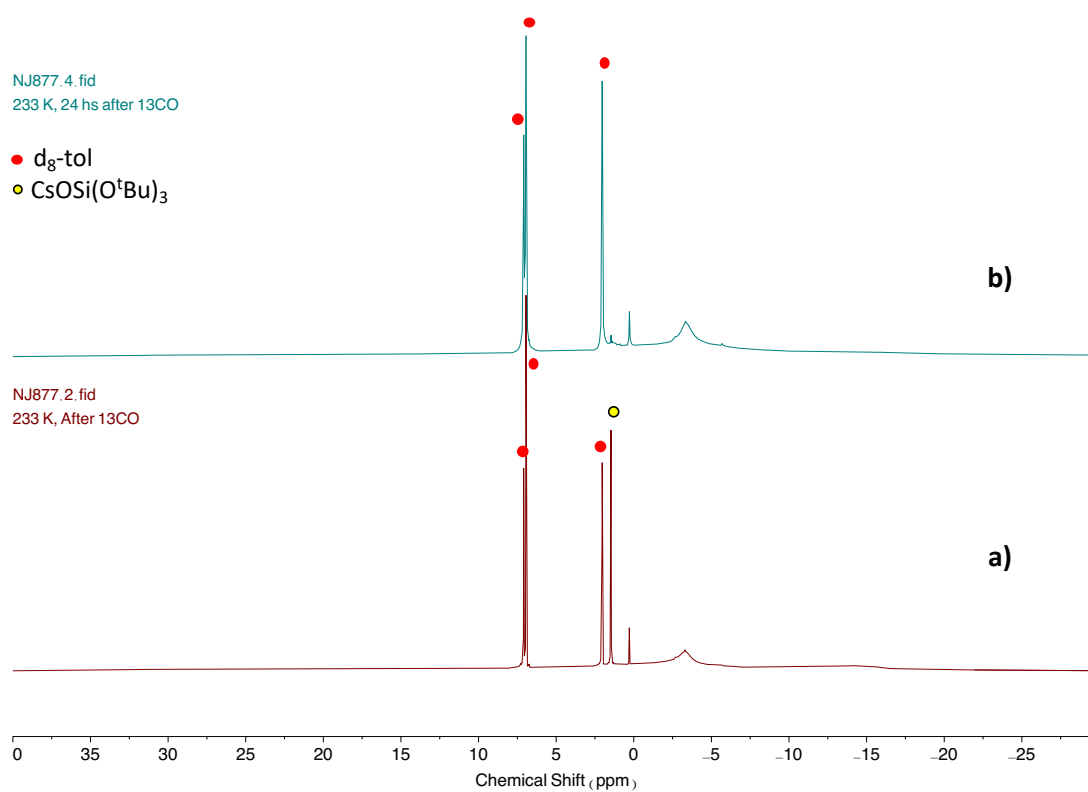


Figure S47: ^1H NMR spectra (400 MHz, d_8 -toluene, 233 K) evolution of the reaction mixture of complex $\text{Cs}_4\text{-(N)}_2$ a) immediately after and b) 24 hs after addition of 5 equiv. of ^{13}CO at 233 K.

NJ877.5.fid
298 K, 24 hs after $^{13}\text{C}\text{O}$

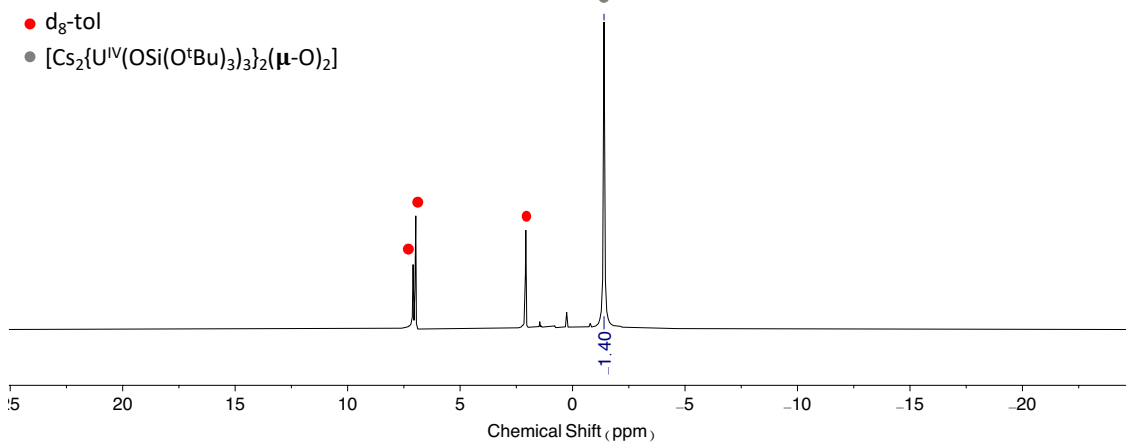


Figure S48: ^1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture of complex $\text{Cs}_4\text{-(N)}_2$ 24 hs after addition of 5 equiv. of $^{13}\text{C}\text{O}$ at 233 K.

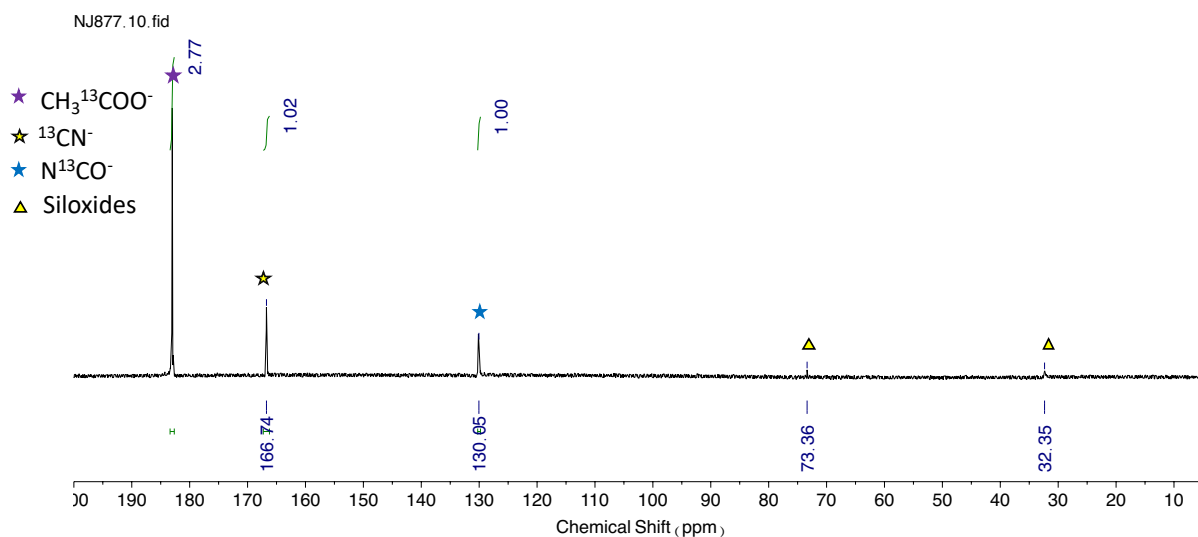


Figure S49: ^{13}C NMR spectrum (151 MHz, D_2O , 298 K) after hydrolysis with $\text{pD}=13$ D_2O of the reaction mixture of complex $\text{Cs}_4\text{-(N)}_2$ 24 hs after addition of 5 equiv. of $^{13}\text{C}\text{O}$ at 233 K.

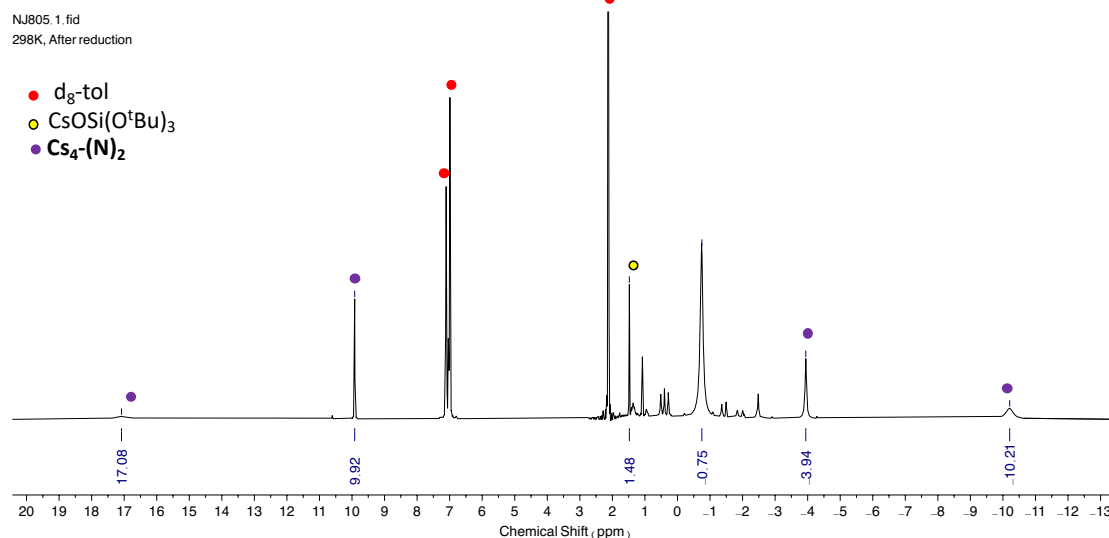


Figure S50: ^1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture obtained after addition of 4 equiv. of CsC_8 to complex **1** after 24 hs at 233 K under a N_2 atmosphere.

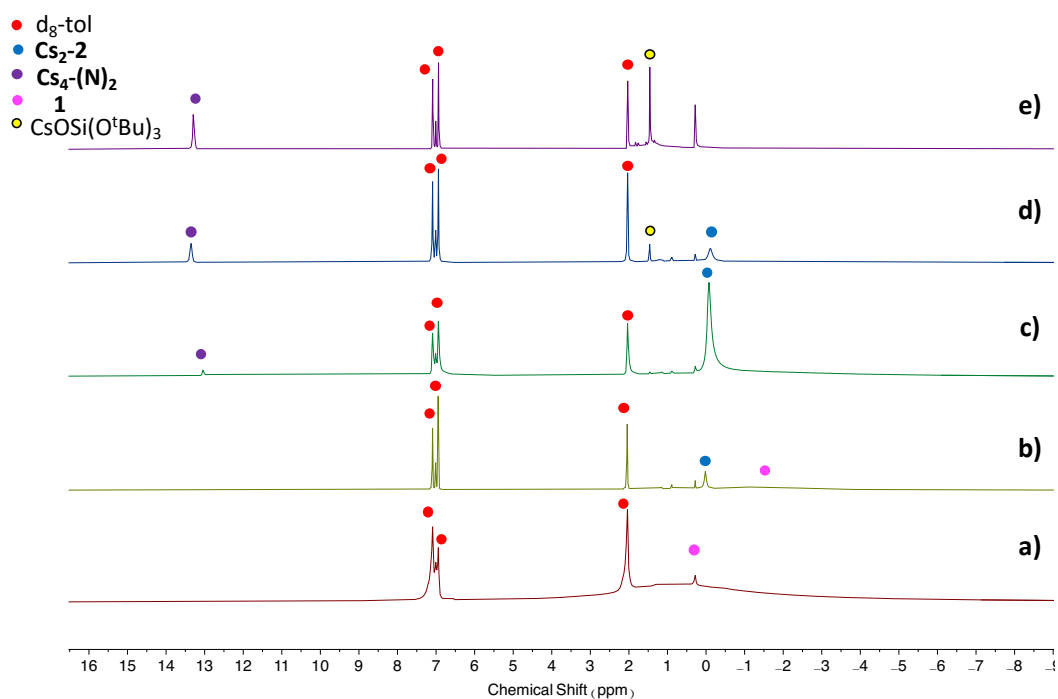


Figure S51: ^1H NMR spectrum (400 MHz, d_8 -toluene, 233 K) evolution of the reaction mixture obtained by addition of 4 equiv. of CsC_8 to complex **1** at 233 K under a N_2 atmosphere a) before b) immediately after, c) 1 h after c) 3 hs after d) 15 hs after, e) 24 hs after.

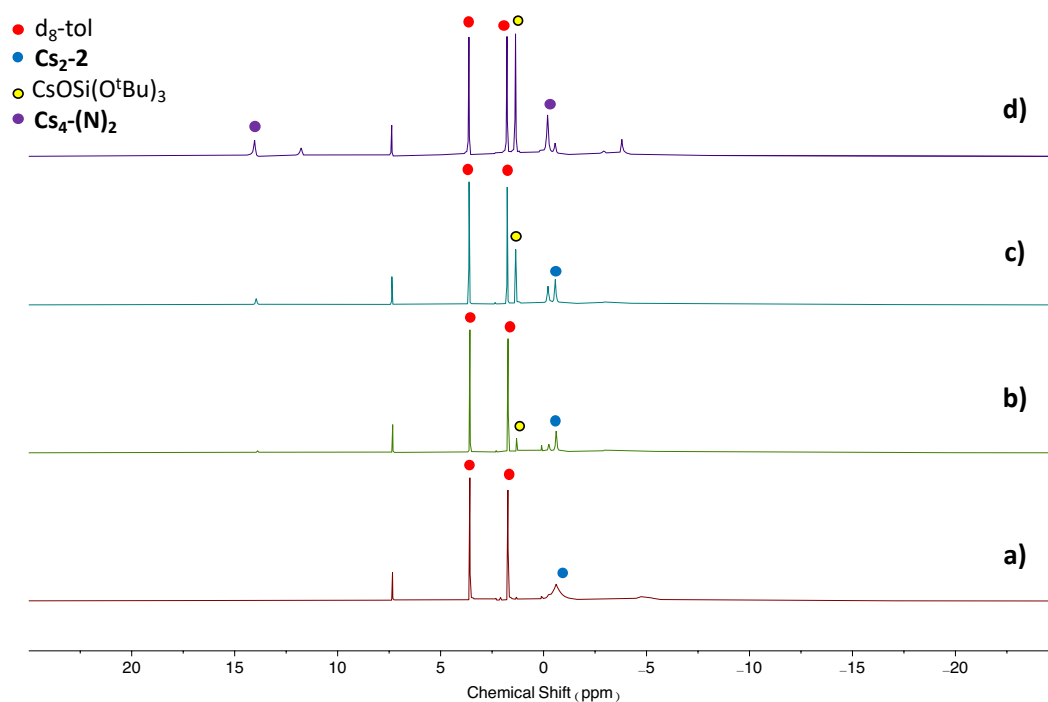


Figure S52: ^1H NMR spectrum (400 MHz, d_8 -THF, 233 K) evolution of the reaction mixture obtained by addition of 2 equiv. of CsC_8 to complex **Cs₂-2** in d_8 -THF at 233 K under a N_2 atmosphere a) before b) immediately after, c) 3 hs after c) 20 hs after.

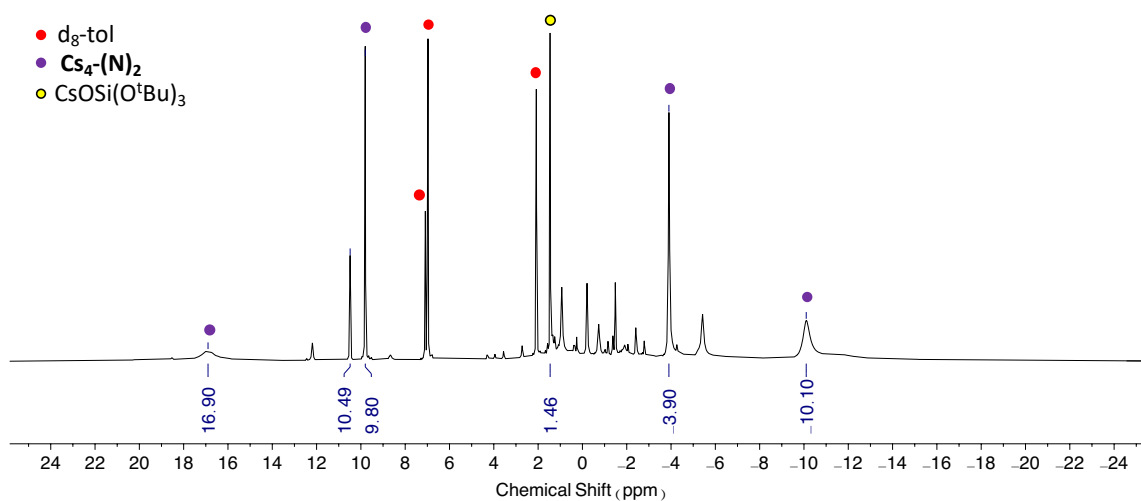


Figure S53: 1H NMR spectrum (400 MHz, d_8 -toluene, 298 K) of the reaction mixture obtained after addition of 2 equiv. of CsC_8 to complex Cs_2-2 in d_8 -THF after 20 hs at 233 K under a N_2 atmosphere.

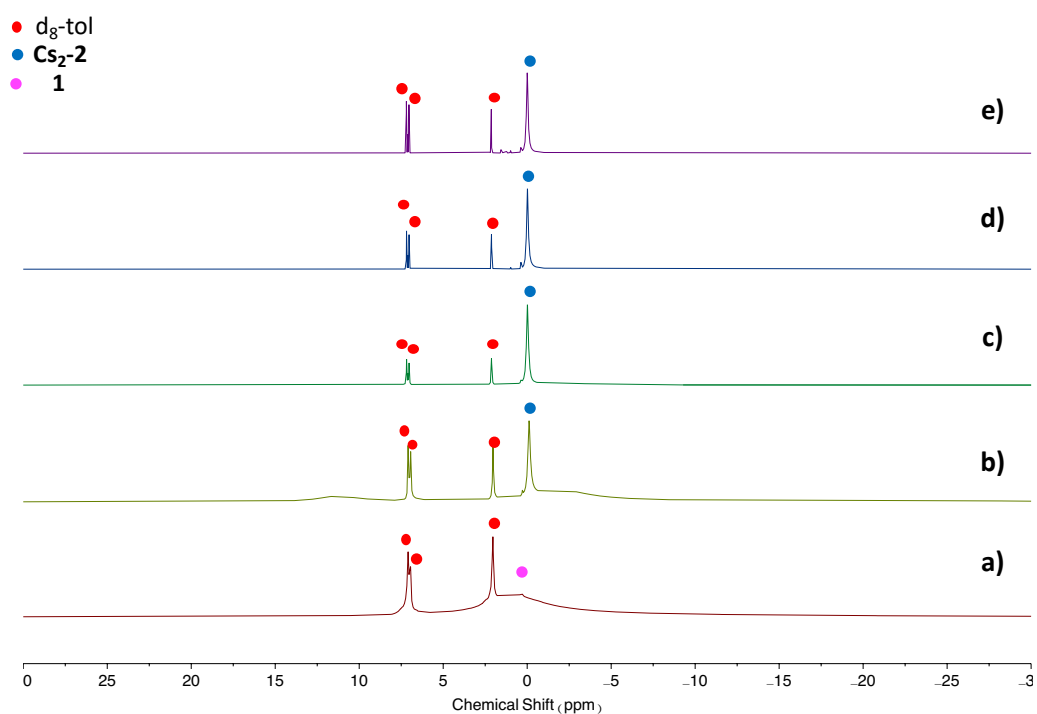


Figure S54: 1H NMR spectrum (400 MHz, d_8 -toluene, 233 K) evolution of the reaction mixture obtained by addition of 4 equiv. of CsC_8 to complex **1** at 233 K under an Ar atmosphere a) before b) immediately after, c) 1 h after c) 3 hs after d) 18 hs after, e) 48 hs after.

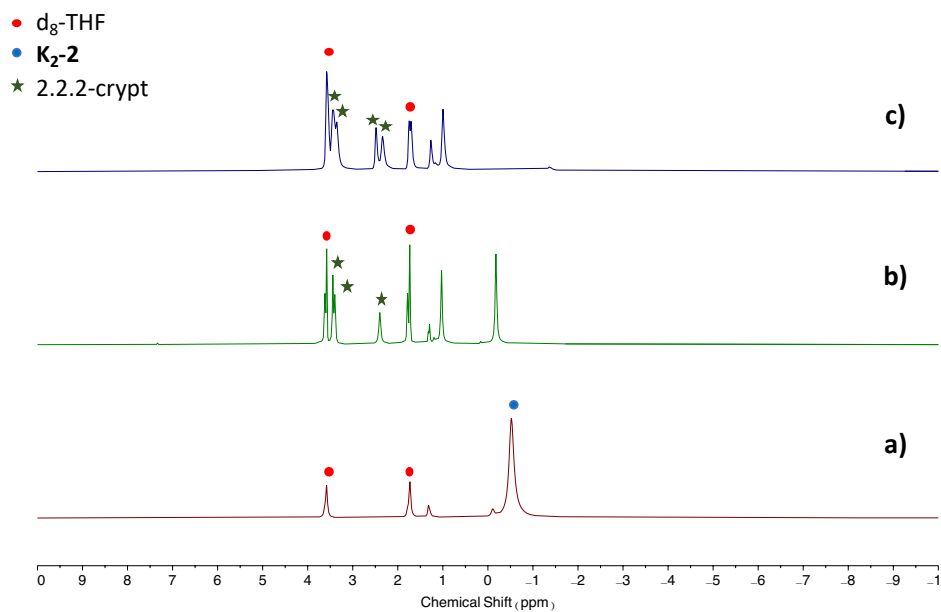


Figure S55: ^1H NMR spectrum (400 MHz, d_8 -THF, 233 K) evolution of the reaction mixture of complex K_2-2 a) before b) after addition of 1 equiv., c) after addition of 2 equiv. of 2.2.2-cryptand at 233 K under an Ar atmosphere.

X-ray crystallography

Suitable crystals were selected and mounted on various Rigaku diffractometers (XtaLAB Synergy R, DW system, HyPix-Arc 150 detector or SuperNova, Dual, Cu at home/near, AtlasS type detectors). The crystals were kept at a steady $T = 140.00(10)$ K during data collection. Data were measured using w scans with Cu K_α radiation. The diffraction patterns were indexed and the total number of runs and images were based on the strategy calculation from the program CrysAlisPro 1.171.41.118a.⁶ The unit cells were refined using CrysAlisPro 1.171.41.118a.⁶ Data reduction, scaling and absorption corrections were performed using CrysAlisPro 1.171.41.118a.⁶

The structures were solved with the **ShelXT**⁷ solution program using dual methods and by using **Olex2** 1.5⁸ as the graphical interface. The models were refined with **ShelXL** 2018/3⁹ using full matrix least squares minimisation on F^2 . All non-hydrogen atoms were refined anisotropically. Some hydrogen atom positions were calculated geometrically and refined using the riding model, but most hydrogen atoms were refined freely. Crystallographic and refinement data are summarized in tables S3-S5. The CCDC numbers 2154518-2154525 for all the compounds contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif

Table S1. Mean values of selected bond lengths (Å) and angles (°) in the complexes **1**, **M₂-2** and **M-3**. All distances are average

Complex	U–U	U1–(μ-O)	U2–(μ-O)	U1–(μ-O)–U2	M1–(μ-O)	M2–(μ-O)
1	4.2128(9)	2.1376(13)	2.0852(13)	172.19(8)	-	-
Rb-3	4.1905(13)	2.265(7)	1.947(18)	168.2(9)	3.730(16)	-
Na-3	3.6659(10)	2.205(17)	22.046(17)	119.1(8)		-
K₂-2	4.2619(10)	2.178(3)	2.120(3)	167(4)	2.913(4)	3.392(4)
Rb₂-2	4.1972(8)	2.135(5)	2.100(5)	164.7(3)	3.007(6)	3.696(6)
Cs₂-2	4.2467(10)	2.128(6)	2.119(6)	178.4(4)	3.352(8)	3.433(8)

Table S2. Mean values of selected bond lengths (Å) and angles (°) in the complexes **M₂-N₂**. All distances are average

Complex	U–U	U1–(μ-O)	U2–(μ-O)	U1–(μ-O)–U2	U–N	N–N
Rb₂-N₂	3.409(2)	2.16(2)	2.19(3)	104(1)	2.20(5)	1.41(1)
K₂-N₂	3.3801(5)	2.127(8)	2.14(1)	105.0(3)	2.279(8)	1.40(1)

In the case of **Rb₂-N₂**, each of the bridging hydrazido and oxo ligands are disordered over two positions found in a difference Fourier map and refined anisotropically

The solid-state molecular structure of **Cs₄-(N)₂** shows the presence of two independent dimers in the unit cell.

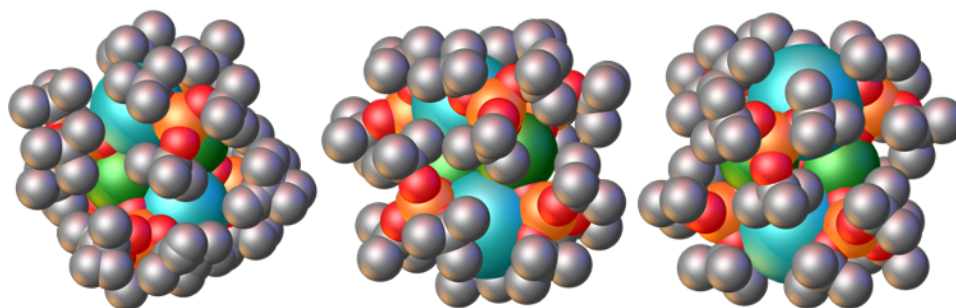


Figure S56: Space filling for the solid-state molecular structures of **K₂-2** (left), **Rb₂-2** (center) and **Cs₂-2** (right)

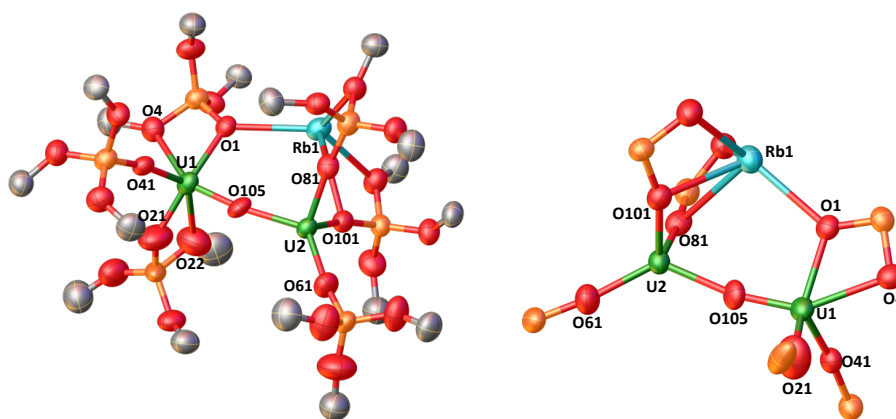


Figure S57: Solid-state molecular structure of $\text{Rb}[\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}]$ (50% probability ellipsoids). Color code: Uranium (green), rubidium (light blue), oxygen (red), carbon (grey), silicon (orange). Hydrogen atoms and $t\text{Bu}$ groups were omitted for clarity. Selected bond distances and angles: U1-O1-U2 : $119.1(8)^\circ$, U1-O1 : $2.205(17) \text{ \AA}$, U2-O1 : $2.046(17) \text{ \AA}$

The solid-state molecular structure of $\text{Rb}[\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}]$, **Rb-3** shows a dimeric U(III)/U(IV) complex with a bridging oxo ligand. U1 is hexa-coordinated in a pseudo octahedral environment, while U2 is tetra-coordinated in a distorted tetrahedral environment by the $\mu\text{-oxo}$ and completed by the oxygen atoms from the ancillary ligands. The two $\text{U}-(\mu\text{-O})$ distances are different ($\text{U1-O105} = 1.947(18) \text{ \AA}$ and $\text{U2-O105} = 2.265(7) \text{ \AA}$) one from the other, suggesting the presence of a localized charge in the uranium centers. The complex shows a slightly bent U-O-U motif with an angle ($168.2(9)^\circ$) comparable to those found in both **K₂-2** ($167.4(2)^\circ$) and **Rb₂-2** ($163.1(5)^\circ$). The Rb^+ cation is not bound to the bridging oxo ($\text{Rb1-O105} = 3.730(16) \text{ \AA}$) and it is penta-coordinated only by 5 oxygen atoms from the siloxide groups.

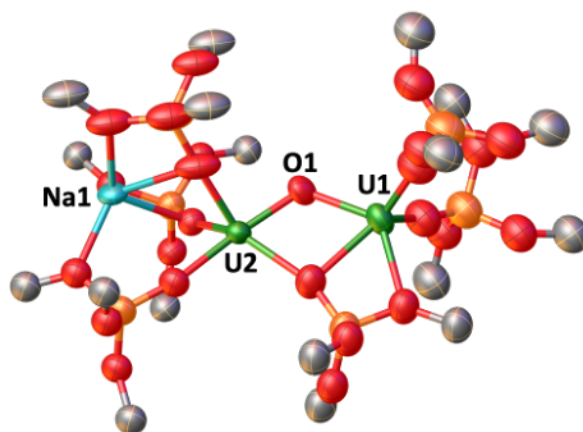


Figure S58: Solid-state molecular structure of **Na-3** (50% probability ellipsoids). Color code: uranium (green), sodium (light blue), oxygen (red), carbon (grey), silicon (orange). Hydrogen atoms and $t\text{Bu}$ groups were omitted for clarity. Selected bond distances and angles: U1-O1-U2 : $119.1(8)^\circ$, U1-O1 : $2.205(17) \text{ \AA}$, U2-O1 : $2.046(17) \text{ \AA}$

The solid-state molecular structure of $[\text{Na}\{\text{U}^{\text{III}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}(\mu\text{-O})\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu}))_3\}]$, complex **Na-3** shows a dimeric U(III)/U(IV) complex, the two U centers are bridged not only by an oxo group, but also by an oxygen atom from one of the siloxide ancillary ligands. U1 is hexa-coordinated in a pseudo octahedral environment, while U2 is penta-coordinated in a distorted square pyramidal environment ($\tau_5 = 0.238$) by the $\mu\text{-oxo}$ and completed by the oxygen atoms from the ancillary ligands. The two $\text{U}-(\mu\text{-O})$ distances are different ($\text{U1-O1A} = 2.065(7) \text{ \AA}$ and $\text{U2-O1A} = 2.214(8) \text{ \AA}$) one from the other, suggesting the presence of a localized charge in the uranium centers. The complex shows a highly bent U-O-U motif with an angle ($119.0(3)^\circ$) when comparable to those found in **K₂-2** ($167.4(2)^\circ$), **Rb₂-2** ($163.1(5)^\circ$) and its Rb analogue ($168.2(9)^\circ$).

Moreover, the complex shows that the two U centres, the oxo and siloxide-oxygen atoms are on a plane, while most of the other oxygen atoms are out of the plane

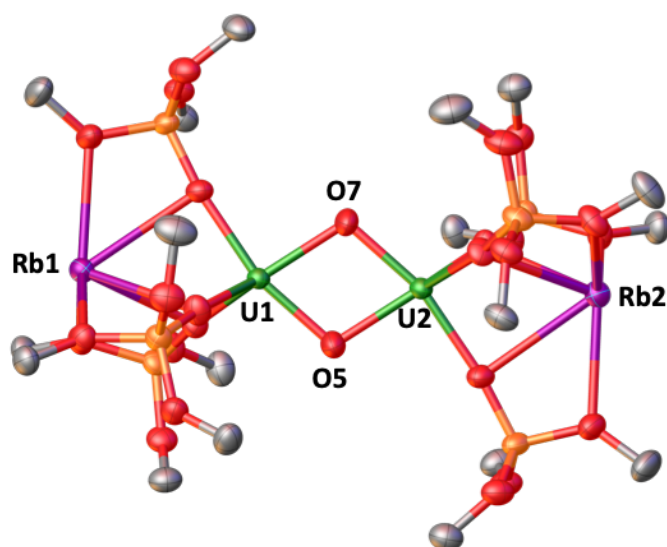


Figure S59: Solid-state molecular structure of $[\text{Rb}_2\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2\}(\mu\text{-O})_2]$ (50% probability ellipsoids). Color cod: uranium (green), rubidium (purple), oxygen (red), carbon (grey), silicon (orange). Hydrogen atoms and $t\text{Bu}$ groups were omitted for clarity.

The solid-state molecular structure of **Rb₂-4** shows a dimeric U(IV) complex in which each U center is pentacoordinated in a distorted square pyramidal environment by three oxygen atoms of the siloxide ancillary ligands and two bridging oxo. The Rb^+ cations are coordinated inside the pockets formed by the siloxide ligands. The two U(IV) centers are held in close proximity at a U-U distance of 3.41805(6) Å. The bridging oxo ligands are disordered over two positions each. The mean U-O-U angle is of 105.0(9) and compares well with the K analogue (106.16 (1) $^\circ$).³ Only two oxo atoms are shown for clarity. The methyl groups of the ligands are omitted for clarity.

The U-O distances of 2.11(2) Å and 2.200(9) are comparable to those reported in the analogous **K₂-4**³ (2.092(5) and 2.182(5) Å) U(IV) and other bis-oxo diuranium complexes¹⁰

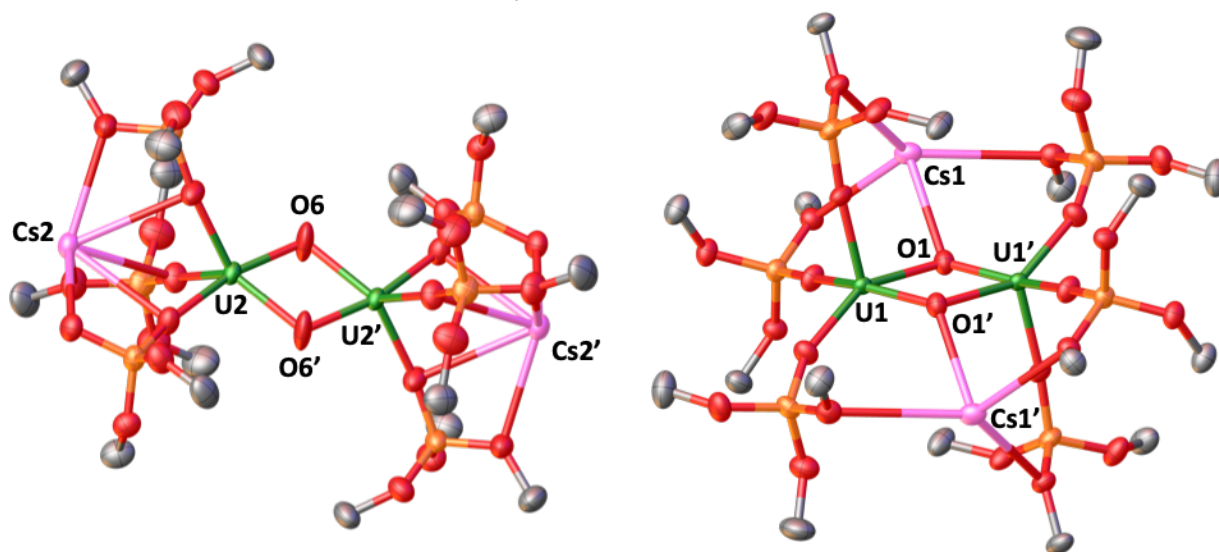


Figure S60: Solid-state molecular structure of $[\text{Cs}_2\{\text{U}^{\text{IV}}(\text{OSi}(\text{O}^t\text{Bu})_3)_2\}(\mu\text{-O})_2]$, **Cs₂-4** (50% probability ellipsoids) with the Cs^+ coordinated by the pockets formed by the siloxide ligands (left) or to the bridging oxo moieties (right) Color cod: uranium (green), cesium (pink), oxygen (red), carbon (grey), silicon (orange). Hydrogen atoms and $t\text{Bu}$ groups were omitted for clarity.

The solid-state molecular structure of **Cs₂-4** shows two dimeric U(IV) complexes in which each U center is pentacoordinated in a distorted square pyramidal environment by three oxygen atoms of the siloxide ancillary ligands and two bridging oxo. The Cs^+ cations are coordinated inside the pockets formed by the siloxide ligands in the isomer on the left of Figure S63, but coordinated to three oxygen atoms of the siloxide ancillary ligands and one of the bridging oxo. The two U(IV) centers are held in close proximity at a U-U distance of 3.48(3) Å. The bridging oxo ligands in the isomer on the left are disordered over two positions each, as was also observed for the analogue **K₂-4**. The mean U-O-U angle is of 108.0(4) $^\circ$ and compares well with the K analogue (106.16 (1) $^\circ$).³ Only two oxo atoms are shown for clarity.

The U-O distances of 2.09(3) Å and 2.212(8) are comparable to those reported in the analogous **K₂-4**³ (2.092(5) and 2.182(5) Å) U(IV) and other bis-oxo diuranium complexes¹⁰

Table S3. X-ray crystallographic data for **M₂-2** and **Rb₂-N₂**.

Compound	Cs₂-2	Rb₂-2 (Hexane)	Rb₂-N₂
Formula	C ₇₂ H ₁₆₂ Cs ₂ O ₂₅ Si ₆ U ₂	C ₇₈ H ₁₇₆ O ₂₅ Rb ₂ Si ₆ U ₂	C ₇₂ H ₁₆₂ N ₂ O ₂₅ Rb ₂ Si ₆ U ₂
Crystal size [mm ³]	0.12×0.07×0.03	0.52×0.44×0.06	0.198×0.110×0.044
Crystal system	Tetragonal	Monoclinic	Triclinic
Space group	I ₄ /a	P21/n	P1
V [Å ³]	42309.8(16)	11211.2(2)	5654.0(2)
a [Å]	25.3833(4)	14.04416(15)	14.0149(3)
b [Å]	25.3833(4)	29.0153(3)	17.5229(3)
c [Å]	65.6666(17)	27.5170(3)	24.7263(6)
α [°]	90	90	83.4471(18)
β [°]	90	91.0486(9)	83.4537(19)
γ [°]	90	90	70.099(2)
Z	16	4	2
Absorption coefficient [mm ⁻¹]	14.977	10.209	10.115
F (000)	18752.0	4744.0	2300
T [K]	140.1(5)	140.00(10)	140.00(10)
Total no. reflexions	113244	57578	143257
Unique reflexions [R(int)]	18706 [0.1469]	21687 [0.0449]	44789 [0.0832]
Final R indice [I>2σ(I)]	0.0556	0.0555	0.0608
Largest diff. peak and hole [eÅ ⁻³]	2.7267 and -2.6391	3.154 and -1.551	1.945 and -2.657
Goof	1.0072	1.092	1.048
CCDC number	2154524	2154518	2154522

Table S4. X-ray crystallographic data for **M-3** and **Cs₄-(N)₂**.

Compound	Rb-3	Na-3	Cs₄-(N)₂
Formula	C ₇₂ H ₁₆₂ O ₂₅ RbSi ₆ U ₂	C ₇₂ H ₁₆₂ NaO ₂₅ Si ₆ U ₂	C ₁₄₄ H ₃₂₄ Cs ₈ N ₄ O ₅₀ Si ₁₂ U ₄
Crystal size [mm ³]	0.126×0.076×0.057	0.23×0.09×0.06	0.60×0.08×0.06
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	P-1	P2 ₁	P-1
V [Å ³]	5114.5(7)	5333.4(2)	11885.2(4)
a [Å]	13.7997(11)	13.8302(3)	14.2492(3)
b [Å]	16.5080(11)	31.0949(4)	30.7972(6)
c [Å]	25.0252(18)	14.0653(4)	30.9557(5)
α [°]	71.888(6)	90	115.8481(18)
β [°]	81.133(6)	118.148(3)	95.2709(16)
γ [°]	71.005(6)	90	98.8528(18)
Z	2	2	2
Absorption coefficient [mm ⁻¹]	10.590	9.643	18.051
F (000)	2198	2146.0	5184.0
T [K]	140.1(5)	140.00(10)	219.99(10)
Total no. reflexions	22172	29907	105668
Unique reflexions [R(int)]	22172	29907	46105 [0.0838]
Final R indice [I>2σ(I)]	0.0858	0.0809	0.0645
Largest diff. peak and hole [eÅ ⁻³]	5.654 and -4.529	2.665 and -1.980	2.984 and -2.052
Goof	0.922	1.052	0.963
CCDC number	2154521	2154525	2154519

Table S5. X-ray crystallographic data for **M₂-4**.

Compound	Rb₂-4 (Toluene) ₂	Cs₂-4 (Toluene)
Formula	C ₈₆ H ₁₇₈ O ₂₆ Rb ₂ Si ₆ U ₂	C ₇₉ H ₁₇₀ Cs ₂ O ₂₆ Si ₆ U ₂
Crystal size [mm ³]	0.41×0.28×0.27	0.28×0.14×0.09
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
V [Å ³]	5863.85(18)	5492.7(3)
a [Å]	14.4840(2)	14.3992(5)
b [Å]	17.5730(3)	14.5329(5)
c [Å]	25.4883(4)	30.7352(7)
α [°]	79.6962(13)	88.132(2)
β [°]	89.4157(13)	79.130(2)
γ [°]	67.0260(16)	60.661(3)
Z	2	2
Absorption coefficient [mm ⁻¹]	9.795	3.724
F (000)	2488.0	2460.0
T [K]	140.0(1)	140.0(3)
Total no. reflexions	68433	53255
Unique reflexions [R(int)]	23858 [0.0269]	19362 [0.0317]
Final R indice [$I > 2\sigma(I)$]	0.0391	0.0542
Largest diff. peak and hole [eÅ ⁻³]	3.019 and -2.322	1.276 and -1.3235
Goof	1.060	1.190
CCDC number	2154523	2154520

SQUID magnetometry

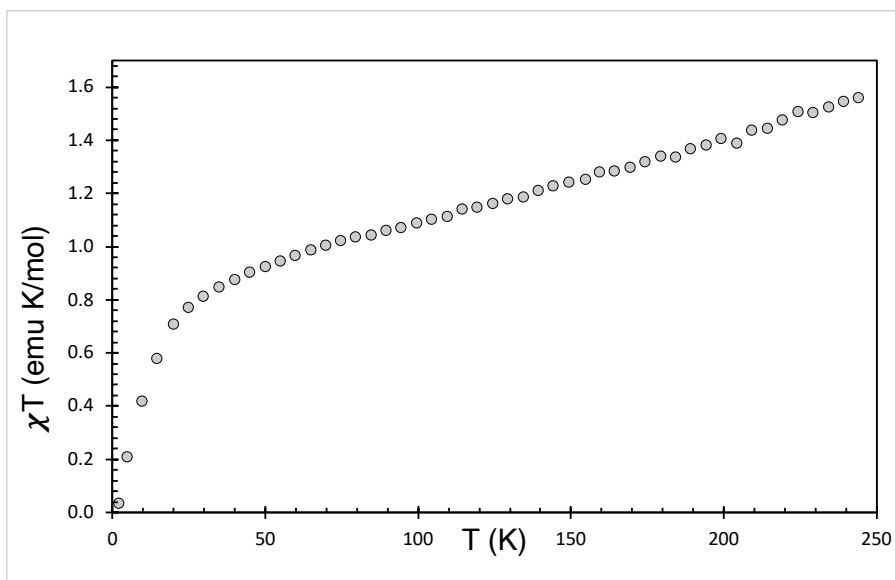


Figure S61: Plot of χT per complex versus temperature data for $\text{Cs}_2\text{-2}$ under an applied field of 1 T

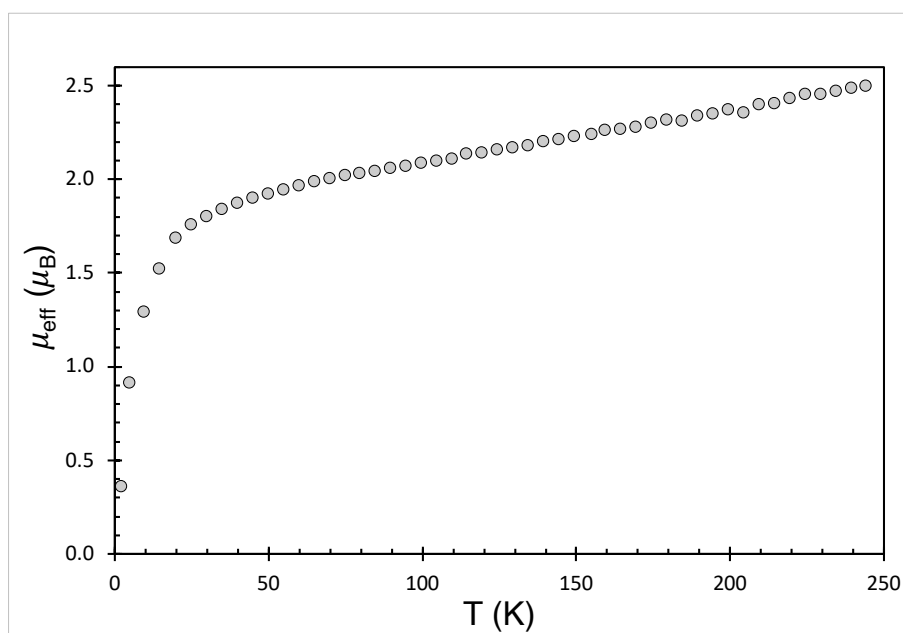


Figure S62: Plot of μ_{eff} per ion versus T data for $\text{Cs}_2\text{-2}$ under an applied field of 1 T

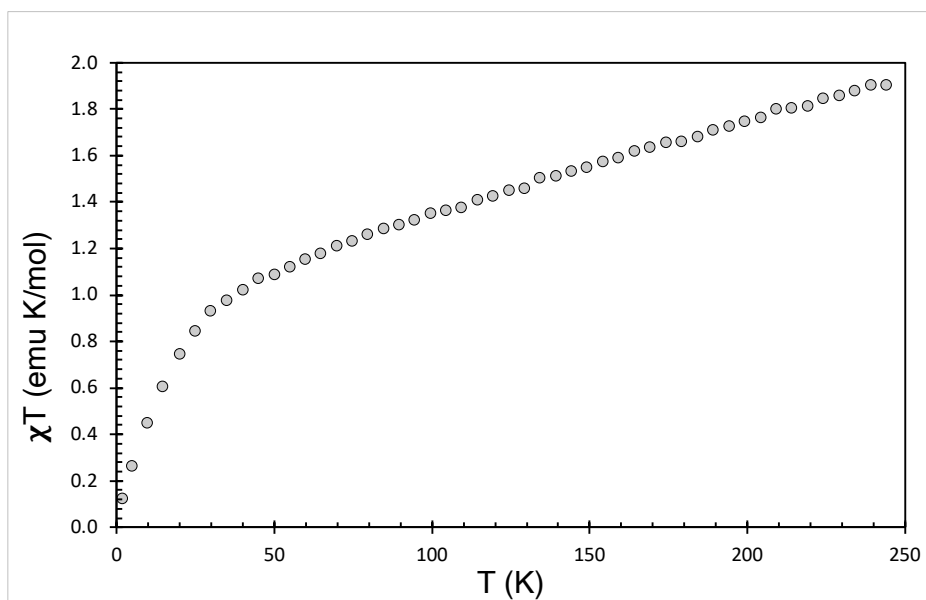


Figure S63: Plot of χT per complex versus temperature data for **Rb₂-2** under an applied field of 1 T

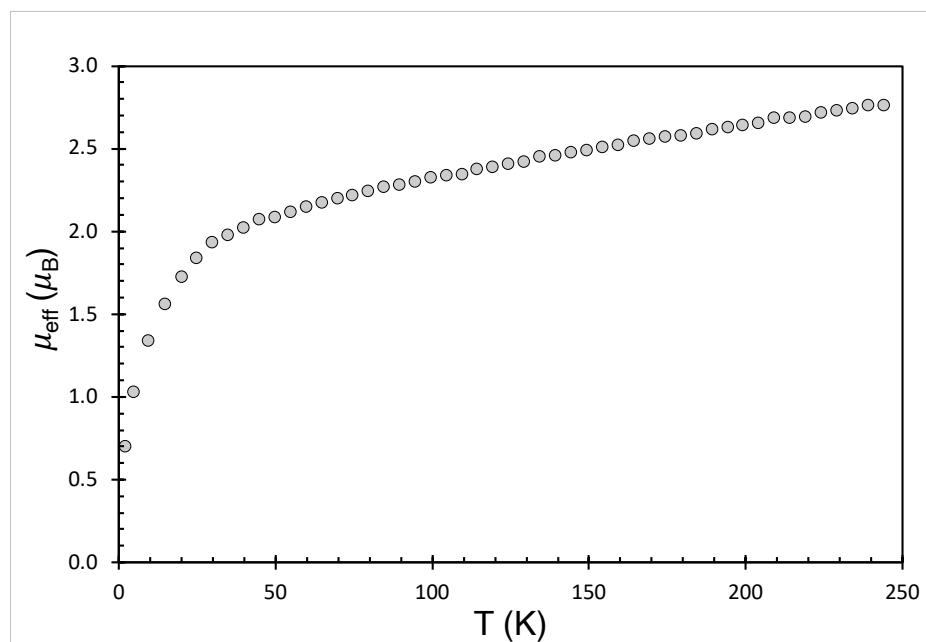


Figure S64: Plot of μ_{eff} per ion versus T data for **Rb₂-2** under an applied field of 1 T

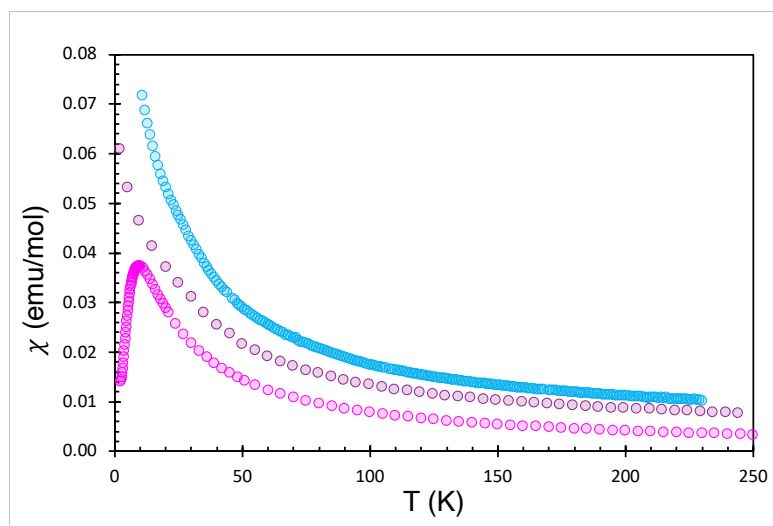


Figure S65: Plot of measured χ (per complex) versus temperature data for $\text{K}_2\text{-2}$ (light blue) (redrawn from ³), $\text{Rb}_2\text{-2}$ (purple) and $\text{Cs}_2\text{-2}$ (pink) under an applied field of 1 T

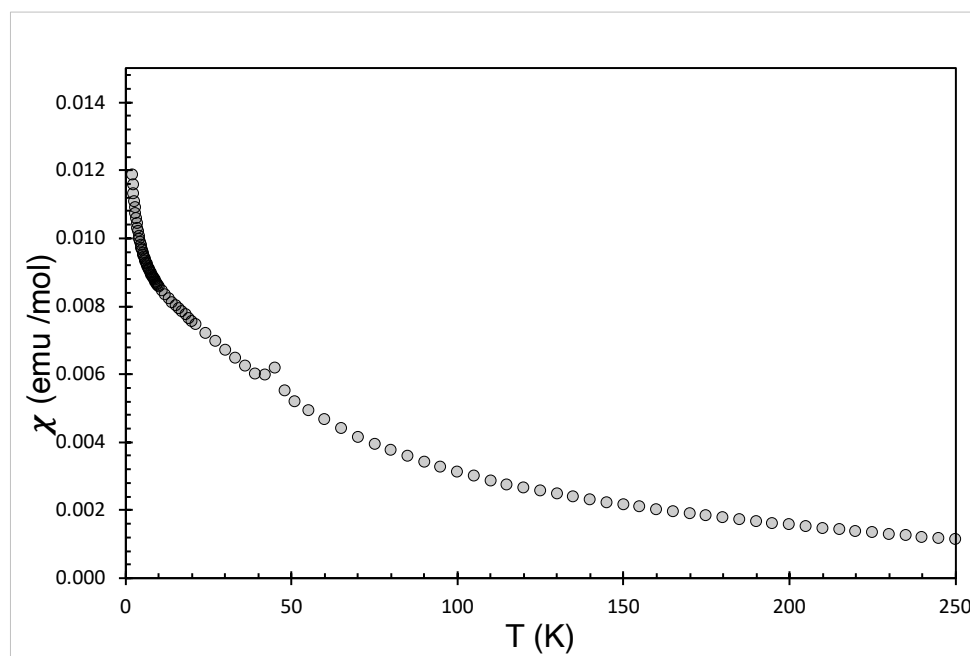


Figure S66: Plot of χ per complex versus temperature data for $\text{Cs}_4\text{-(N)}_2$ under an applied field of 1 T

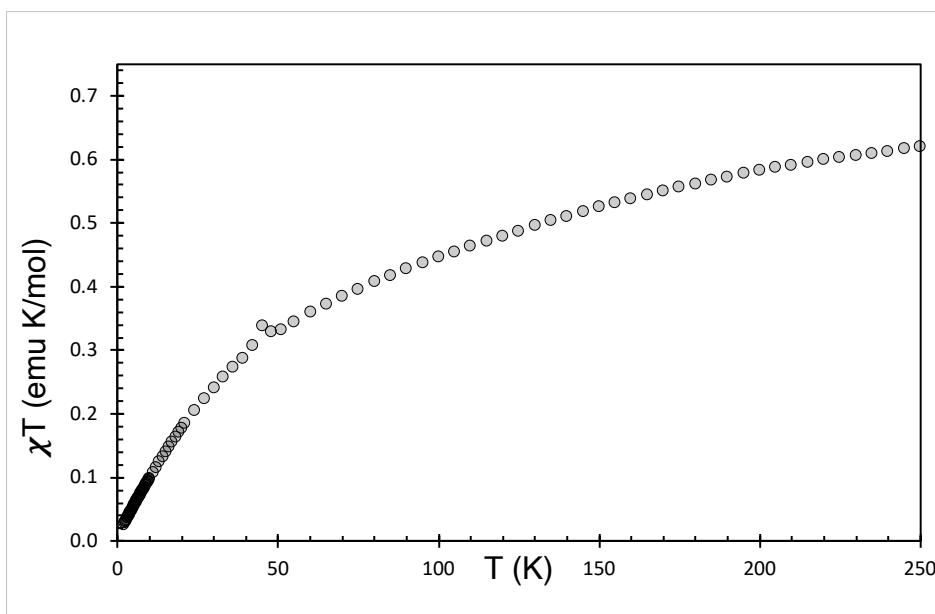


Figure S67: Plot of χT per complex versus temperature data for $\text{Cs}_4\text{-(N)}_2$ under an applied field of 1 T

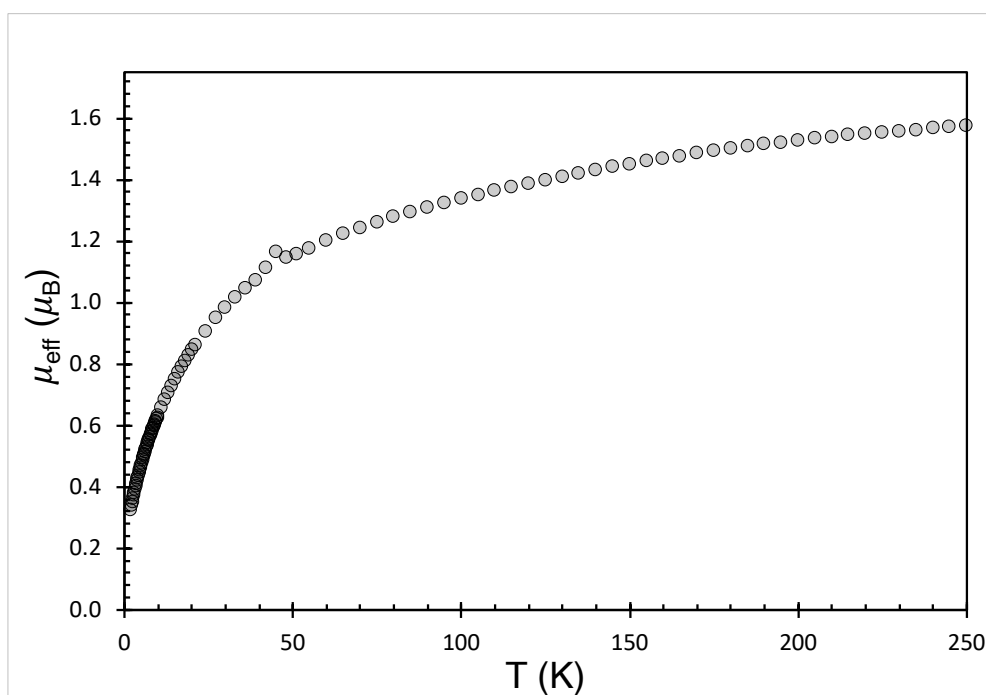


Figure S68: Plot of μ_{eff} per ion versus temperature data for $\text{Cs}_4\text{-(N)}_2$ under an applied field of 1 T

Electrochemistry

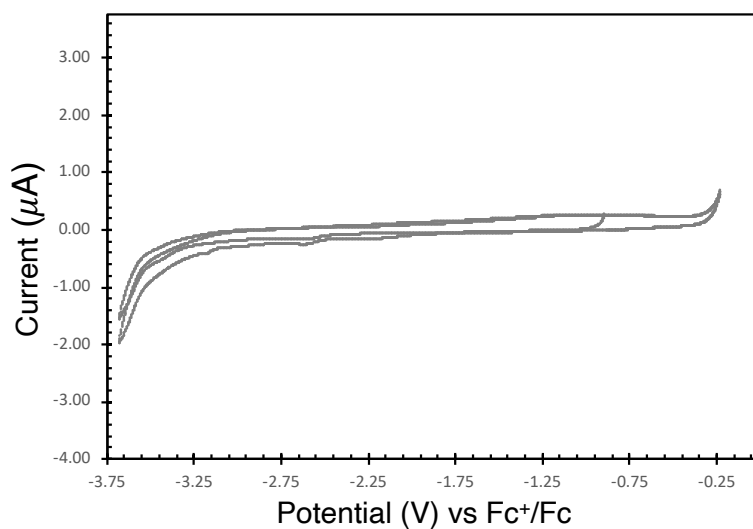


Figure S69: Cyclic voltammogram recorded in 0.1 M [NBu₄][BPh₄] in THF solution at 25°C in absence of compound (blank), at a scan rate of 100 mV/sec a, referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

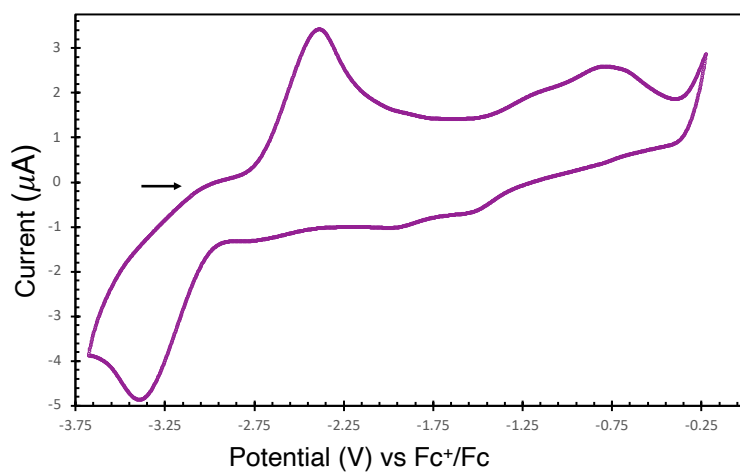


Figure S70: Cyclic voltammogram of complex **Rb₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec a, referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

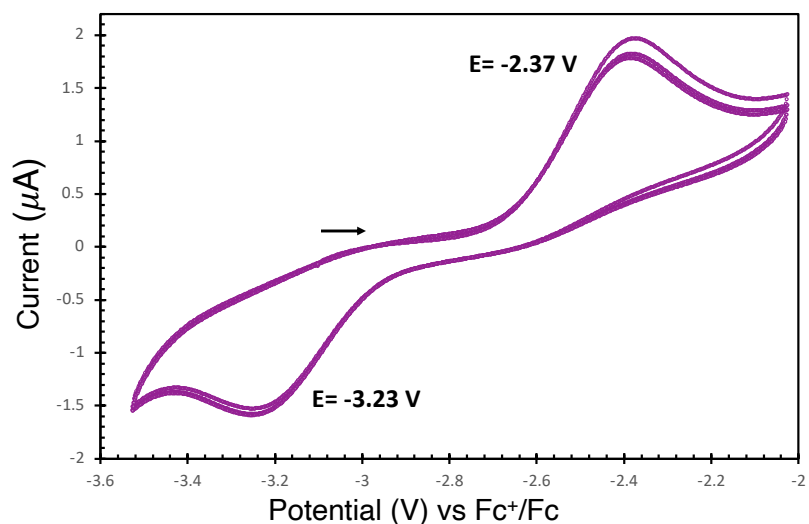


Figure S71: Reduction region of cyclic voltammogram of complex **Rb₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec a, referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

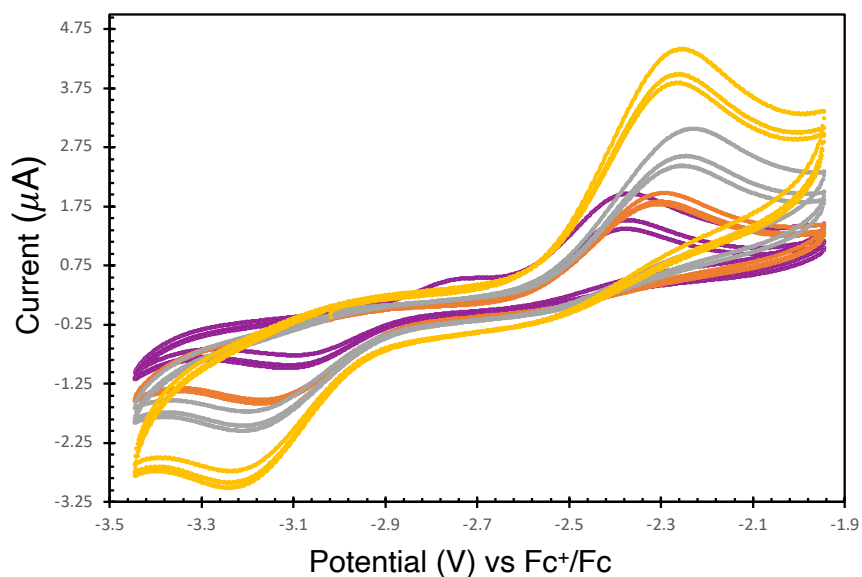


Figure S72: Reduction region of cyclic voltammogram of complex **Rb₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.0 mM THF solution at 25°C, at different scan rates (purple: 50 mV/sec, orange: 100 mV/sec, grey: 200 mV/sec, yellow: 500 mV/sec), referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

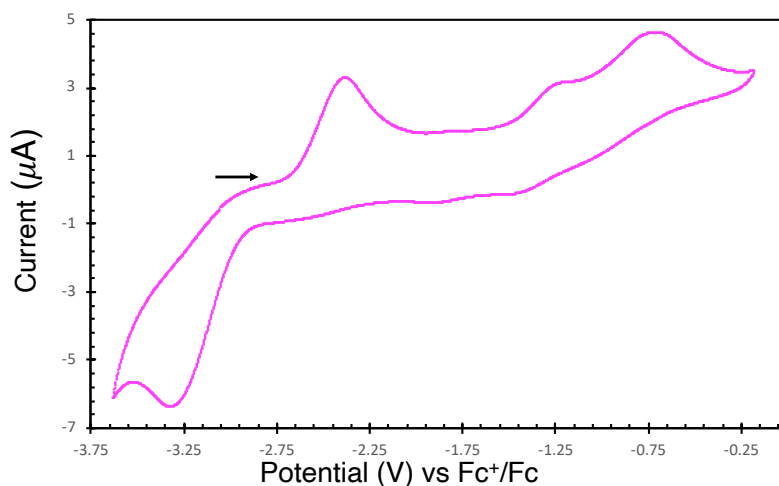


Figure S73: Cyclic voltammogram of complex **Cs₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.5 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

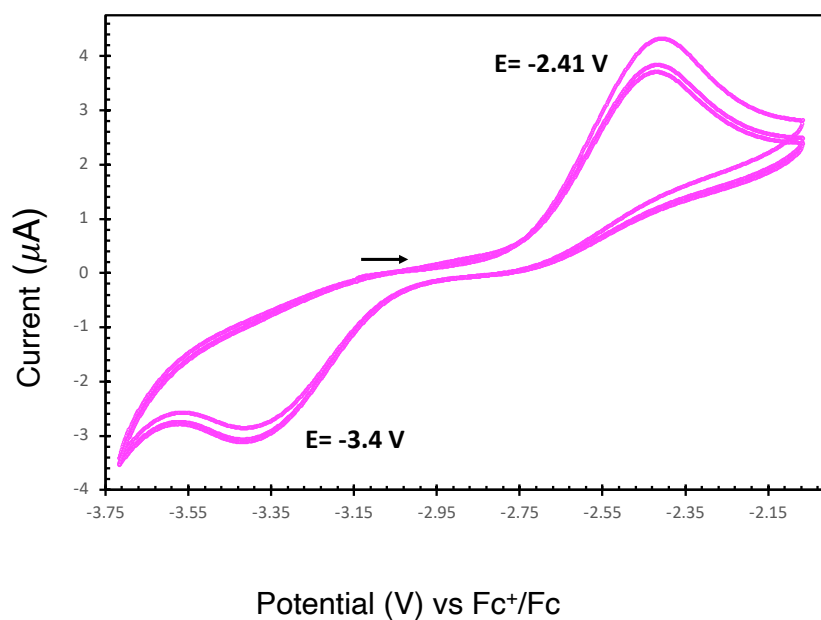


Figure S74: Reduction region of cyclic voltammogram of complex **Cs₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.5 mM THF solution at 25°C, at a scan rate of 100 mV/sec a, referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

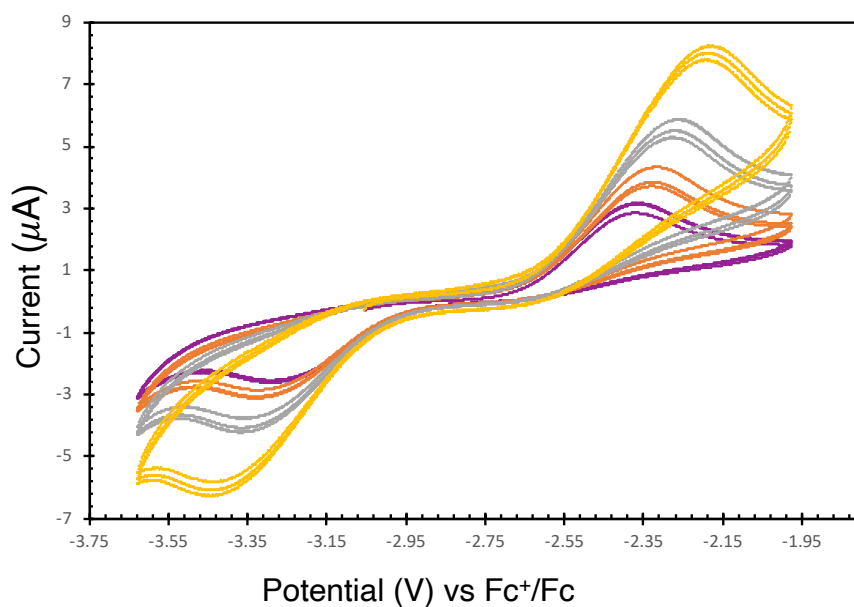


Figure S75: Reduction region of cyclic voltammogram of complex **Cs₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.5 mM THF solution at 25°C, at different scan rates (purple: 50 mV/sec, orange: 100 mV/sec, grey: 200 mV/sec, yellow: 500 mV/sec), referenced against [Fe(C₅H₅)₂]⁺/ [Fe(C₅H₅)₂]

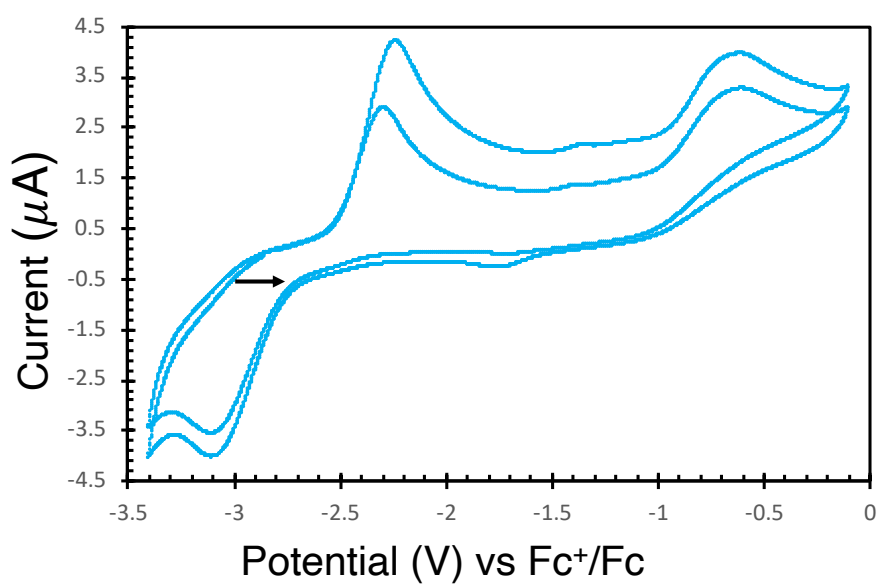


Figure S76: Cyclic voltammogram of complex **K₂-2** recorded in 0.1 M [NBu₄][BPh₄] in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against [Fe(C₅H₅)₂]^{+/0}

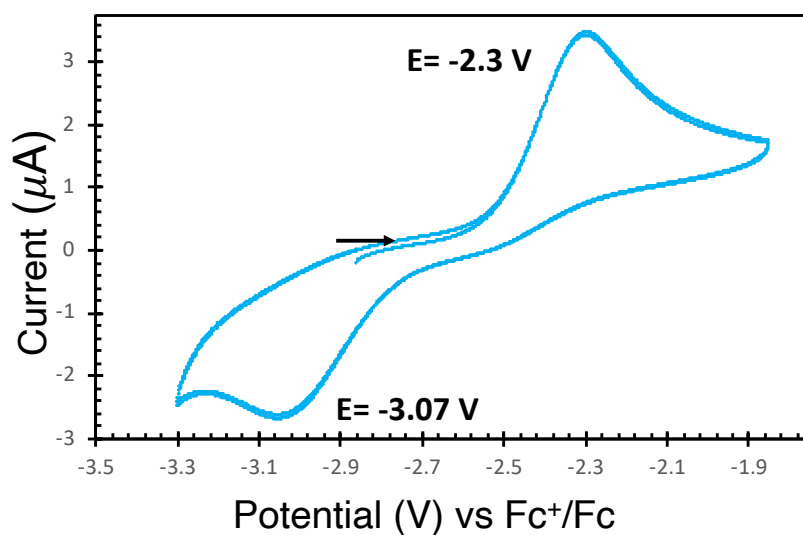


Figure S77: Reduction region of cyclic voltammogram of complex $\text{K}_2\text{-2}$ recorded in 0.1 M $[\text{NBu}_4][\text{BPh}_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[\text{Fe}(\text{C}_5\text{H}_5)_2]^{+/0}$

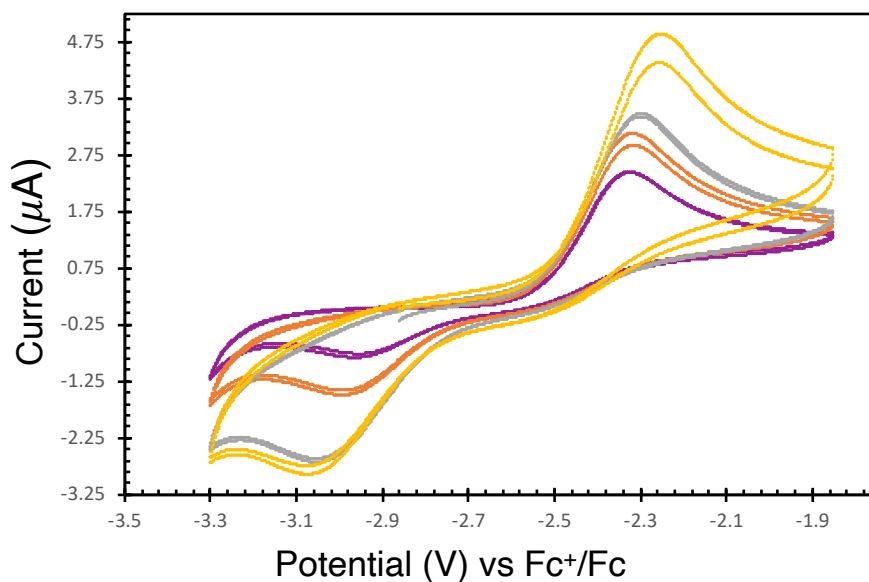


Figure S78: Reduction region of cyclic voltammogram of complex $\text{K}_2\text{-2}$ recorded in 0.1 M $[\text{NBu}_4][\text{BPh}_4]$ in 3.0 mM THF solution at 25°C, at different scan rates (purple: 50 mV/sec, orange: 75 mV/sec, grey: 100 mV/sec, yellow: 200 mV/sec), referenced against $[\text{Fe}(\text{C}_5\text{H}_5)_2]^{+/0}$

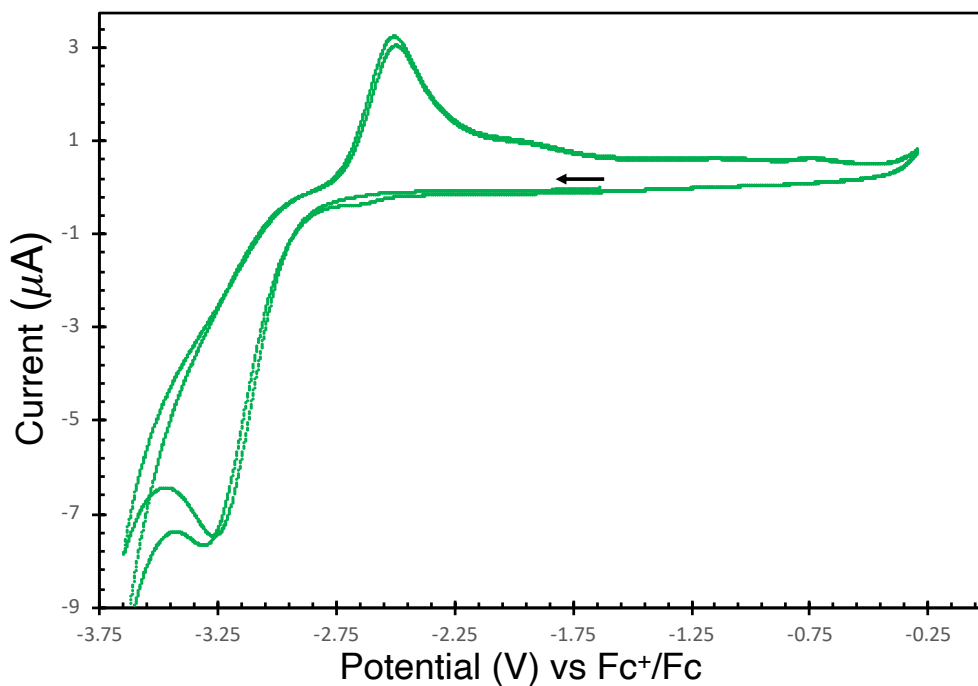


Figure S79: Cyclic voltammogram of complex **1** recorded in 0.1 M $[\text{NBu}_4][\text{BPh}_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[\text{Fe}(\text{C}_5\text{H}_5)_2]^{+/0}$

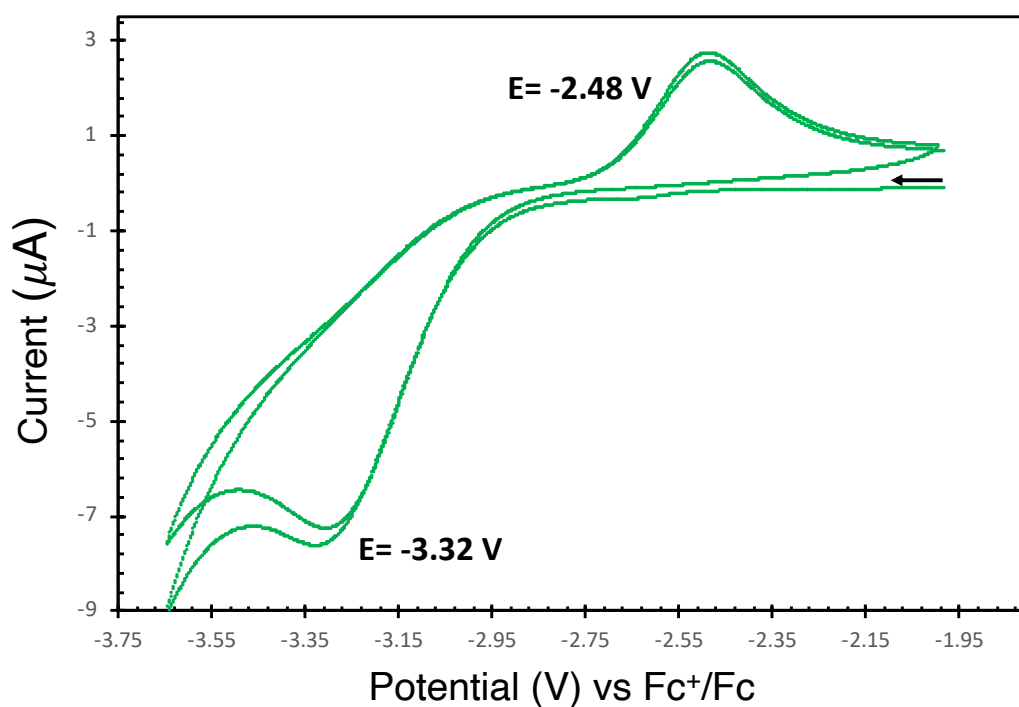


Figure S80: Reduction region of cyclic voltammogram of complex **1** recorded in 0.1 M $[\text{NBu}_4][\text{BPh}_4]$ in 3.0 mM THF solution at 25°C, at a scan rate of 100 mV/sec, referenced against $[\text{Fe}(\text{C}_5\text{H}_5)_2]^{+/0}$

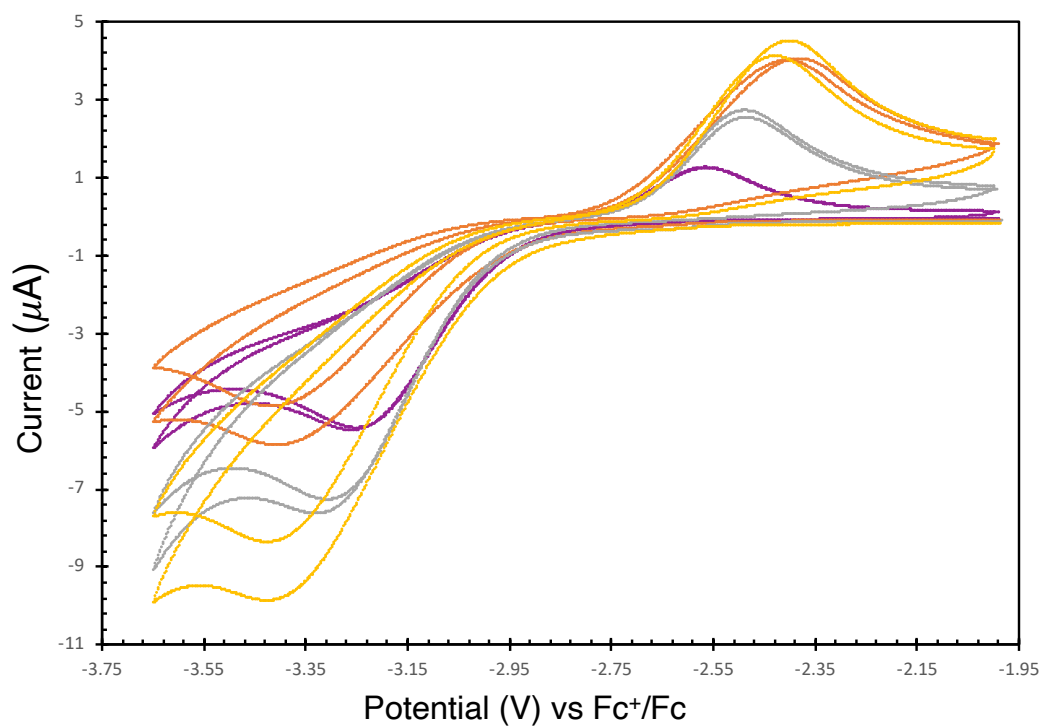


Figure S81: Reduction region of cyclic voltammogram of complex **1** recorded in 0.1 M [NBu₄][BPh₄] in 3.0 mM THF solution at 25°C, at different scan rates (purple: 50 mV/sec, orange: 75 mV/sec, grey: 100 mV/sec; yellow: 200 mV/sec), referenced against [Fe(C₅H₅)₂]⁺⁰

EPR data

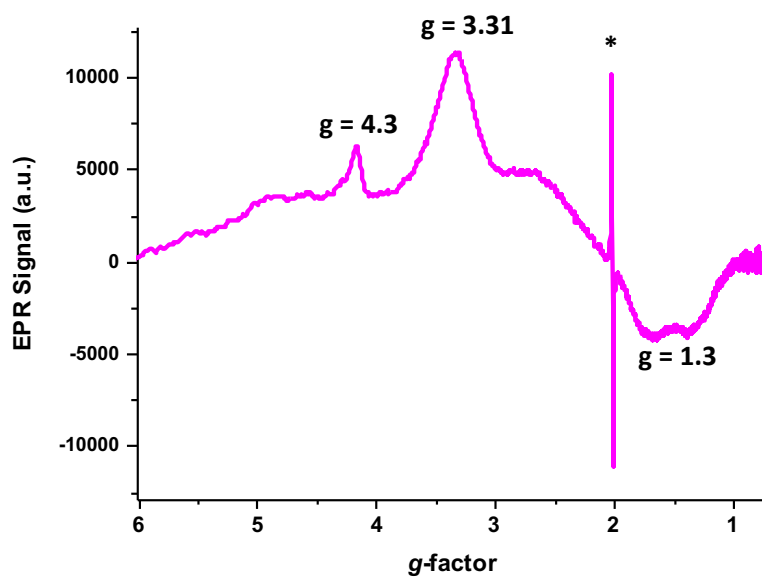


Figure S82: X-band EPR spectrum of frozen 20 mM solution of complex $\text{Rb}_2\text{-N}_2$ in toluene:hexane (1:1) glass at 6 K. * indicates a radical impurity present in the solution. ($\nu = 9.397588$ GHz, $P = 0.6332$ mW, amplitude modulation 5 G, frequency modulation 100 kHz).

Computational Details

The optimization of three different spin states for uranium complexes were carried out by employing DFT hybrid functional (B3PW91)¹¹ along with small core pseudopotential Stuttgart basis set for uranium, rubidium, cesium and silicon atoms with additional polarization functions for rubidium, cesium and silicon atoms.¹² Pople basis sets (6-31G**) were employed for the rest of the atoms.¹³ Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.¹⁴ The density was analyzed using the NBO technic with three different versions of the program NBO3.1, NBO5.0 and NBO6.0

Bonding orbitals from NBO analysis for ground state spin (s=3) for K₂-2

(0.92139) BD (1) U 1 - O 32(Alpha)
(6.17%) 0.2484* U1 s(0.27%)p16.98(4.51%)d99.99(68.53%)f99.99(26.68%)g 0.07(0.02%)
(93.83%) 0.9687* O32 s(1.84%)p53.35(98.16%)d 0.00(0.00%)
(0.91548) BD (2) U 1 - O 32(Alpha)
(5.77%) 0.2401* U1 s(0.10%)p47.58(4.99%)d99.99(73.49%)f99.99(21.39%)g 0.24(0.02%)
(94.23%) 0.9707* O32 s(0.09%)p99.99(99.90%)d 0.02(0.00%)
(0.95011) BD (1) U 2 - O 32(Beta)
(6.90%) 0.2627* U2 s(0.03%)p99.99(3.43%)d99.99(60.23%)f99.99(36.29%)g 1.39(0.03%)
(93.10%) 0.9649* O32 s(1.47%)p67.20(98.53%)d 0.00(0.00%)
(0.94798) BD (2) U 2 - O 32(Beta)
(6.92%) 0.2630* U2 s(0.06%)p46.17(2.89%)d99.99(59.97%)f99.99(37.04%)g 0.59(0.04%)
(93.08%) 0.9648* O32 s(2.41%)p40.51(97.59%)d 0.00(0.00%)

Bonding orbitals from NBO analysis for ground state spin (s=1) for K₂-N₂

(0.97361) BD (1) U 1 - O 12(Alpha)
(11.06%) 0.3326* U1 s(7.90%)p 0.90(7.13%)d 4.82(38.07%) f 5.94(46.88%)g 0.00(0.03%)
(88.94%) 0.9431* O12 s(43.23%)p 1.31(56.74%)d 0.00(0.02%)
(0.90969) BD (2) U 1 - O 12(Alpha)
(10.18%) 0.3191* U1 s(1.16%)p 3.96(4.59%)d30.35(35.19%)f50.89(59.00%)g 0.06(0.07%)
(89.82%) 0.9477* O12 s(1.38%)p71.37(98.57%)d 0.03(0.05%)
(0.90149) BD (3) U 1 - O 12(Alpha)
(11.50%) 0.3391* U1 s(0.17%)p21.03(3.53%)d99.99(43.18%)f99.99(53.09%)g 0.17(0.03%)
(88.50%) 0.9408* O 12 s(0.24%)p99.99(99.71%)d 0.19(0.05%)
(0.92760) BD (1) U 1 - N 13(Alpha)
(18.90%) 0.4347* U1 s(11.16%)p 1.02(11.33%)d 3.26(36.36%) f 3.69(41.12%)g 0.00(0.03%)
(81.10%) 0.9006* N13 s(46.97%)p 1.13(52.98%)d 0.00(0.05%)
(0.88634) BD (2) U 1 - N 13(Alpha)
(14.29%) 0.3780* U 1 s(0.47%)p11.62(5.50%)d36.33(17.20%)f99.99(76.81%)g 0.04(0.02%)
(85.71%) 0.9258* N 13 s(19.43%)p 4.14(80.49%)d 0.00(0.08%)
(0.87270) BD (1) U 1 - N 14(Alpha)
(17.32%) 0.4161* U 1 s(12.81%)p 0.74(9.42%)d 3.75(47.97%) f 2.32(29.77%)g 0.00(0.02%)
(82.68%) 0.9093* N 14 s(37.95%)p 1.63(62.00%)d 0.00(0.06%)
(0.96321) BD (1) U 2 - O 12(Alpha)
(11.85%) 0.3442* U 2 s(7.44%)p 0.77(5.71%)d 5.20(38.64%) f 6.48(48.18%)g 0.00(0.03%)
(88.15%) 0.9389* O 12 s(55.10%)p 0.81(44.88%)d 0.00(0.02%)
(0.93524) BD (1) U 2 - N 14(Alpha)
(20.92%) 0.4574* U 2 s(6.32%)p 1.30(8.23%)d 5.52(34.92%) f 7.98(50.49%)g 0.00(0.03%)
(79.08%) 0.8893* N 14 s(34.44%)p 1.90(65.50%)d 0.00(0.06%)
(0.86486) BD (2) U 2 - N 14(Alpha)
(19.67%) 0.4435* U 2 s(2.76%)p 2.68(7.42%)d 3.72(10.28%) f28.77(79.53%)g 0.01(0.02%)
(80.33%) 0.8963* N 14 s(6.07%)p15.45(93.83%)d 0.02(0.09%)
(0.97739) BD (1) U 1 - O 12(Beta)
(10.07%) 0.3173* U 1 s(7.48%)p 0.99(7.37%)d 5.37(40.16%)f 6.01(44.96%)g 0.00(0.03%)
(89.93%) 0.9483* O 12 s(42.02%)p 1.38(57.96%)d 0.00(0.02%)
(0.91478) BD (2) U 1 - O 12(Beta)
(8.94%) 0.2990* U 1 s(1.74%)p 2.98(5.19%)d21.31(37.12%)f32.06(55.85%)g 0.05(0.09%)
(91.06%) 0.9542* O 12 s(2.23%)p43.85(97.72%)d 0.02(0.05%)
(0.91341) BD (3) U 1 - O 12(Beta)
(9.57%) 0.3093* U 1 s(0.31%)p14.31(4.51%)d99.99(42.44%)f99.99(52.71%)g 0.12(0.04%)
(90.43%) 0.9510* O 12 s(0.37%)p99.99(99.59%)d 0.12(0.04%)
(0.95297) BD (1) U 1 - N 13(Beta)
(13.55%) 0.3681* U 1 s(10.28%)p 1.20(12.36%)d 3.79(38.93%)f 3.74(38.40%)g 0.00(0.03%)

(86.45%) 0.9298* N 13 s(53.14%)p 0.88(46.81%)d 0.00(0.04%)
 (0.90140) BD (2) U 1 - N 13(Beta)
 (11.87%) 0.3445* U 1 s(0.07%)p53.58(3.73%)d99.99(17.17%)f99.99(79.00%)g 0.46(0.03%)
 (88.13%) 0.9388* N 13 s(6.12%)p15.32(93.79%)d 0.01(0.09%)
 (0.91146) BD (1) U 1 - N 14(Beta)
 (13.40%) 0.3660* U 1 s(12.98%)p 0.85(11.01%)d 3.46(44.96%)f 2.39(31.03%)g 0.00(0.02%)
 (86.60%) 0.9306* N 14 s(44.70%)p 1.24(55.25%)d 0.00(0.05%)
 (0.96561) BD (1) U 2 - O 12(Beta)
 (10.62%) 0.3259* U 2 s(7.50%)p 0.82(6.14%)d 5.45(40.88%)f 6.06(45.44%)g 0.00(0.03%)
 (89.38%) 0.9454* O 12 s(55.35%)p 0.81(44.63%)d 0.00(0.02%)
 (0.95352) BD (1) U 2 - N 14(Beta)
 (14.76%) 0.3842* U 2 s(6.45%)p 1.40(9.00%)d 6.01(38.72%)f 7.11(45.81%)g 0.00(0.03%)
 (85.24%) 0.9232* N 14 s(36.22%)p 1.76(63.72%)d 0.00(0.06%)
 (0.88712) BD (2) U 2 - N 14(Beta)
 (15.09%) 0.3885* U 2 s(0.58%)p 9.01(5.21%)d25.23(14.59%)f99.99(79.58%)g 0.06(0.03%)
 (84.91%) 0.9215* N 14 s(0.13%)p99.99(99.78%)d 0.70(0.09%)

Bonding orbitals from NBO analysis for ground state spin (s=1) for K₄-(N)₂

BD (1) U 1 - O 17(Alpha)
 (18.12%) 0.4257* U 1 s(0.01%)p99.99(1.59%)d99.99(48.96%) f99.99(49.35%)g 8.00(0.09%)
 (81.88%) 0.9049* O 17 s(0.08%)p99.99(99.85%)d 0.79(0.07%)
 BD (2) U 1 - O 17(Alpha)
 (17.91%) 0.4232* U 1 s(0.01%)p 1.00(0.99%)d52.69(51.92%) f47.66(46.97%)g 0.12(0.12%)
 (82.09%) 0.9060* O 17 s(2.65%)p36.71(97.29%)d 0.02(0.06%)
 BD (3) U 1 - O 17(Alpha)
 (20.03%) 0.4476* U 1 s(2.47%)p 0.43(1.07%)d17.24(42.65%) f21.66(53.58%)g 0.09(0.22%)
 (79.97%) 0.8943* O 17 s(30.41%)p 2.29(69.55%)d 0.00(0.04%)
 BD (1) U 1 - N 38(Alpha)
 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%)
 (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)
 BD (1) U 1 - N 39(Alpha)
 (29.84%) 0.5462* U 1 s(2.64%)p 0.62(1.62%)d19.31(50.95%) f16.94(44.70%)g 0.04(0.09%)
 (70.16%) 0.8376* N 39 s(39.60%)p 1.52(60.23%)d 0.00(0.16%)
 BD (2) U 1 - N 39(Alpha)
 (27.75%) 0.5268* U 1 s(0.03%)p99.99(3.92%)d99.99(46.32%) f99.99(49.66%)g 2.88(0.07%)
 (72.25%) 0.8500* N 39 s(0.09%)p99.99(99.78%)d 1.55(0.14%)
 BD (3) U 1 - N 39(Alpha)
 (28.97%) 0.5383* U 1 s(0.01%)p99.99(1.28%)d99.99(47.79%) f99.99(50.89%)g 3.47(0.04%)
 (71.03%) 0.8428* N 39 s(0.06%)p99.99(99.81%)d 2.35(0.13%)
 BD (1) U 2 - N 38(Alpha)
 (18.30%) 0.4277* U 2 s(9.05%)p 0.18(1.61%)d 4.38(39.69%) f 5.48(49.61%)g 0.00(0.03%)
 (81.70%) 0.9039* N 38 s(43.26%)p 1.31(56.73%)d 0.00(0.01%)
 BD (1) U 2 - N 39(Alpha)
 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%)
 (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)
 BD (1) U 1 - O 17(Beta)
 (18.16%) 0.4262* U 1 s(0.01%)p 1.00(1.59%)d30.77(49.00%)f30.96(49.30%)g 0.06(0.09%)
 (81.84%) 0.9046* O 17 s(0.03%)p99.99(99.90%)d 2.00(0.07%)
 BD (2) U 1 - O 17(Beta)
 (17.82%) 0.4221* U 1 s(0.02%)p59.27(0.93%)d99.99(51.79%)f99.99(47.14%)g 7.50(0.12%)
 (82.18%) 0.9066* O 17 s(2.97%)p32.65(96.97%)d 0.02(0.06%)
 BD (3) U 1 - O 17(Beta)
 (19.96%) 0.4468* U 1 s(2.50%)p 0.41(1.02%)d17.42(43.46%)f21.16(52.80%)g 0.09(0.22%)
 (80.04%) 0.8946* O 17 s(30.27%)p 2.30(69.69%)d 0.00(0.04%)
 BD (1) U 1 - N 38(Beta)
 (18.50%) 0.4301* U 1 s(10.58%)p 0.69(7.28%)d 4.93(52.11%)f 2.83(29.99%)g 0.00(0.04%)
 (81.50%) 0.9028* N 38 s(44.33%)p 1.26(55.66%)d 0.00(0.01%)
 BD (1) U 1 - N 39(Beta)
 (29.77%) 0.5457* U 1 s(2.25%)p 0.71(1.60%)d22.51(50.76%)f20.09(45.29%)g 0.04(0.09%)
 (70.23%) 0.8380* N 39 s(36.58%)p 1.73(63.26%)d 0.00(0.16%)
 BD (2) U 1 - N 39(Beta)
 (28.19%) 0.5309* U 1 s(0.03%)p76.69(2.43%)d99.99(47.62%)f99.99(49.85%)g 2.09(0.07%)
 (71.81%) 0.8474* N 39 s(0.16%)p99.99(99.71%)d 0.86(0.14%)
 BD (3) U 1 - N 39(Beta)

(28.55%) 0.5343* U 1 s(0.01%)p99.99(2.30%)d99.99(46.20%)f99.99(51.42%)g 3.98(0.06%)
 (71.45%) 0.8453* N 39 s(0.26%)p99.99(99.60%)d 0.53(0.14%)
 BD (1) U 2 - N 38(Beta)
 (15.43%) 0.3928* U 2 s(9.82%)p 0.20(1.99%)d 4.55(44.73%)f 4.42(43.42%)g 0.00(0.04%)
 (84.57%) 0.9196* N 38 s(47.87%)p 1.09(52.12%)d 0.00(0.01%)
 BD (1) U 2 - N 39(Beta)
 (11.39%) 0.3374* U 2 s(12.53%)p 0.58(7.32%)d 3.99(50.04%)f 2.40(30.10%)g 0.00(0.01%)
 (88.61%) 0.9414* N 39 s(63.07%)p 0.58(36.89%)d 0.00(0.03%)

Bonding orbitals from NBO analysis for ground state spin (s=3) for Rb₂-2

BD (1) U 1 - O 35(Alpha)
 (9.78%) 0.3128* U 1 s(0.69%)p 3.00(2.07%)d65.60(45.37%) f74.96(51.85%)g 0.02(0.02%)
 (90.22%) 0.9498* O 35 s(0.17%)p99.99(99.83%)d 0.00(0.00%)
 BD (2) U 1 - O 35(Alpha)
 (9.77%) 0.3126* U 1 s(0.62%)p 4.42(2.73%)d66.60(41.16%) f89.78(55.48%)g 0.03(0.02%)
 (90.23%) 0.9499* O 35 s(0.62%)p99.99(99.38%)d 0.00(0.00%)
 BD (1) U 2 - O 35(Beta)
 (6.23%) 0.2496* U 2 s(0.01%)p 1.00(3.19%)d18.85(60.15%)f11.47(36.62%)g 0.01(0.04%)
 (93.77%) 0.9684* O 35 s(1.54%)p64.10(98.46%)d 0.00(0.00%)
 BD (2) U 2 - O 35(Beta)
 (6.15%) 0.2481* U 2 s(0.01%)p 1.00(3.73%)d15.88(59.25%)f 9.91(36.98%)g 0.01(0.04%)
 (93.85%) 0.9687* O 35 s(0.31%)p99.99(99.69%)d 0.00(0.00%)

Bonding orbitals from NBO analysis for ground state spin (s=1) for Rb₂-N₂

BD (1) U 1 - O 11(Alpha)
 (10.82%) 0.3290* U 1 s(7.64%)p 0.88(6.70%)d 5.04(38.49%) f 6.17(47.13%)g 0.00(0.03%)
 (89.18%) 0.9443* O 11 s(43.32%)p 1.31(56.65%)d 0.00(0.02%)
 BD (2) U 1 - O 11(Alpha)
 (10.07%) 0.3174* U 1 s(1.25%)p 3.81(4.76%)d28.11(35.19%) f46.91(58.73%)g 0.05(0.07%)
 (89.93%) 0.9483* O 11 s(1.28%)p77.27(98.68%)d 0.04(0.05%)
 BD (3) U 1 - O 11(Alpha)
 (11.45%) 0.3383* U 1 s(0.18%)p18.89(3.42%)d99.99(42.96%) f99.99(53.40%)g 0.16(0.03%)
 (88.55%) 0.9410* O 11 s(0.18%)p99.99(99.77%)d 0.25(0.05%)
 BD (1) U 1 - N 36(Alpha)
 (18.86%) 0.4343* U 1 s(10.44%)p 1.05(10.96%)d 3.52(36.73%) f 4.01(41.84%)g 0.00(0.03%)
 (81.14%) 0.9008* N 36 s(46.67%)p 1.14(53.28%)d 0.00(0.05%)
 BD (2) U 1 - N 36(Alpha)
 (14.44%) 0.3800* U 1 s(0.38%)p14.51(5.55%)d44.80(17.15%) f99.99(76.90%)g 0.04(0.02%)
 (85.56%) 0.9250* N 36 s(20.03%)p 3.99(79.89%)d 0.00(0.08%)
 BD (1) U 1 - N 37(Alpha)
 (17.29%) 0.4159* U 1 s(12.10%)p 0.75(9.08%)d 4.06(49.11%) f 2.45(29.69%)g 0.00(0.02%)
 (82.71%) 0.9094* N 37 s(37.39%)p 1.67(62.55%)d 0.00(0.06%)
 BD (1) U 2 - O 11(Alpha)
 (11.69%) 0.3419* U 2 s(7.11%)p 0.74(5.27%)d 5.46(38.78%) f 6.87(48.80%)g 0.00(0.03%)
 (88.31%) 0.9397* O 11 s(55.18%)p 0.81(44.80%)d 0.00(0.02%)
 BD (1) U 2 - N 37(Alpha)
 (21.10%) 0.4593* U 2 s(5.68%)p 1.41(8.00%)d 6.19(35.16%) f 9.01(51.14%)g 0.00(0.03%)
 (78.90%) 0.8883* N 37 s(33.80%)p 1.96(66.13%)d 0.00(0.06%)
 BD (2) U 2 - N 37(Alpha)
 (19.94%) 0.4466* U 2 s(2.49%)p 3.13(7.78%)d 4.12(10.24%) f31.95(79.47%)g 0.01(0.01%)
 (80.06%) 0.8947* N 37 s(6.68%)p13.96(93.23%)d 0.01(0.09%)
 BD (1) U 1 - O 11(Beta)
 (10.43%) 0.3229* U 1 s(8.46%)p 0.09(0.78%)d 3.86(32.61%)f 6.87(58.08%)g 0.01(0.07%)
 (89.57%) 0.9464* O 11 s(19.67%)p 4.08(80.30%)d 0.00(0.03%)
 BD (2) U 1 - O 11(Beta)
 (9.58%) 0.3095* U 1 s(0.06%)p69.16(4.29%)d99.99(44.70%)f99.99(50.92%)g 0.55(0.03%)
 (90.42%) 0.9509* O 11 s(0.00%)p 1.00(99.95%)d 0.00(0.04%)
 BD (1) U 1 - N 36(Beta)
 (13.39%) 0.3659* U 1 s(9.07%)p 1.13(10.29%)d 4.14(37.53%)f 4.75(43.09%)g 0.00(0.03%)
 (86.61%) 0.9307* N 36 s(53.68%)p 0.86(46.27%)d 0.00(0.04%)
 BD (2) U 1 - N 36(Beta)
 (11.81%) 0.3436* U 1 s(0.09%)p43.65(3.71%)d99.99(17.14%)f99.99(79.04%)g 0.37(0.03%)
 (88.19%) 0.9391* N 36 s(5.81%)p16.19(94.10%)d 0.02(0.09%)
 BD (1) U 1 - N 37(Beta)

(13.11%) 0.3621* U 1 s(11.68%)p 0.84(9.82%)d 3.67(42.82%)f 3.05(35.66%)g 0.00(0.02%)
 (86.89%) 0.9321* N 37 s(44.68%)p 1.24(55.27%)d 0.00(0.05%)
 BD (1) U 2 - O 11(Beta)
 (10.69%) 0.3270* U 2 s(5.93%)p 0.19(1.14%)d 6.07(35.98%)f 9.60(56.89%)g 0.01(0.07%)
 (89.31%) 0.9450* O 11 s(19.58%)p 4.10(80.38%)d 0.00(0.03%)
 BD (1) U 2 - N 37(Beta)
 (14.47%) 0.3804* U 2 s(6.32%)p 1.36(8.62%)d 6.01(37.97%)f 7.45(47.06%)g 0.00(0.03%)
 (85.53%) 0.9248* N 37 s(35.84%)p 1.79(64.10%)d 0.00(0.06%)
 BD (2) U 2 - N 37(Beta)
 (15.00%) 0.3872* U 2 s(0.48%)p10.86(5.19%)d31.39(14.99%)f99.99(79.32%)g 0.06(0.03%)
 (85.00%) 0.9220* N 37 s(0.10%)p99.99(99.80%)d 0.88(0.09%)

Bonding orbitals from NBO analysis for ground state spin (s=1) for Rb₄-(N)₂

BD (1) U 1 - O 17(Alpha)
 (18.19%) 0.4265* U 1 s(0.01%)p 1.00(1.36%)d36.10(49.03%)f36.45(49.51%)g 0.07(0.10%)
 (81.81%) 0.9045* O 17 s(0.42%)p99.99(99.51%)d 0.15(0.06%)
 BD (2) U 1 - O 17(Alpha)
 (18.21%) 0.4267* U 1 s(0.10%)p 7.09(0.74%)d99.99(51.85%)f99.99(47.16%)g 1.33(0.14%)
 (81.79%) 0.9044* O 17 s(6.98%)p13.32(92.96%)d 0.01(0.06%)
 BD (3) U 1 - O 17(Alpha)
 (19.84%) 0.4454* U 1 s(1.76%)p 0.72(1.27%)d24.17(42.60%)f30.73(54.17%)g 0.11(0.19%)
 (80.16%) 0.8953* O 17 s(25.75%)p 2.88(74.20%)d 0.00(0.04%)
 BD (1) U 1 - N 38(Alpha)
 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%)f 3.11(29.03%)g 0.00(0.04%)
 (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)
 BD (1) U 1 - N 39(Alpha)
 (29.80%) 0.5459* U 1 s(2.19%)p 0.65(1.43%)d23.74(51.92%)f20.29(44.36%)g 0.05(0.10%)
 (70.20%) 0.8379* N 39 s(39.00%)p 1.56(60.84%)d 0.00(0.17%)
 BD (2) U 1 - N 39(Alpha)
 (27.80%) 0.5273* U 1 s(0.05%)p75.34(4.05%)d99.99(46.20%)f99.99(49.62%)g 1.36(0.07%)
 (72.20%) 0.8497* N 39 s(0.07%)p99.99(99.79%)d 2.04(0.14%)
 BD (3) U 1 - N 39(Alpha)
 (29.15%) 0.5399* U 1 s(0.05%)p25.84(1.20%)d99.99(48.07%)f99.99(50.64%)g 0.90(0.04%)
 (70.85%) 0.8417* N 39 s(0.02%)p99.99(99.84%)d 6.11(0.14%)
 BD (1) U 2 - N 38(Alpha)
 (18.41%) 0.4291* U 2 s(8.60%)p 0.16(1.40%)d 4.55(39.10%)f 5.92(50.87%)g 0.00(0.03%)
 (81.59%) 0.9032* N 38 s(42.89%)p 1.33(57.10%)d 0.00(0.02%)
 BD (1) U 2 - N 39(Alpha)
 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%)f 2.28(29.26%)g 0.00(0.01%)
 (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)
 BD (1) U 1 - O 17(Beta)
 (18.25%) 0.4272* U 1 s(0.01%)p99.99(1.33%)d99.99(49.08%)f99.99(49.48%)g 8.48(0.10%)
 (81.75%) 0.9042* O 17 s(0.72%)p99.99(99.22%)d 0.09(0.06%)
 BD (2) U 1 - O 17(Beta)
 (18.06%) 0.4249* U 1 s(0.11%)p 7.34(0.79%)d99.99(51.52%)f99.99(47.45%)g 1.26(0.14%)
 (81.94%) 0.9052* O 17 s(6.20%)p15.13(93.75%)d 0.01(0.06%)
 BD (3) U 1 - O 17(Beta)
 (19.81%) 0.4450* U 1 s(1.78%)p 0.65(1.15%)d24.47(43.61%)f29.88(53.26%)g 0.11(0.20%)
 (80.19%) 0.8955* O 17 s(26.38%)p 2.79(73.58%)d 0.00(0.04%)
 BD (1) U 1 - N 38(Beta)
 (18.24%) 0.4270* U 1 s(9.48%)p 0.71(6.76%)d 5.65(53.55%)f 3.18(30.18%)g 0.00(0.04%)
 (81.76%) 0.9042* N 38 s(44.56%)p 1.24(55.43%)d 0.00(0.01%)
 BD (1) U 1 - N 39(Beta)
 (29.77%) 0.5456* U 1 s(1.87%)p 0.76(1.42%)d27.67(51.61%)f24.12(45.00%)g 0.05(0.10%)
 (70.23%) 0.8380* N 39 s(36.01%)p 1.77(63.82%)d 0.00(0.17%)
 BD (2) U 1 - N 39(Beta)
 (28.21%) 0.5311* U 1 s(0.05%)p52.20(2.86%)d99.99(47.01%)f99.99(50.01%)g 1.29(0.07%)
 (71.79%) 0.8473* N 39 s(0.18%)p99.99(99.67%)d 0.77(0.14%)
 BD (3) U 1 - N 39(Beta)
 (28.72%) 0.5359* U 1 s(0.03%)p66.18(1.95%)d99.99(47.04%)f99.99(50.93%)g 1.72(0.05%)
 (71.28%) 0.8443* N 39 s(0.12%)p99.99(99.74%)d 1.23(0.14%)
 BD (1) U 2 - N 38(Beta)
 (15.45%) 0.3931* U 2 s(9.44%)p 0.18(1.72%)d 4.71(44.44%)f 4.70(44.36%)g 0.00(0.04%)
 (84.55%) 0.9195* N 38 s(47.69%)p 1.10(52.29%)d 0.00(0.02%)

BD (1) U 2 - N 39(Beta)
(11.26%) 0.3356* U 2 s(12.10%)p 0.58(7.06%)d 4.18(50.62%)f 2.50(30.21%)g 0.00(0.01%)
(88.74%) 0.9420* N 39 s(63.75%)p 0.57(36.22%)d 0.00(0.03%)

Bonding orbitals from NBO analysis for ground state spin (s=3) for Cs₂-2

BD (1) U 1 - O 11(Alpha)
(7.43%) 0.2725* U 1 s(0.03%)p99.99(3.79%)d99.99(61.69%)f99.99(34.47%)g 0.78(0.02%)
(92.57%) 0.9622* O 11 s(0.18%)p99.99(99.82%)d 0.00(0.00%)

BD (2) U 1 - O 11(Alpha)
(7.29%) 0.2700* U 1 s(0.04%)p97.26(3.70%)d99.99(61.55%)f99.99(34.70%)g 0.53(0.02%)
(92.71%) 0.9629* O 11 s(0.20%)p99.99(99.80%)d 0.00(0.00%)

BD (1) U 2 - O 11(Beta)
(6.15%) 0.2479* U 2 s(0.00%)p 1.00(3.86%)d15.66(60.48%) f 9.23(35.63%)g 0.01(0.03%)
(93.85%) 0.9688* O 11 s(0.14%)p99.99(99.86%)d 0.00(0.00%)

BD (2) U 2 - O 11(Beta)
(6.05%) 0.2460* U 2 s(0.01%)p 1.00(2.70%)d22.00(59.31%) f14.08(37.95%)g 0.01(0.03%)
(93.95%) 0.9693* O 11 s(0.09%)p99.99(99.91%)d 0.00(0.00%)

(0.92978) BD (1) U 2 - O 11

Bonding orbitals from NBO analysis for ground state spin (s=1) for Cs₂-N₂

(0.93642) BD (1) U 1 - O 11(Alpha)
(12.17%) 0.3488* U 1 s(6.81%)p 0.07(0.46%)d 4.23(28.84%) f 9.37(63.83%)g 0.01(0.06%)
(87.83%) 0.9372* O 11 s(15.03%)p 5.65(84.93%)d 0.00(0.03%)

(0.90951) BD (2) U 1 - O 11(Alpha)
(12.04%) 0.3470* U 1 s(0.34%)p 9.63(3.26%)d99.99(42.70%) f99.99(53.67%)g 0.08(0.03%)
(87.96%) 0.9379* O 11 s(0.18%)p99.99(99.77%)d 0.24(0.04%)

(0.88685) BD (1) U 1 - N 36(Alpha)
(17.95%) 0.4237* U 1 s(8.06%)p 1.36(10.93%)d 4.38(35.33%) f 5.66(45.65%)g 0.00(0.03%)
(82.05%) 0.9058* N 36 s(52.66%)p 0.90(47.31%)d 0.00(0.04%)

(0.86424) BD (2) U 1 - N 36(Alpha)
(12.41%) 0.3522* U 1 s(0.19%)p37.26(6.93%)d87.67(16.32%) f99.99(76.54%)g 0.10(0.02%)
(87.59%) 0.9359* N 36 s(21.75%)p 3.59(78.17%)d 0.00(0.08%)

(0.91434) BD (1) U 1 - N 37(Alpha)
(14.18%) 0.3765* U 1 s(9.37%)p 0.86(8.02%)d 5.03(47.09%) f 3.79(35.50%)g 0.00(0.02%)
(85.82%) 0.9264* N 37 s(43.22%)p 1.31(56.72%)d 0.00(0.06%)

(0.92978) BD (1) U 2 - O 11(Alpha)
(11.73%) 0.3426* U 2 s(6.20%)p 0.13(0.79%)d 5.24(32.51%) f 9.74(60.43%)g 0.01(0.07%)
(88.27%) 0.9395* O 11 s(15.05%)p 5.64(84.91%)d 0.00(0.04%)

(0.84741) BD (1) U 2 - N 36(Alpha)
(26.50%) 0.5148* U 2 s(2.81%)p 0.63(1.78%)d 4.01(11.28%) f29.88(84.11%)g 0.01(0.02%)
(73.50%) 0.8573* N 36 s(0.36%)p99.99(99.54%)d 0.29(0.10%)

(0.92734) BD (1) U 2 - N 37(Alpha)
(21.01%) 0.4583* U 2 s(6.56%)p 0.44(2.86%)d 5.56(36.52%) f 8.23(54.02%)g 0.01(0.04%)
(78.99%) 0.8888* N 37 s(35.40%)p 1.82(64.54%)d 0.00(0.06%)

(0.94800) BD (1) U 1 - O 11(Beta)
(9.62%) 0.3102* U 1 s(5.14%)p 0.31(1.61%)d 7.09(36.42%)f11.05(56.76%)g 0.01(0.07%)
(90.38%) 0.9507* O 11 s(7.66%)p12.05(92.31%)d 0.00(0.03%)

(0.91953) BD (2) U 1 - O 11(Beta)
(9.72%) 0.3118* U 1 s(0.47%)p 7.14(3.37%)d91.77(43.27%)f99.99(52.86%)g 0.07(0.03%)
(90.28%) 0.9501* O 11 s(0.03%)p99.99(99.93%)d 1.48(0.04%)

(0.89868) BD (3) U 1 - O 11(Beta)
(8.10%) 0.2846* U 1 s(0.50%)p10.70(5.31%)d83.64(41.51%)f99.99(52.65%)g 0.07(0.03%)
(91.90%) 0.9586* O 11 s(25.70%)p 2.89(74.26%)d 0.00(0.03%)

(0.93294) BD (1) U 1 - N 36(Beta)
(11.93%) 0.3454* U 1 s(5.44%)p 2.22(12.08%)d 7.56(41.13%)f 7.59(41.32%)g 0.01(0.03%)
(88.07%) 0.9384* N 36 s(67.97%)p 0.47(32.00%)d 0.00(0.03%)

(0.90055) BD (2) U 1 - N 36(Beta)
(10.86%) 0.3295* U 1 s(0.16%)p36.26(5.94%)d85.02(13.92%)f99.99(79.94%)g 0.20(0.03%)
(89.14%) 0.9441* N 36 s(7.93%)p11.59(91.98%)d 0.01(0.09%)

(0.88176) BD (1) U 2 - N 36(Beta)
(14.69%) 0.3833* U 2 s(2.47%)p 1.08(2.65%)d11.19(27.59%)f27.28(67.25%)g 0.02(0.04%)
(85.31%) 0.9236* N 36 s(1.51%)p65.33(98.40%)d 0.06(0.09%)

(0.92674) BD (1) U 2 - N 37(Beta)
(18.62%) 0.4315* U 2 s(3.74%)p 0.32(1.21%)d 9.04(33.78%)f16.39(61.23%)g 0.01(0.05%)

(81.38%) 0.9021* N 37 s(9.53%)p 9.49(90.39%)d 0.01(0.08%)

Bonding orbitals from NBO analysis for ground state spin (s=1) for Cs₄-(N)₂

(0.98145) BD (1) U 1 - O 17(Alpha)
(18.90%) 0.4347* U 1 s(0.26%)p 3.65(0.96%)d99.99(47.74%) f99.99(50.87%)g 0.64(0.17%)
(81.10%) 0.9006* O 17 s(11.92%)p 7.38(88.02%)d 0.00(0.05%)
(0.97951) BD (2) U 1 - O 17(Alpha)
(18.61%) 0.4314* U 1 s(0.56%)p 1.44(0.80%)d84.47(47.01%) f92.45(51.46%)g 0.31(0.17%)
(81.39%) 0.9022* O 17 s(15.89%)p 5.29(84.06%)d 0.00(0.05%)
(0.99101) BD (3) U 1 - O 17(Alpha)
(18.11%) 0.4256* U 1 s(0.14%)p11.20(1.57%)d99.99(48.88%) f99.99(49.32%)g 0.67(0.09%)
(81.89%) 0.9049* O 17 s(2.21%)p44.32(97.73%)d 0.03(0.06%)
(0.95720) BD (1) U 1 - N 38(Alpha)
(17.03%) 0.4126* U 1 s(5.26%)p 1.49(7.84%)d10.97(57.72%) f 5.54(29.13%)g 0.01(0.04%)
(82.97%) 0.9109* N 38 s(51.94%)p 0.92(48.04%)d 0.00(0.01%)
(0.94228) BD (1) U 1 - N 39(Alpha)
(28.91%) 0.5377* U 1 s(1.18%)p 1.14(1.34%)d45.77(53.90%) f36.90(43.46%)g 0.10(0.11%)
(71.09%) 0.8431* N 39 s(39.14%)p 1.55(60.69%)d 0.00(0.18%)
(0.92407) BD (2) U 1 - N 39(Alpha)
(27.83%) 0.5276* U 1 s(0.24%)p17.03(4.13%)d99.99(45.44%) f99.99(50.12%)g 0.29(0.07%)
(72.17%) 0.8495* N 39 s(0.06%)p99.99(99.79%)d 2.76(0.16%)
(0.94234) BD (3) U 1 - N 39(Alpha)
(29.33%) 0.5415* U 1 s(0.08%)p13.75(1.15%)d99.99(47.63%) f99.99(51.10%)g 0.49(0.04%)
(70.67%) 0.8407* N 39 s(0.01%)p99.99(99.84%)d11.56(0.15%)
(0.96571) BD (1) U 2 - N 38(Alpha)
(18.09%) 0.4253* U 2 s(8.65%)p 0.21(1.81%)d 4.50(38.93%) f 5.84(50.57%)g 0.00(0.03%)
(81.91%) 0.9050* N 38 s(41.54%)p 1.41(58.44%)d 0.00(0.02%)
(0.91784) BD (1) U 2 - N 39(Alpha)
(12.21%) 0.3494* U 2 s(12.50%)p 0.62(7.78%)d 4.14(51.70%) f 2.24(28.01%)g 0.00(0.01%)
(87.79%) 0.9370* N 39 s(60.86%)p 0.64(39.10%)d 0.00(0.04%)
(0.97930) BD (1) U 1 - O 17(Beta)
(18.94%) 0.4352* U 1 s(0.31%)p 2.80(0.87%)d99.99(47.82%)f99.99(50.82%)g 0.59(0.18%)
(81.06%) 0.9003* O 17 s(13.56%)p 6.37(86.39%)d 0.00(0.05%)
(0.98214) BD (2) U 1 - O 17(Beta)
(18.39%) 0.4288* U 1 s(0.47%)p 1.78(0.83%)d99.99(47.75%)f99.99(50.79%)g 0.34(0.16%)
(81.61%) 0.9034* O 17 s(13.17%)p 6.59(86.78%)d 0.00(0.05%)
(0.99034) BD (3) U 1 - O 17(Beta)
(18.17%) 0.4262* U 1 s(0.14%)p10.09(1.46%)d99.99(48.80%)f99.99(49.50%)g 0.68(0.10%)
(81.83%) 0.9046* O 17 s(3.39%)p28.50(96.55%)d 0.02(0.06%)
(0.96308) BD (1) U 1 - N 38(Beta)
(16.92%) 0.4114* U 1 s(5.16%)p 1.40(7.20%)d11.04(56.93%)f 5.95(30.67%)g 0.01(0.04%)
(83.08%) 0.9115* N 38 s(45.78%)p 1.18(54.20%)d 0.00(0.01%)
(0.94563) BD (1) U 1 - N 39(Beta)
(28.98%) 0.5384* U 1 s(0.94%)p 1.36(1.28%)d56.91(53.71%)f46.58(43.96%)g 0.12(0.11%)
(71.02%) 0.8427* N 39 s(36.08%)p 1.77(63.74%)d 0.00(0.18%)
(0.92965) BD (2) U 1 - N 39(Beta)
(27.97%) 0.5289* U 1 s(0.17%)p20.08(3.48%)d99.99(45.61%)f99.99(50.66%)g 0.43(0.07%)
(72.03%) 0.8487* N 39 s(0.16%)p99.99(99.68%)d 0.98(0.16%)
(0.94758) BD (3) U 1 - N 39(Beta)
(29.07%) 0.5392* U 1 s(0.09%)p15.69(1.42%)d99.99(47.13%)f99.99(51.31%)g 0.48(0.04%)
(70.93%) 0.8422* N 39 s(0.03%)p99.99(99.82%)d 5.15(0.15%)
(0.96701) BD (1) U 2 - N 38(Beta)
(15.14%) 0.3890* U 2 s(9.46%)p 0.23(2.22%)d 4.67(44.16%)f 4.67(44.13%)g 0.00(0.04%)
(84.86%) 0.9212* N 38 s(46.09%)p 1.17(53.90%)d 0.00(0.02%)
(0.92368) BD (1) U 2 - N 39(Beta)
(11.30%) 0.3362* U 2 s(11.51%)p 0.68(7.85%)d 4.46(51.37%)f 2.54(29.25%)g 0.00(0.01%)
(88.70%) 0.9418* N 39 s(63.80%)p 0.57(36.16%)d 0.00(0.04%)

Table ST1: Computed Wiberg bond index and natural charges for **K₂-2**, **K₂-N₂** and **K₄-(N)₂**

Atom Label	Wiberg bond index						Natural charges		
	K ₂ -2	K ₂ -2	K ₂ -N ₂	K ₂ -N ₂	K ₄ -(N) ₂	K ₄ -(N) ₂	K ₂ -2	K ₂ -N ₂	K ₄ -(N) ₂
U1	0.0000	0.1317	0.0000	0.3864	0.0000	0.4015	1.61924	1.56803	1.18292
U2	0.1317	0.0000	0.3864	0.0000	0.4015	0.0000	1.63570	1.56878	1.53497
O (μ_2)	0.6055	0.7868	0.9966	0.9879	1.8185	0.0211	-1.17306	-0.76635	-0.73185
N1			1.0520	0.8446	1.4138	1.3088		-0.54552	-1.03536
N2			0.8421	1.0544	2.2841	0.6111		-0.54696	-0.73627

Table ST2: Computed Wiberg bond index for **Rb₂-2**, **Rb₂-N₂** and **Rb₄-(N)₂**

Atom Label	Wiberg bond index						Natural charges		
	Rb ₂ -2	Rb ₂ -2	Rb ₂ -N ₂	Rb ₂ -N ₂	Rb ₄ -(N) ₂	U2ON2Rb4	Rb ₂ -2	Rb ₂ -N ₂	Rb ₄ -(N) ₂
U1	0.0000	0.0216	0.0000	0.0871	0.0000	0.0944	1.65808	1.58509	1.18649
U2	0.0216	0.0000	0.0871	0.0000	0.0944	0.0000	1.66459	1.58333	1.52597
O (μ_2)	0.1633	0.1687	0.2363	0.2355	0.4546	0.0051	-1.17262	-0.77677	-0.73344
N1			0.2495	0.2052	0.3545	0.3091		-0.55181	-1.03032
N2			0.2050	0.2497	0.5751	0.1465		-0.55171	-0.73013

Table ST3: Computed Wiberg bond index for **Cs₂-2**, **Cs₂-N₂** and **Cs₄-(N)₂**

Atom Label	Wiberg bond index						Natural charges		
	Cs ₂ -2	Cs ₂ -2	Cs ₂ -N ₂	Cs ₂ -N ₂	Cs ₄ -(N) ₂	Cs ₄ -(N) ₂	Cs ₂ -2	Cs ₂ -N ₂	Cs ₄ -(N) ₂
U1	0.0000	0.0230	0.0000	0.0836	0.0000	0.0982	1.58368	1.60269	1.10202
U2	0.0230	0.0000	0.0836	0.0000	0.0982	0.0000	1.63980	1.62503	1.43110
O (μ_2)	0.1642	0.1666	0.2353	0.2306	0.0049	0.1474	-1.17532	-0.79451	-1.19414
N1			0.2463	0.1986	0.3473	0.3125		-0.55274	-1.08683
N2			0.2005	0.2422	0.5753	0.1490		-0.55672	-0.75886

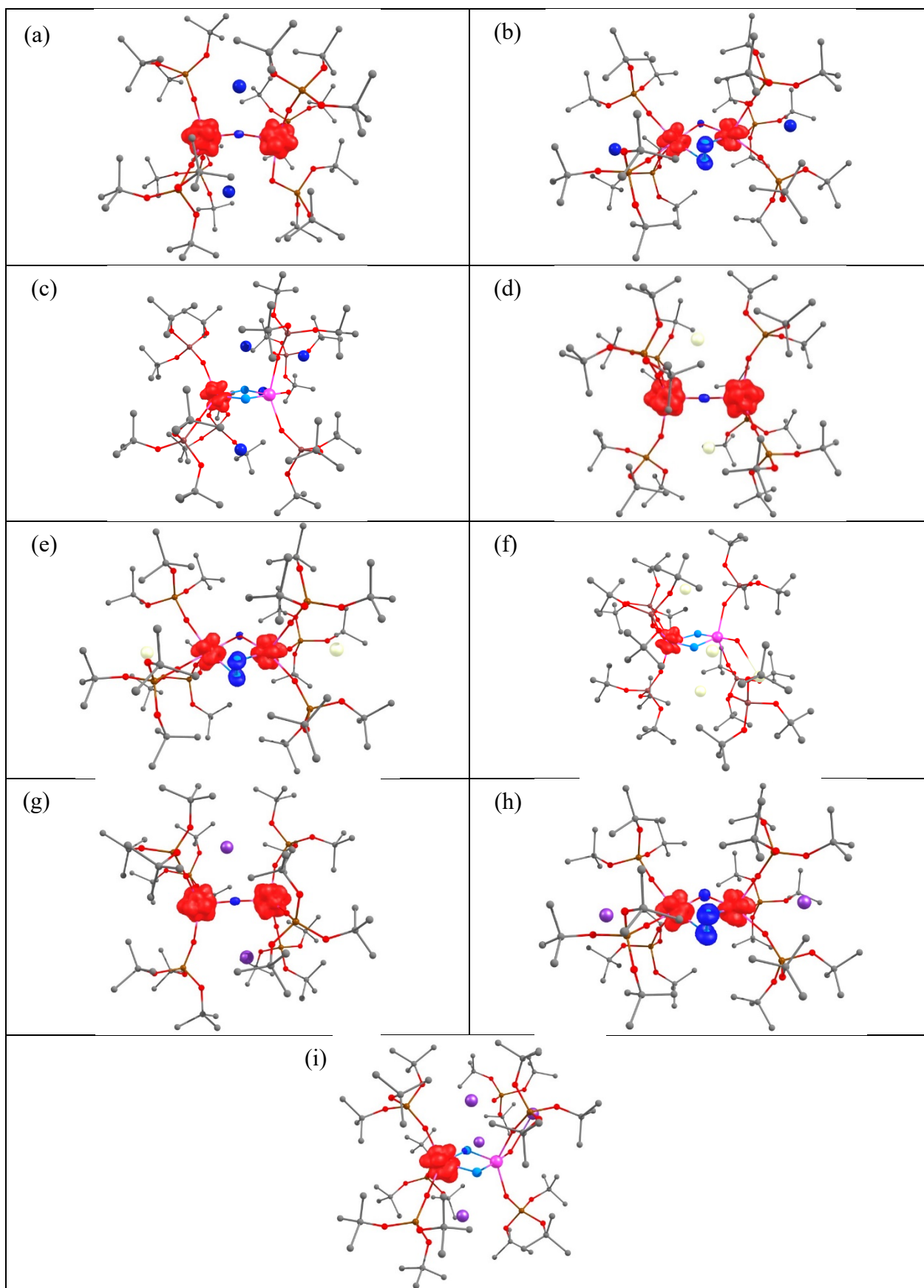


Figure SF1: Computed spin density plots for (a) $\text{K}_2\text{-2}$, $s=3$ (b) $\text{K}_2\text{-N}_2$, $s=1$ (c) $\text{K}_4\text{-(N)}_2$, $s=1$ (d) $\text{Rb}_2\text{-2}$, $s=3$ (e) $\text{Rb}_2\text{-N}_2$, $s=1$ (f) $\text{Rb}_4\text{-(N)}_2$, $s=1$ (g) $\text{Cs}_2\text{-2}$, $s=3$ (h) $\text{Cs}_2\text{-N}_2$, $s=1$ (i) $\text{Cs}_4\text{-N}_2$, $s=1$.

Table ST4: DFT computed spin densities

Atom Label	Spin densities								
	K ₂ -2	K ₂ -N ₂	K ₄ -(N) ₂	Rb ₂ -2	Rb ₂ -N ₂	Rb ₄ -(N) ₂	Cs ₂ -2	Cs ₂ -N ₂	Cs ₄ -(N) ₂
U1	3.08	1.27	-0.01	3.10	1.29	-0.01	3.11	1.30	0.00
U2	3.10	1.27	2.18	3.10	1.29	2.19	3.10	1.32	2.18
O (μ ₂)	-0.09	-0.08	0.00	-0.09	-0.08	0.00	-0.09	-0.08	0.00
N1		-0.18	-0.09		-0.20	-0.09		-0.23	-0.09
N2		-0.18	-0.03		-0.20	-0.03		-0.23	-0.03

Table ST5: DFT computed NBO second order perturbation analysis for K₂-2, s=3 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
BD (1) U 1 - O 32 (6.17%) 0.2484* U 1 s(0.27%)p16.98(4.51%)d99.99(68.53%) f99.99(26.68%)g 0.07(0.02%) (93.83%) 0.9687* O 32 s(1.84%)p53.35(98.16%)d 0.00(0.00%)	LP*(4) U 2 s(0.42%)p 3.06(1.27%)d99.99(87.52%) f25.94(10.77%)g 0.06(0.02%)	13.81
BD (2) U 1 - O 32 (5.77%) 0.2401* U 1 s(0.10%)p47.58(4.99%)d99.99(73.49%) f99.99(21.39%)g 0.24(0.02%) (94.23%) 0.9707* O 32 s(0.09%)p99.99(99.90%)d 0.02(0.00%)	LP*(5) U 2 s(0.56%)p 7.08(3.97%)d99.99(80.69%) f26.31(14.77%)g 0.01(0.01%)	14.10
LP (1) O 32 s(45.90%)p 1.18(54.10%)d 0.00(0.00%)	LP*(4) U 1 s(0.75%)p 2.77(2.07%)d99.99(77.35%) f26.53(19.83%)g 0.01(0.01%)	35.78
LP (2) O 32 s(52.16%)p 0.92(47.83%)d 0.00(0.01%)	LP*(4) U 1 s(0.75%)p 2.77(2.07%)d99.99(77.35%) f26.53(19.83%)g 0.01(0.01%)	10.92
LP (2) O 32 s(52.16%)p 0.92(47.83%)d 0.00(0.01%)	LP*(3) U 2 s(0.72%)p 7.41(5.31%)d99.99(76.78%) f24.02(17.19%)g 0.01(0.01%)	13.67
LP (2) O 32 s(52.16%)p 0.92(47.83%)d 0.00(0.01%)	LP*(4) U 2 s(0.42%)p 3.06(1.27%)d99.99(87.52%) f25.94(10.77%)g 0.06(0.02%)	22.06

Table ST6: DFT computed NBO second order perturbation analysis for K_2-N_2 , $s=1$ spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<p><u>BD (2) U 1 - O 12</u> (10.18%) 0.3191* U 1 s(1.16%)p 3.96(4.59%)d30.35(35.19%)f50.89(59.00%)g 0.06(0.07%) (89.82%) 0.9477* O 12 s(1.38%)p71.37(98.57%)d 0.03(0.05%)</p>	<p><u>LP*(3) U 2</u> s(0.36%)p 0.78(0.28%)d99.99(57.18%)f99.99(42.18%)g 0.01(0.00%)</p>	14.66
<p><u>BD (3) U 1 - O 12</u> (11.50%) 0.3391* U 1 s(0.17%)p21.03(3.53%)d99.99(43.18%) f99.99(53.09%)g 0.17(0.03%) (88.50%) 0.9408* O 12 s(0.24%)p99.99(99.71%)d 0.19(0.05%)</p>	<p><u>LP*(5) U 2</u> s(0.66%)p 0.64(0.42%)d89.12(59.07%)f60.11(39.84%)g 0.01(0.01%)</p>	18.54
<p><u>BD (2) U 1 - N 13</u> (14.29%) 0.3780* U 1 s(0.47%)p11.62(5.50%)d36.33(17.20%) f99.99(76.81%)g 0.04(0.02%) (85.71%) 0.9258* N 13 s(19.43%)p 4.14(80.49%)d 0.00(0.08%)</p>	<p><u>LP*(2) U 2</u> s(2.00%)p 0.79(1.58%)d15.22(30.46%)f32.95(65.93%)g 0.01(0.03%)</p>	10.59
<p><u>BD (1) U 1 - N 14</u> (17.32%) 0.4161* U 1 s(12.81%)p 0.74(9.42%)d 3.75(47.97%)f 2.32(29.77%)g 0.00(0.02%) (82.68%) 0.9093* N 14 s(37.95%)p 1.63(62.00%)d 0.00(0.06%)</p>	<p><u>LP*(6) U 2</u> s(45.44%)p 0.36(16.23%)d 0.08(3.53%)f 0.77(34.77%)g 0.00(0.03%)</p>	11.76
<p><u>BD (1) U 2 - O 12</u> (11.85%) 0.3442* U 2 s(7.44%)p 0.77(5.71%)d 5.20(38.64%)f 6.48(48.18%)g 0.00(0.03%) (88.15%) 0.9389* O 12 s(55.10%)p 0.81(44.88%)d 0.00(0.02%)</p>	<p><u>LP*(8) U 1</u> s(0.09%)p99.99(61.21%)d99.99(16.40%)f99.99(22.26%)g 0.40(0.04%)</p>	10.30
<p><u>BD (1) N 13 - N 14</u> (50.00%) 0.7071* N 13 s(21.47%)p 3.65(78.34%)d 0.01(0.20%) (50.00%) 0.7071* N 14 s(21.51%)p 3.64(78.29%)d 0.01(0.20%)</p>	<p><u>LP*(2) U 2</u> s(2.00%)p 0.79(1.58%)d15.22(30.46%)f32.95(65.93%)g 0.01(0.03%)</p>	11.37
<p><u>LP (1) N 13</u> s(12.10%)p 7.25(87.78%)d 0.01(0.11%)</p>	<p><u>LP*(2) U 2</u> s(2.00%)p 0.79(1.58%)d15.22(30.46%)f32.95(65.93%)g 0.01(0.03%)</p>	40.30

Table ST7: DFT computed NBO second order perturbation analysis for $K_4-(N)_2$, $s=1$ spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
BD (3) U 1 - O 17 (20.03%) 0.4476* U 1 s(2.47%)p 0.43(1.07%)d17.24(42.65%)f21.66(53.58%)g 0.09(0.22%) (79.97%) 0.8943* O 17 s(30.41%)p 2.29(69.55%)d 0.00(0.04%)	LP*(4) U 2 s(0.34%)p 5.25(1.77%)d99.99(69.40%)f84.78(28.49%)g 0.03(0.01%)	10.84
BD (3) U 1 - O 17 (20.03%) 0.4476* U 1 s(2.47%)p 0.43(1.07%)d17.24(42.65%)f21.66(53.58%)g 0.09(0.22%) (79.97%) 0.8943* O 17 s(30.41%)p 2.29(69.55%)d 0.00(0.04%)	LP*(8) U 2 s(28.52%)p 0.02(0.59%)d 1.70(48.46%) f 0.79(22.42%)g 0.00(0.01%)	35.87
BD (3) U 1 - O 17 (20.03%) 0.4476* U 1 s(2.47%)p 0.43(1.07%)d17.24(42.65%)f21.66(53.58%)g 0.09(0.22%) (79.97%) 0.8943* O 17 s(30.41%)p 2.29(69.55%)d 0.00(0.04%)	LP*(11) U 2 s(1.26%)p12.20(15.37%)d 5.75(7.24%)f60.42(76.10%)g 0.02(0.03%)	560.78
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(1) U 1 s(1.24%)p 1.16(1.45%)d45.77(56.83%)f32.60(40.47%)g 0.01(0.01%)	37.73
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(5) U 1 s(0.75%)p 7.00(5.22%)d53.06(39.56%)f73.06(54.47%)g 0.01(0.01%)	95.62
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(9) U 1 s(0.06%)p59.51(3.44%)d65.89(3.81%)f99.99(92.48%)g 3.45(0.20%)	163.49
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(3) U 2 s(0.75%)p 3.57(2.67%)d80.56(60.24%)f48.59(36.33%)g 0.02(0.02%)	140.84
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(4) U 2 s(0.34%)p 5.25(1.77%)d99.99(69.40%)f84.78(28.49%)g 0.03(0.01%)	22.23
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(7) U 2 s(37.53%)p 0.03(1.21%)d 0.54(20.21%) f 1.09(41.02%)g 0.00(0.02%)	113.58
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(9) U 2 s(0.13%)p99.99(21.96%)d48.76(6.10%)f99.99(71.81%)g 0.05(0.01%)	71.48
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(11) U 2 s(1.26%)p12.20(15.37%)d 5.75(7.24%)f60.42(76.10%)g 0.02(0.03%)	222.68
BD (2) U 1 - N 39 (27.75%) 0.5268* U 1 s(0.03%)p99.99(3.92%)d99.99(46.32%) f99.99(49.66%)g 2.88(0.07%)	LP*(4) U 2 s(0.34%)p 5.25(1.77%)d99.99(69.40%)f84.78(28.49%)g 0.03(0.01%)	451.09

(72.25%) 0.8500* N 39 s(0.09%)p99.99(99.78%)d 1.55(0.14%)		
BD (1) U 2 - N 38 (18.30%) 0.4277* U 2 s(9.05%)p 0.18(1.61%)d 4.38(39.69%) f 5.48(49.61%)g 0.00(0.03%) (81.70%) 0.9039* N 38 s(43.26%)p 1.31(56.73%)d 0.00(0.01%)	LP*(1) U 1 s(1.24%)p 1.16(1.45%)d45.77(56.83%) f32.60(40.47%)g 0.01(0.01%)	36.79
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(2) U 1 s(11.41%)p 2.09(23.89%)d 0.40(4.59%) f 5.26(60.04%)g 0.01(0.07%)	6021.46
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(5) U 1 s(0.75%)p 7.00(5.22%)d53.06(39.56%) f73.06(54.47%)g 0.01(0.01%)	232.93
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(9) U 1 s(0.06%)p59.51(3.44%)d65.89(3.81%)f99.99(92.48%)g 3.45(0.20%)	586.78
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(3) U 2 s(0.75%)p 3.57(2.67%)d80.56(60.24%) f48.59(36.33%)g 0.02(0.02%)	119.39
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(5) U 2 s(0.05%)p10.19(0.46%)d99.99(78.41%)f99.99(21.07%)g 0.20(0.01%)	355.39
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(6) U 2 s(0.88%)p 2.10(1.84%)d84.36(73.87%) f26.72(23.40%)g 0.01(0.01%)	39.24
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(7) U 2 s(37.53%)p 0.03(1.21%)d 0.54(20.21%) f 1.09(41.02%)g 0.00(0.02%)	609.38
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(8) U 2 s(28.52%)p 0.02(0.59%)d 1.70(48.46%) f 0.79(22.42%)g 0.00(0.01%)	66.31
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(9) U 2 s(0.13%)p99.99(21.96%)d48.76(6.10%) f99.99(71.81%)g 0.05(0.01%)	50.71
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(10) U 2 s(0.03%)p99.99(20.29%)d99.99(28.74%) f99.99(50.92%)g 0.70(0.02%)	933.92
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(9) U 1 s(0.06%)p59.51(3.44%)d65.89(3.81%)f99.99(92.48%)g 3.45(0.20%)	68.89

LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(3) U 2 s(0.75%)p 3.57(2.67%)d80.56(60.24%)f48.59(36.33%)g 0.02(0.02%)	19.97
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(5) U 2 s(0.05%)p10.19(0.46%)d99.99(78.41%)f99.99(21.07%)g 0.20(0.01%)	44.40
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(7) U 2 s(37.53%)p 0.03(1.21%)d 0.54(20.21%) f 1.09(41.02%)g 0.00(0.02%)	10.34
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(11) U 2 s(1.26%)p12.20(15.37%)d 5.75(7.24%) f60.42(76.10%)g 0.02(0.03%)	31.43
LP (1) N 38 s(6.20%)p15.14(93.77%)d 0.01(0.04%)	LP*(1) U 1 s(1.24%)p 1.16(1.45%)d45.77(56.83%)f32.60(40.47%)g 0.01(0.01%)	70.11
LP (2) N 38 s(0.28%)p99.99(99.68%)d 0.15(0.04%)	LP*(1) U 1 s(1.24%)p 1.16(1.45%)d45.77(56.83%)f32.60(40.47%)g 0.01(0.01%)	145.05
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(9) K 5 s(0.16%)p36.79(5.92%)d99.99(93.92%)	94.87
LP (1) O 17 s(66.87%)p 0.50(33.13%)d 0.00(0.00%)	LP*(4) K 6 s(64.59%)p 0.55(35.28%)d 0.00(0.13%)	24.04
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(4) K 4 s(59.10%)p 0.69(40.79%)d 0.00(0.11%)	658.27
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(4) K 4 s(59.10%)p 0.69(40.79%)d 0.00(0.11%)	41.48
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(4) K 5 s(62.34%)p 0.60(37.16%)d 0.01(0.49%)	29.69
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(9) K 5 s(0.16%)p36.79(5.92%)d99.99(93.92%)	442.69
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(4) K 5 s(62.34%)p 0.60(37.16%)d 0.01(0.49%)	52.42
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(9) K 5 s(0.16%)p36.79(5.92%)d99.99(93.92%)	190.85

BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(4) K 6 s(64.59%)p 0.55(35.28%)d 0.00(0.13%)	2004.94
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(6) K 6 s(0.53%)p 1.58(0.83%)d99.99(98.64%)	34.08
BD (1) U 1 - N 38 (18.68%) 0.4322* U 1 s(10.38%)p 0.76(7.87%)d 5.09(52.83%) f 2.78(28.89%)g 0.00(0.04%) (81.32%) 0.9018* N 38 s(50.24%)p 0.99(49.74%)d 0.00(0.01%)	LP*(7) K 6 s(0.39%)p 8.48(3.28%)d99.99(96.33%)	62.66
BD (2) U 1 - N 39 (27.75%) 0.5268* U 1 s(0.03%)p99.99(3.92%)d99.99(46.32%) f99.99(49.66%)g 2.88(0.07%) (72.25%) 0.8500* N 39 s(0.09%)p99.99(99.78%)d 1.55(0.14%)	LP*(6) K 6 s(0.53%)p 1.58(0.83%)d99.99(98.64%)	143.93
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(4) K 6 s(64.59%)p 0.55(35.28%)d 0.00(0.13%)	137.27
BD (1) U 2 - N 39 (12.40%) 0.3521* U 2 s(13.37%)p 0.54(7.19%)d 3.75(50.19%) f 2.19(29.25%)g 0.00(0.01%) (87.60%) 0.9359* N 39 s(60.32%)p 0.66(39.64%)d 0.00(0.04%)	LP*(5) K 6 s(1.24%)p 0.99(1.23%)d78.35(97.52%)	62.33

Table S78: DFT computed NBO second order perturbation analysis for **Rb₂-2**, s=3 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
LP(1) O 35 s(96.83%)p 0.03(3.16%)d 0.00(0.01%)	LP*(4) U 1 s(0.88%)p 3.40(2.99%)d91.70(80.83%) f17.32(15.27%)g 0.02(0.02%)	28.55
BD (1) U 1 - O 35 (9.78%) 0.3128* U 1 s(0.69%)p 3.00(2.07%)d65.60(45.37%) f74.96(51.85%)g 0.02(0.02%) (90.22%) 0.9498* O 35 s(0.17%)p99.99(99.83%)d 0.00(0.00%)	LP*(4) U 2 s(0.90%)p 4.20(3.80%)d93.26(84.38%) f12.05(10.90%)g 0.02(0.02%)	6.16
LP(1) O 35 s(96.83%)p 0.03(3.16%)d 0.00(0.01%)	LP*(4) U 2 s(0.90%)p 4.20(3.80%)d93.26(84.38%) f12.05(10.90%)g 0.02(0.02%)	13.17
LP(2) O 35 s(2.37%)p41.19(97.63%)d 0.00(0.00%)	LP*(3) U 2 s(2.41%)p 4.10(9.89%)d31.96(77.13%) f 4.37(10.55%)g 0.01(0.01%)	9.59

Table ST9: DFT computed NBO second order perturbation analysis for **Rb₂-N₂**, s=1 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<p><u>BD (2) U 1 - O 11</u> (10.07%) 0.3174* U 1 s(1.25%)p 3.81(4.76%)d28.11(35.19%)f46.91(58.73%)g 0.05(0.07%) (89.93%) 0.9483* O 11 s(1.28%)p77.27(98.68%)d 0.04(0.05%)</p>	<p><u>LP*(3) U 2</u> s(0.24%)p 1.65(0.40%)d99.99(60.30%)f99.99(39.05%)g 0.01(0.00%)</p>	14.96
<p><u>BD (3) U 1 - O 11</u> (11.45%) 0.3383* U 1 s(0.18%)p18.89(3.42%)d99.99(42.96%) f99.99(53.40%)g 0.16(0.03%) (88.55%) 0.9410* O 11 s(0.18%)p99.99(99.77%)d 0.25(0.05%)</p>	<p><u>LP*(5) U 2</u> s(0.68%)p 0.50(0.34%)d84.28(57.36%)f61.14(41.61%)g 0.01(0.01%)</p>	19.52
<p><u>BD (2) U 1 - N 36</u> (14.44%) 0.3800* U 1 s(0.38%)p14.51(5.55%)d44.80(17.15%) f99.99(76.90%)g 0.04(0.02%) (85.56%) 0.9250* N 36 s(20.03%)p 3.99(79.89%)d 0.00(0.08%)</p>	<p><u>LP*(2) U 2</u> s(1.60%)p 1.11(1.78%)d19.66(31.48%)f40.66(65.11%)g 0.02(0.03%)</p>	10.71
<p><u>BD (1) U 1 - N 37</u> (17.29%) 0.4159* U 1 s(12.10%)p 0.75(9.08%)d 4.06(49.11%)f 2.45(29.69%)g 0.00(0.02%) (82.71%) 0.9094* N 37 s(37.39%)p 1.67(62.55%)d 0.00(0.06%)</p>	<p><u>LP*(6) U 2</u> s(42.96%)p 0.44(18.69%)d 0.15(6.38%)f 0.74(31.95%)g 0.00(0.02%)</p>	12.04
<p><u>BD (1) U 2 - O 11</u> (11.69%) 0.3419* U 2 s(7.11%)p 0.74(5.27%)d 5.46(38.78%)f 6.87(48.80%)g 0.00(0.03%) (88.31%) 0.9397* O 11 s(55.18%)p 0.81(44.80%)d 0.00(0.02%)</p>	<p><u>LP*(8) U 1</u> s(0.07%)p99.99(59.45%)d99.99(16.50%)f99.99(23.95%)g 0.47(0.03%)</p>	9.43
<p><u>BD (1) N 36 - N 37</u> (50.03%) 0.7073* N 36 s(22.17%)p 3.50(77.64%)d 0.01(0.19%) (49.97%) 0.7069* N 37 s(22.11%)p 3.51(77.69%)d 0.01(0.20%)</p>	<p><u>LP*(2) U 2</u> s(1.60%)p 1.11(1.78%)d19.66(31.48%)f40.66(65.11%)g 0.02(0.03%)</p>	11.00
<p>LP (1) N 36 s(11.11%)p 7.99(88.77%)d 0.01(0.12%)</p>	<p><u>LP*(2) U 2</u> s(1.60%)p 1.11(1.78%)d19.66(31.48%)f40.66(65.11%)g 0.02(0.03%)</p>	38.77

Table ST10: DFT computed NBO second order perturbation analysis for **Rb₄-(N)₂**, s=1 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<p><u>BD (3) U 1 - O 17</u> (19.84%) 0.4454* U 1 s(1.76%)p 0.72(1.27%)d24.17(42.60%)f30.73(54.17%)g 0.11(0.19%) (80.16%) 0.8953* O 17 s(25.75%)p 2.88(74.20%)d 0.00(0.04%)</p>	<p><u>LP*(4) U 2</u> s(0.36%)p 4.73(1.71%)d99.99(69.14%)f79.38(28.77%)g 0.03(0.01%)</p>	52.84
<p><u>BD (3) U 1 - O 17</u> (19.84%) 0.4454* U 1 s(1.76%)p 0.72(1.27%)d24.17(42.60%)f30.73(54.17%)g 0.11(0.19%) (80.16%) 0.8953* O 17 s(25.75%)p 2.88(74.20%)d 0.00(0.04%)</p>	<p><u>LP*(6) U 2</u> s(1.21%)p 1.81(2.20%)d65.55(79.59%)f13.99(16.99%)g 0.00(0.01%)</p>	118.34
<p><u>BD (1) U 1 - N 38</u> (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%)f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)</p>	<p><u>LP*(1) U 1</u> s(1.19%)p 1.30(1.55%)d48.63(57.69%)f33.35(39.57%)g 0.01(0.01%)</p>	20.83
<p><u>BD (1) U 1 - N 38</u> (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%)f 3.11(29.03%)g 0.00(0.04%)</p>	<p><u>LP*(5) U 1</u> s(0.66%)p 6.70(4.42%)d59.58(39.26%)f84.46(55.66%)g 0.01(0.01%)</p>	115.79

(81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)		
BD (1) U 1 - N 38 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%) f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)	LP*(9) U 1 s(0.20%)p22.66(4.50%)d22.37(4.44%) f99.99(90.65%)g 1.07(0.21%)	243.94
BD (1) U 1 - N 38 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%) f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)	LP*(3) U 2 s(0.68%)p 4.14(2.81%)d87.93(59.67%) f54.26(36.82%)g 0.03(0.02%)	363.17
BD (1) U 1 - N 38 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%) f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)	LP*(4) U 2 s(0.36%)p 4.73(1.71%)d99.99(69.14%) f79.38(28.77%)g 0.03(0.01%)	32.61
BD (1) U 1 - N 38 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%) f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)	LP*(9) U 2 s(0.14%)p99.99(22.66%)d40.40(5.83%) f99.99(71.35%)g 0.05(0.01%)	31.42
BD (1) U 1 - N 38 (18.42%) 0.4292* U 1 s(9.33%)p 0.79(7.34%)d 5.82(54.26%) f 3.11(29.03%)g 0.00(0.04%) (81.58%) 0.9032* N 38 s(50.74%)p 0.97(49.25%)d 0.00(0.01%)	LP*(11) U 2 s(1.04%)p28.69(29.74%)d 7.30(7.57%) f59.44(61.62%)g 0.03(0.03%)	155.42
BD (2) U 1 - N 39 (27.80%) 0.5273* U 1 s(0.05%)p75.34(4.05%)d99.99(46.20%) f99.99(49.62%)g 1.36(0.07%) (72.20%) 0.8497* N 39 s(0.07%)p99.99(99.79%)d 2.04(0.14%)	LP*(1) U 1 s(1.19%)p 1.30(1.55%)d48.63(57.69%) f33.35(39.57%)g 0.01(0.01%)	30.17
BD (3) U 1 - N 39 (29.15%) 0.5399* U 1 s(0.05%)p25.84(1.20%)d99.99(48.07%) f99.99(50.64%)g 0.90(0.04%) (70.85%) 0.8417* N 39 s(0.02%)p99.99(99.84%)d 6.11(0.14%)	LP*(1) U 1 s(1.19%)p 1.30(1.55%)d48.63(57.69%) f33.35(39.57%)g 0.01(0.01%)	15.15
BD (1) U 2 - N 39 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	LP*(5) U 1 s(0.66%)p 6.70(4.42%)d59.58(39.26%) f84.46(55.66%)g 0.01(0.01%)	188.75
BD (1) U 2 - N 39 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	LP*(9) U 1 s(0.20%)p22.66(4.50%)d22.37(4.44%) f99.99(90.65%)g 1.07(0.21%)	279.76
BD (1) U 2 - N 39 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	LP*(3) U 2 s(0.68%)p 4.14(2.81%)d87.93(59.67%) f54.26(36.82%)g 0.03(0.02%)	123.82
BD (1) U 2 - N 39 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	LP*(5) U 2 s(0.12%)p 5.37(0.63%)d99.99(72.55%) f99.99(26.69%)g 0.07(0.01%)	385.19
BD (1) U 2 - N 39 (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	LP*(6) U 2 s(1.21%)p 1.81(2.20%)d65.55(79.59%) f13.99(16.99%)g 0.00(0.01%)	25.67

<u>BD (1) U 2 - N 39</u> (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	<u>LP*(7) U 2</u> s(35.83%)p 0.04(1.52%)d 0.61(21.82%) f 1.14(40.81%)g 0.00(0.01%)	1629.09
<u>BD (1) U 2 - N 39</u> (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	<u>LP*(8) U 2</u> s(31.61%)p 0.01(0.45%)d 1.51(47.87%) f 0.63(20.05%)g 0.00(0.01%)	748.26
<u>BD (1) U 2 - N 39</u> (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	<u>LP*(9) U 2</u> s(0.14%)p99.99(22.66%)d40.40(5.83%) f99.99(71.35%)g 0.05(0.01%)	15.95
<u>BD (1) U 2 - N 39</u> (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	<u>LP*(10) U 2</u> s(0.01%)p 1.00(18.20%)d 1.60(29.12%) f 2.89(52.65%)g 0.00(0.02%)	259.10
<u>LP (1) N 38</u> s(6.00%)p15.66(93.96%)d 0.01(0.04%)	<u>LP*(1) U 1</u> s(1.19%)p 1.30(1.55%)d48.63(57.69%) f33.35(39.57%)g 0.01(0.01%)	16.99
<u>LP (2) N 38</u> s(0.35%)p99.99(99.60%)d 0.12(0.04%)	<u>LP*(1) U 1</u> s(1.19%)p 1.30(1.55%)d48.63(57.69%) f33.35(39.57%)g 0.01(0.01%)	154.86
<u>BD (1) U 1 - O 17</u> (18.19%) 0.4265* U 1 s(0.01%)p 1.00(1.36%)d36.10(49.03%)f36.45(49.51%)g 0.07(0.10%) (81.81%) 0.9045* O 17 s(0.42%)p99.99(99.51%)d 0.15(0.06%)	<u>LP*(4)Rb 5</u> s(58.95%)p 0.70(40.98%)d 0.00(0.08%)	18.58
<u>BD (2) U 1 - O 17</u> (18.21%) 0.4267* U 1 s(0.10%)p 7.09(0.74%)d99.99(51.85%)f99.99(47.16%)g 1.33(0.14%) (81.79%) 0.9044* O 17 s(6.98%)p13.32(92.96%)d 0.01(0.06%)	<u>LP*(4)Rb 5</u> s(58.95%)p 0.70(40.98%)d 0.00(0.08%)	12.35
<u>BD (3) U 1 - O 17</u> (19.84%) 0.4454* U 1 s(1.76%)p 0.72(1.27%)d24.17(42.60%)f30.73(54.17%)g 0.11(0.19%) (80.16%) 0.8953* O 17 s(25.75%)p 2.88(74.20%)d 0.00(0.04%)	<u>LP*(4)Rb 5</u> s(58.95%)p 0.70(40.98%)d 0.00(0.08%)	17.57
<u>BD (1) U 2 - N 38</u> (18.41%) 0.4291* U 2 s(8.60%)p 0.16(1.40%)d 4.55(39.10%) f 5.92(50.87%)g 0.00(0.03%) (81.59%) 0.9032* N 38 s(42.89%)p 1.33(57.10%)d 0.00(0.02%)	<u>LP*(4)Rb 5</u> s(58.95%)p 0.70(40.98%)d 0.00(0.08%)	29.49
<u>BD (1) U 2 - N 39</u> (12.24%) 0.3498* U 2 s(12.85%)p 0.55(7.02%)d 3.96(50.86%) f 2.28(29.26%)g 0.00(0.01%) (87.76%) 0.9368* N 39 s(60.96%)p 0.64(39.00%)d 0.00(0.04%)	<u>LP*(4)Rb 6</u> s(54.39%)p 0.84(45.58%)d 0.00(0.03%)	386.66

Table ST11: DFT computed NBO second order perturbation analysis for **Cs₂-2**, s=3 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<u>LP (1) O 11</u> s(68.34%)p 0.46(31.65%)d 0.00(0.01%)	<u>395. LP*(4) U 1</u> s(0.57%)p 4.44(2.51%)d99.99(90.64%)f11.10(6.27%)g 0.04(0.02%)	30.98
<u>LP (1) O 11</u> s(68.34%)p 0.46(31.65%)d 0.00(0.01%)	<u>LP*(4) U 2</u> s(1.36%)p 4.33(5.90%)d56.34(76.72%)f11.76(16.01%)g 0.01(0.02%)	6.03
<u>LP (1) O 11</u> s(68.34%)p 0.46(31.65%)d 0.00(0.01%)	<u>LP*(5) U 2</u> s(0.15%)p17.06(2.54%)d99.99(88.59%) f58.44(8.70%)g 0.08(0.01%)	6.68
<u>LP (2) O 11</u> s(31.26%)p 2.20(68.73%)d 0.00(0.01%)	<u>LP*(4) U 2</u> s(1.36%)p 4.33(5.90%)d56.34(76.72%)f11.76(16.01%)g 0.01(0.02%)	21.99
<u>LP (2) O 11</u> s(31.26%)p 2.20(68.73%)d 0.00(0.01%)	<u>LP*(5) U 2</u> s(0.15%)p17.06(2.54%)d99.99(88.59%) f58.44(8.70%)g 0.08(0.01%)	12.63

Table ST12: DFT computed NBO second order perturbation analysis for **Cs₂-N₂**, s=1 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<u>BD (1) U 1 - O 11</u> (12.17%) 0.3488* U 1 s(6.81%)p 0.07(0.46%)d 4.23(28.84%) f 9.37(63.83%)g 0.01(0.06%) (87.83%) 0.9372* O 11 s(15.03%)p 5.65(84.93%)d 0.00(0.03%)	<u>LP*(9) U 2</u> s(0.55%)p0.63(0.35%)d99.99(66.64%)f58.68(32.45%)g 0.01(0.00%)	11.15
<u>BD (1) U 1 - N 36</u> (17.95%) 0.4237* U 1 s(8.06%)p 1.36(10.93%)d 4.38(35.33%) f 5.66(45.65%)g 0.00(0.03%) (82.05%) 0.9058* N 36 s(52.66%)p 0.90(47.31%)d 0.00(0.04%)	<u>LP*(9) U 2</u> s(0.55%)p0.63(0.35%)d99.99(66.64%)f58.68(32.45%)g 0.01(0.00%)	10.89
<u>BD (2) U 1 - N 36</u> (12.41%) 0.3522* U 1 s(0.19%)p37.26(6.93%)d87.67(16.32%) f99.99(76.54%)g 0.10(0.02%) (87.59%) 0.9359* N 36 s(21.75%)p 3.59(78.17%)d 0.00(0.08%)	<u>LP*(3) U 2</u> s(0.41%)p0.74(0.31%)d78.71(32.48%)f99.99(66.80%)g 0.02(0.01%)	13.88
<u>BD (1) U 2 - O 11</u> (11.73%) 0.3426* U 2 s(6.20%)p 0.13(0.79%)d 5.24(32.51%) f 9.74(60.43%)g 0.01(0.07%) (88.27%) 0.9395* O 11 s(15.05%)p 5.64(84.91%)d 0.00(0.04%)	<u>LP*(2) U 1</u> s(1.10%)p 0.69(0.76%)d73.24(80.23%) f16.35(17.91%)g 0.01(0.01%)	15.82
<u>BD (1) U 2 - N 36</u> (26.50%) 0.5148* U 2 s(2.81%)p 0.63(1.78%)d 4.01(11.28%) f29.88(84.11%)g 0.01(0.02%) (73.50%) 0.8573* N 36 s(0.36%)p99.99(99.54%)d 0.29(0.10%)	<u>LP*(2) U 1</u> s(1.10%)p 0.69(0.76%)d73.24(80.23%) f16.35(17.91%)g 0.01(0.01%)	11.94

Table ST13: DFT computed NBO second order perturbation analysis for **Cs₄-(N)₂**, s=1 spin state

Donor NBO	Acceptor NBO	E(2) kcal/mol
<u>BD (1) U 2 - N 39</u> (12.21%) 0.3494* U 2 s(12.50%)p 0.62(7.78%)d 4.14(51.70%)f 2.24(28.01%)g 0.00(0.01%) (87.79%) 0.9370* N 39 s(60.86%)p 0.64(39.10%)d 0.00(0.04%)	<u>LP*(3) U 1</u> s(12.50%)p 4.43(55.33%)d 0.44(5.52%)f 2.13(26.61%)g 0.00(0.04%)	21.71
<u>LP (1) O 17</u> s(70.00%)p 0.43(30.00%)d 0.00(0.00%)	<u>LP*(7) U 1</u> s(8.43%)p 6.97(58.72%)d 1.43(12.07%) f 2.45(20.66%)g 0.01(0.12%)	14.24
<u>LP (1) N 38</u> s(6.41%)p14.58(93.55%)d 0.01(0.04%)	<u>LP*(3) U 2</u> s(0.53%)p 6.08(3.23%)d99.99(57.53%) f72.71(38.68%)g 0.03(0.02%)	42.34
<u>LP (2) N 38</u> s(0.07%)p99.99(99.88%)d 0.57(0.04%)	<u>LP*(1) U 1</u> s(0.71%)p2.90(2.06%)d82.90(58.72%)f54.36(38.51%)g 0.01(0.01%)	53.86
<u>LP (2) N 38</u> s(0.07%)p99.99(99.88%)d 0.57(0.04%)	<u>LP*(4) U 2</u> s(0.30%)p 5.67(1.71%)d99.99(69.59%) f94.37(28.39%)g 0.04(0.01%)	36.25
<u>LP (1) N 38</u> s(6.41%)p14.58(93.55%)d 0.01(0.04%)	<u>LP*(3) U 1</u> s(12.50%)p 4.43(55.33%)d 0.44(5.52%)f 2.13(26.61%)g 0.00(0.04%)	8.27

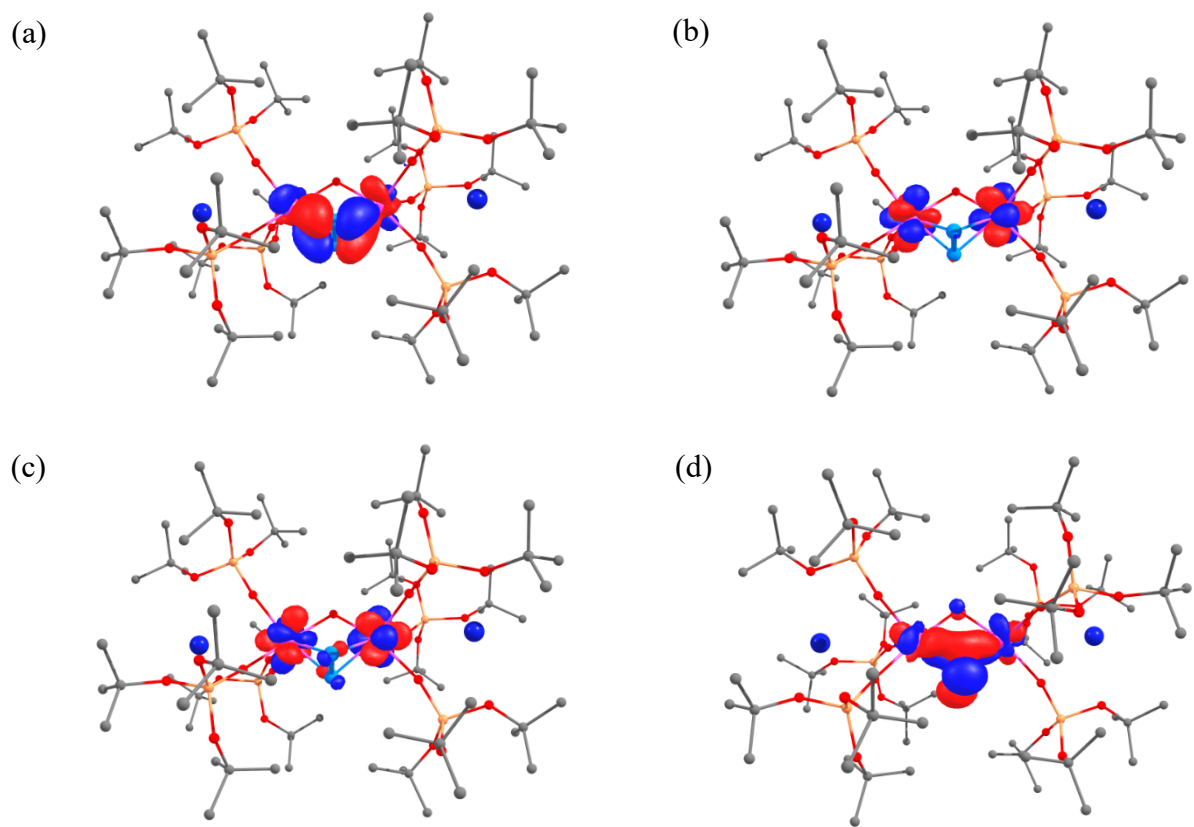


Figure SF2: DFT computed MO's (a) HOMO-3 (b) HOMO-2 (c) HOMO-1 (d) HOMO of K_2-N_2

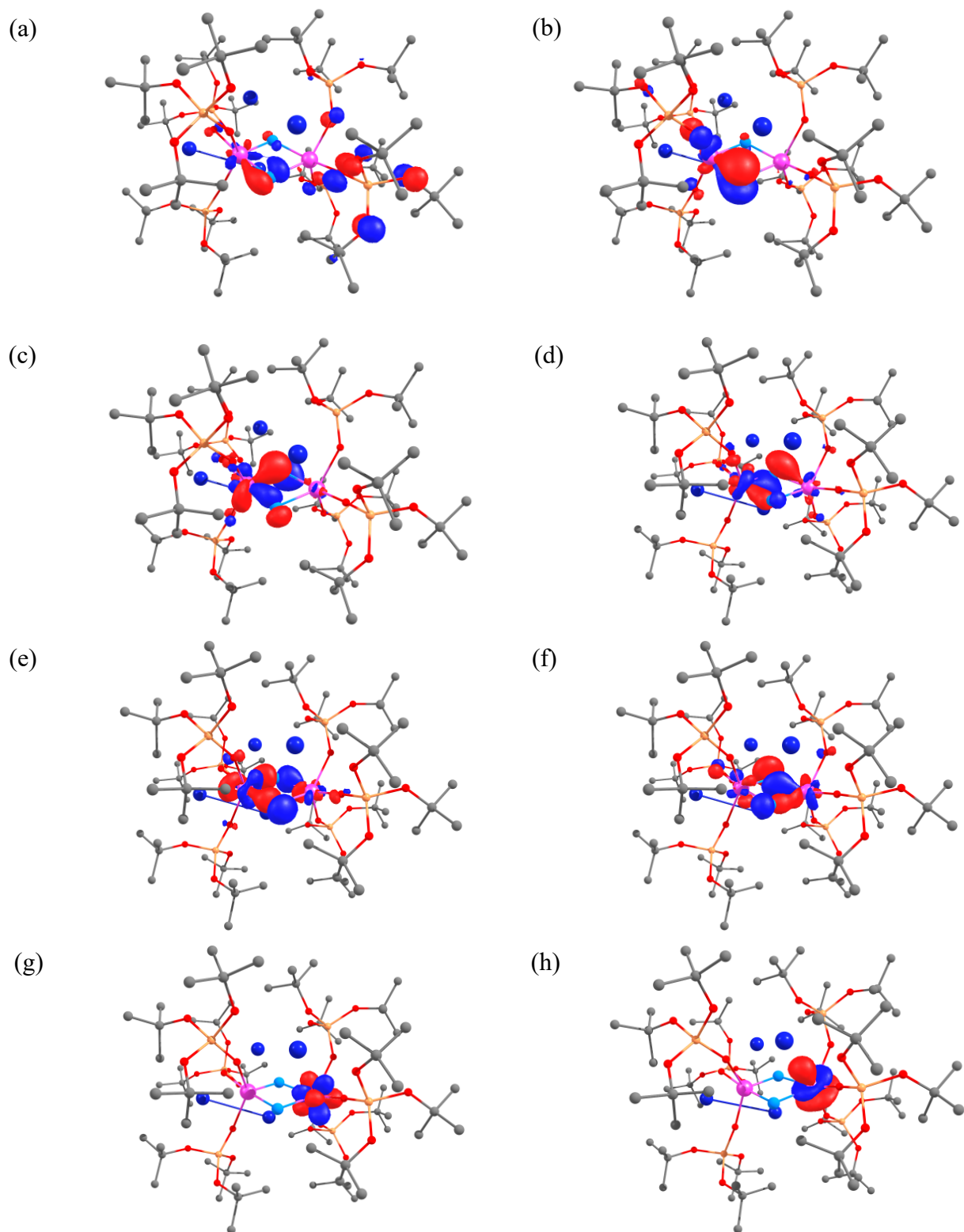


Figure SF3: DFT computed MO's (a) HOMO-8 (b) HOMO-6 (c) HOMO-5 (d) HOMO-4 (e) HOMO-3 (f) HOMO-2 (g) HOMO-1 (h) HOMO of K_4-N_2

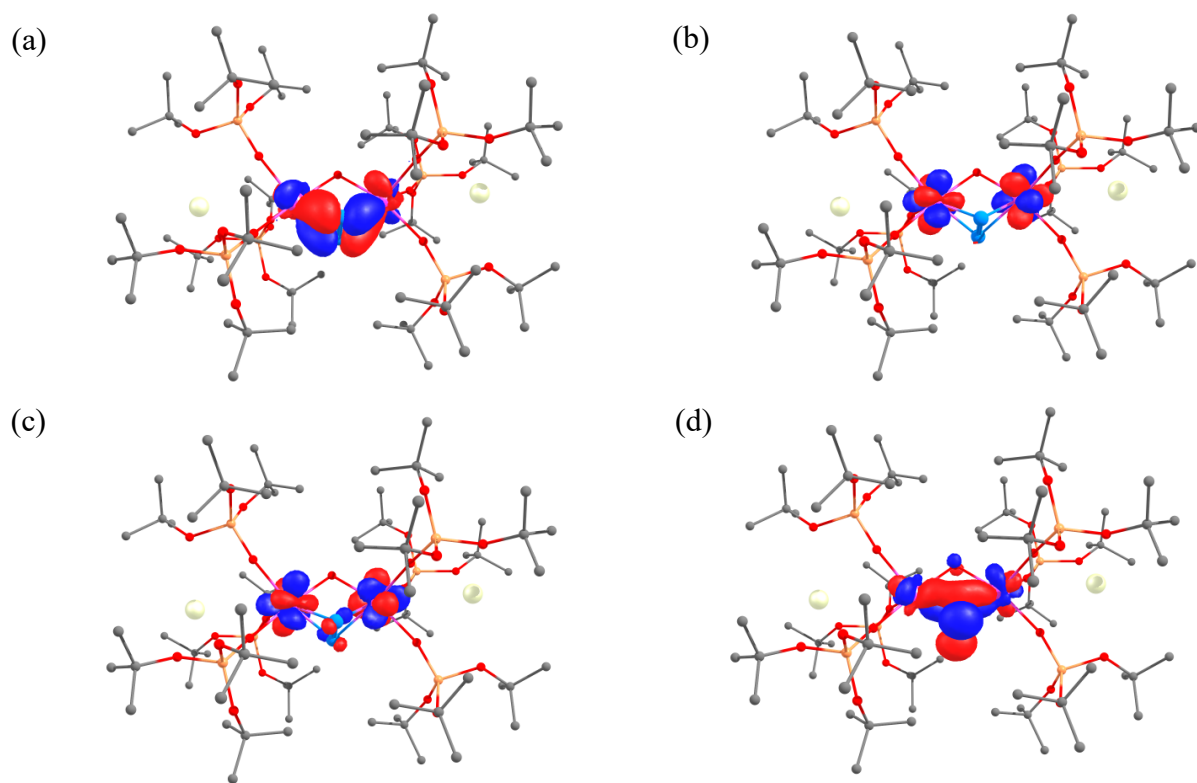


Figure SF4: DFT computed MO's (a) HOMO-3 (b) HOMO-2 (c) HOMO-1 (d) HOMO of $\text{Rb}_2\text{-N}_2$

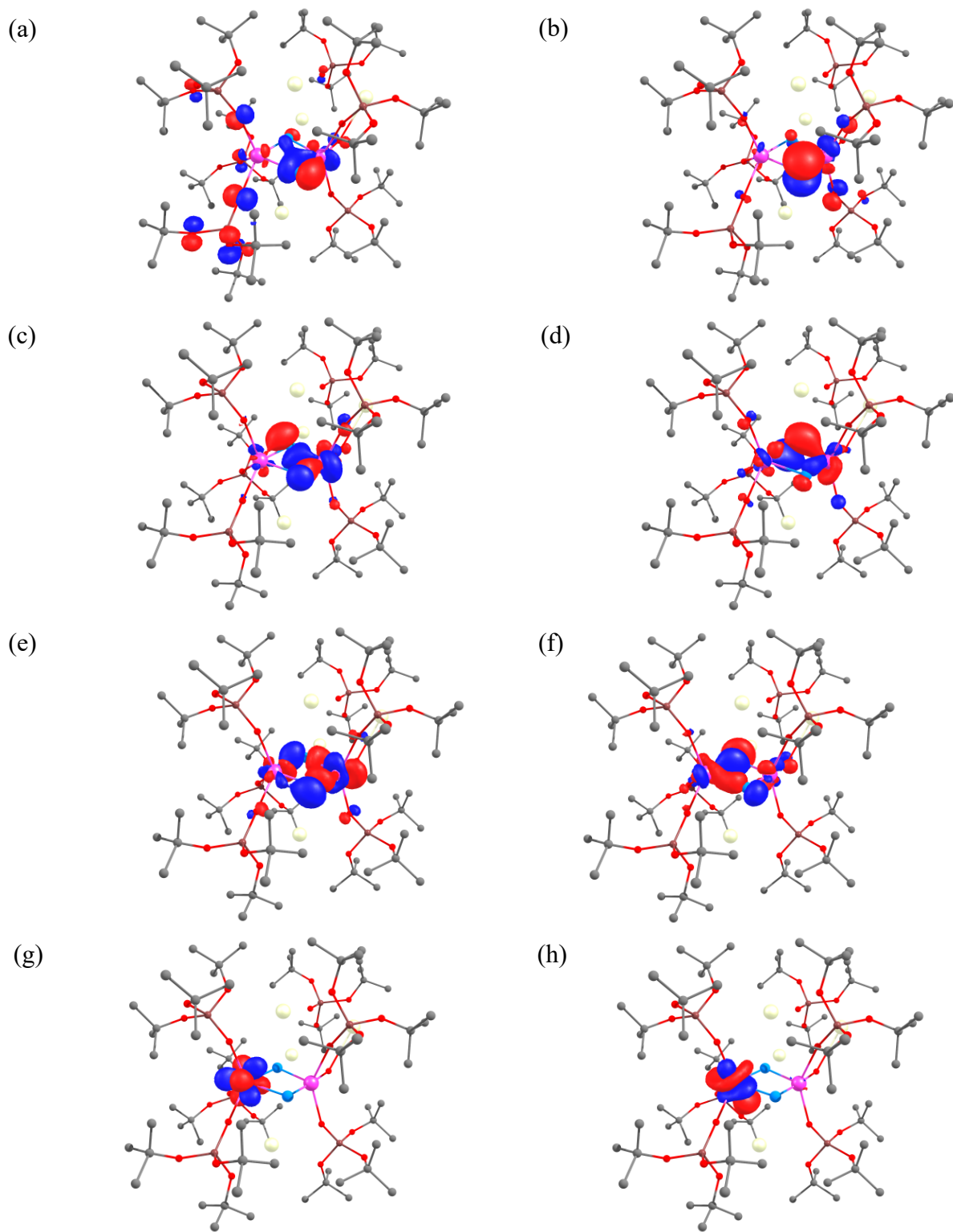


Figure SF5: DFT computed MO's (a) HOMO-8 (b) HOMO-6 (c) HOMO-5 (d) HOMO-4 (e) HOMO-3 (f) HOMO-2 (g) HOMO-1 (h) HOMO of $\text{Rb}_4\text{-N}_2$

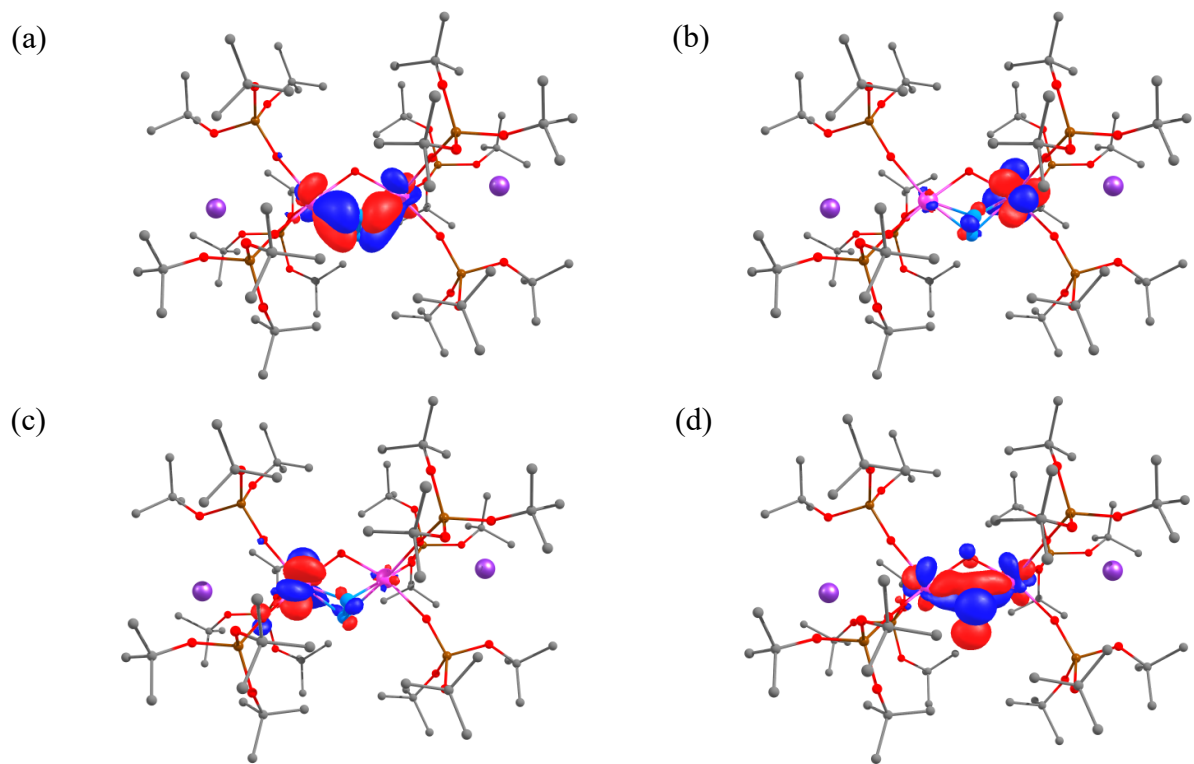


Figure SF6: DFT computed MO's (a) HOMO-3 (b) HOMO-2 (c) HOMO-1 (d) HOMO of $\text{Cs}_2\text{-N}_2$

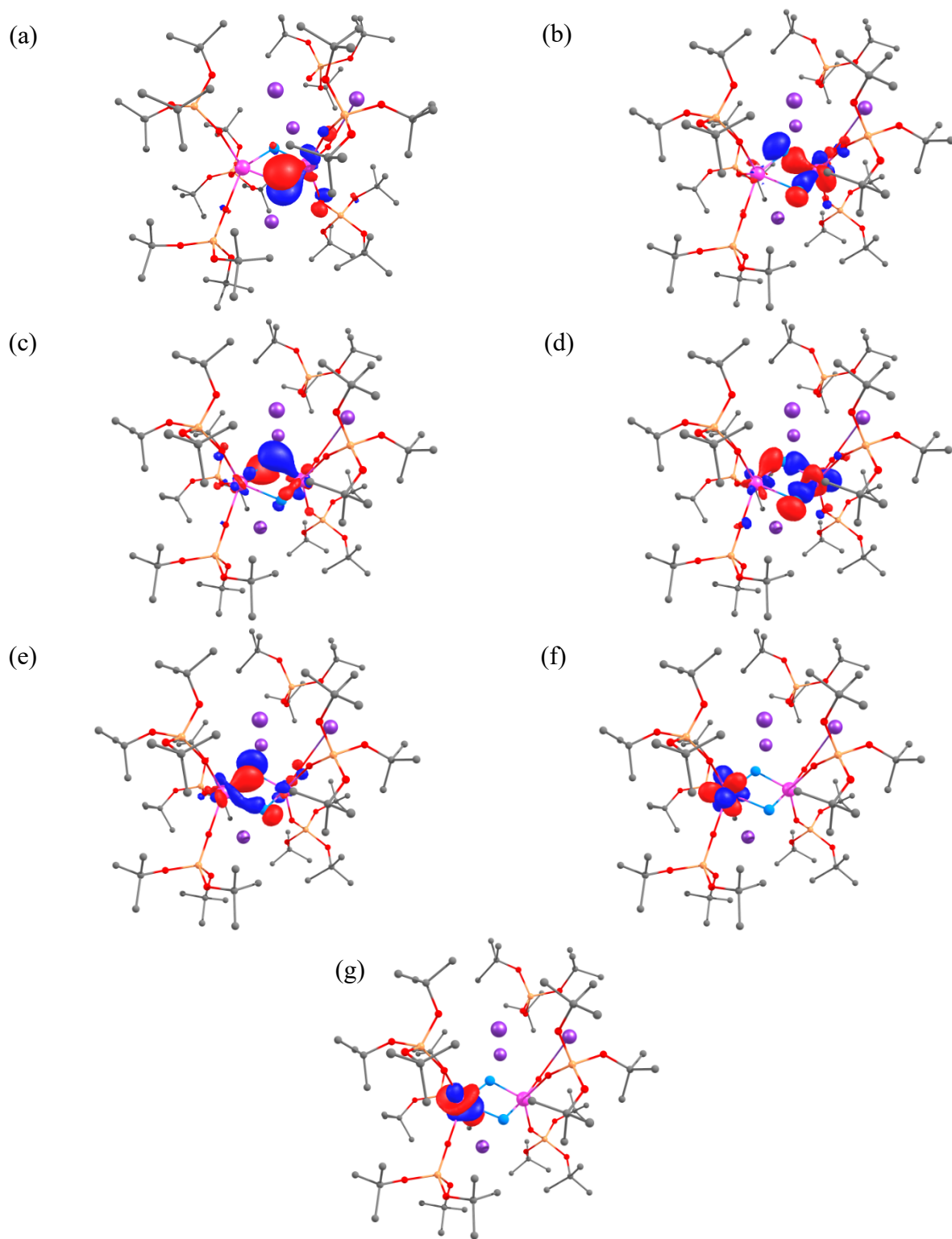


Figure SF7: DFT computed MO's (a) HOMO-6 (b) HOMO-5 (c) HOMO-4 (d) HOMO-3 (e) HOMO-2 (f) HOMO-1 (g) HOMO of $\text{Cs}_4\text{-(N)}_2$

Optimized Coordinates

K₂-2

U	-3.075568000	6.751435000	23.344141000
U	1.184865000	7.177224000	23.486604000
K	-0.718223000	10.025067000	24.478713000
K	-0.547974000	3.875218000	23.555791000
Si	-4.677065000	9.382560000	24.536030000
Si	-3.945450000	6.749225000	19.633129000
Si	-3.744941000	3.300422000	25.004583000
Si	1.639345000	10.567952000	21.701505000
Si	1.678361000	8.746366000	26.974657000
Si	2.777693000	3.887441000	22.311122000
O	-3.138942000	8.861590000	24.478038000
O	-5.442944000	8.068869000	23.760644000
O	-5.316096000	9.697037000	26.049909000
O	-5.032309000	10.747528000	23.645634000
O	-3.438693000	6.598545000	21.178656000
O	-2.712229000	6.469524000	18.528103000
O	-5.217365000	5.679682000	19.430878000
O	-4.568167000	8.247012000	19.220871000
O	-3.366305000	4.643911000	24.165511000
O	-4.709459000	2.201156000	24.189977000
O	1.358584000	9.120715000	22.398495000
O	0.670121000	11.649669000	22.577894000
O	1.149504000	10.725443000	20.115099000
O	3.244015000	11.038820000	21.688067000
O	1.402095000	8.026292000	25.539418000
O	0.682728000	10.118953000	26.953066000
O	3.216190000	9.339828000	27.233409000
O	1.368508000	7.758040000	28.288060000
O	2.007615000	5.081305000	23.109392000
O	1.624843000	2.644748000	22.217470000
O	3.203622000	4.205186000	20.730456000
O	-0.867469000	6.686720000	23.421492000
C	-6.799803000	7.901307000	23.264795000
C	-6.902356000	6.438710000	22.841421000
H	-7.919172000	6.211239000	22.505058000
H	-6.665735000	5.777471000	23.679347000
H	-6.219378000	6.224558000	22.013972000
C	-7.022824000	8.814307000	22.061836000
H	-8.024271000	8.649850000	21.649982000
H	-6.290918000	8.600369000	21.278840000
H	-6.928255000	9.863309000	22.348578000
C	-7.796872000	8.209162000	24.380540000
H	-8.819765000	8.072645000	24.014794000
H	-7.693411000	9.239162000	24.731696000
H	-7.648837000	7.537931000	25.231879000
C	-5.129340000	9.065842000	27.324989000
C	-4.776916000	7.588857000	27.172270000
H	-4.691882000	7.114178000	28.154494000
H	-3.820970000	7.469802000	26.654379000
H	-5.548100000	7.065442000	26.601281000
C	-6.452512000	9.228127000	28.075226000
H	-6.378657000	8.816474000	29.087035000
H	-7.258749000	8.709790000	27.548717000
H	-6.718907000	10.286704000	28.151818000
C	-4.008525000	9.804128000	28.056731000
H	-3.848937000	9.386434000	29.056453000
H	-4.253735000	10.865652000	28.162320000
H	-3.077417000	9.711828000	27.490949000
C	-5.217773000	12.122871000	24.012674000
C	-6.575189000	12.300710000	24.696662000
H	-6.747363000	13.354299000	24.941825000

H	-6.619575000	11.711780000	25.614929000
H	-7.378813000	11.972669000	24.029948000
C	-4.083276000	12.583566000	24.929679000
H	-4.186925000	13.645430000	25.176606000
H	-3.120025000	12.447543000	24.426890000
H	-4.084024000	12.011442000	25.861042000
C	-5.185077000	12.906372000	22.699742000
H	-5.323833000	13.976880000	22.883403000
H	-5.981798000	12.565171000	22.032694000
H	-4.229126000	12.761354000	22.188794000
C	-1.703984000	5.452643000	18.537459000
C	-0.578175000	5.871570000	19.485715000
H	0.239726000	5.143438000	19.478549000
H	-0.956172000	5.973809000	20.506973000
H	-0.175663000	6.841809000	19.178828000
C	-2.292608000	4.105573000	18.960717000
H	-1.525789000	3.325008000	18.919700000
H	-3.114323000	3.816207000	18.299843000
H	-2.682636000	4.160849000	19.981510000
C	-1.183820000	5.372325000	17.100577000
H	-0.385051000	4.628227000	17.014931000
H	-0.787404000	6.342536000	16.786450000
H	-1.991969000	5.096806000	16.416351000
C	-6.180971000	5.589181000	18.370110000
C	-6.705375000	4.152403000	18.410668000
H	-7.479866000	3.997909000	17.652032000
H	-7.133357000	3.933923000	19.393273000
H	-5.892558000	3.443355000	18.224271000
C	-5.551848000	5.877460000	17.005207000
H	-6.299194000	5.759678000	16.213045000
H	-4.725583000	5.190115000	16.804558000
H	-5.164733000	6.898334000	16.964762000
C	-7.318376000	6.574439000	18.650286000
H	-8.095841000	6.499775000	17.881861000
H	-6.932639000	7.596122000	18.667077000
H	-7.772520000	6.359343000	19.622192000
C	-3.896373000	9.482116000	18.924745000
C	-3.370738000	9.438836000	17.487800000
H	-2.876126000	10.381335000	17.229439000
H	-4.198467000	9.286044000	16.787495000
H	-2.660679000	8.618253000	17.366759000
C	-4.958722000	10.574231000	19.060181000
H	-4.538318000	11.554247000	18.810808000
H	-5.341630000	10.610606000	20.083531000
H	-5.795478000	10.376512000	18.382929000
C	-2.760830000	9.725709000	19.917422000
H	-2.259012000	10.674142000	19.705880000
H	-2.011472000	8.931265000	19.859566000
H	-3.152192000	9.760929000	20.938850000
O	-2.220843000	2.621375000	25.354085000
C	-1.854768000	1.571884000	26.271915000
C	-2.019798000	2.053904000	27.714420000
H	-1.679253000	1.284456000	28.415514000
H	-3.061830000	2.295743000	27.924624000
H	-1.425134000	2.957404000	27.878787000
C	-2.680572000	0.310203000	26.018404000
H	-2.372437000	-0.487808000	26.702242000
H	-2.537482000	-0.044731000	24.993402000
H	-3.745323000	0.497828000	26.166938000
C	-0.378051000	1.281943000	25.997312000
H	0.232831000	2.173070000	26.177321000
H	-0.232018000	0.954794000	24.962956000
H	-0.008929000	0.489032000	26.655454000
C	-4.753429000	1.781704000	22.819164000

C	-3.360812000	1.813417000	22.187741000
H	-3.391513000	1.429925000	21.163359000
H	-2.663590000	1.200668000	22.767435000
H	-2.998387000	2.845280000	22.148231000
C	-5.293522000	0.350299000	22.837229000
H	-5.390708000	-0.041926000	21.819793000
H	-6.279215000	0.324984000	23.311385000
H	-4.625629000	-0.307257000	23.401673000
C	-5.701804000	2.701996000	22.053502000
H	-5.796739000	2.382194000	21.011406000
H	-5.331567000	3.729696000	22.058096000
H	-6.696671000	2.684399000	22.509360000
O	-4.510375000	3.529616000	26.467637000
C	-5.853944000	3.304511000	26.929351000
C	-6.141617000	1.803829000	27.016754000
H	-5.437883000	1.316922000	27.699430000
H	-6.058092000	1.340920000	26.031263000
H	-7.153284000	1.632155000	27.399896000
C	-6.858418000	3.986206000	26.001917000
H	-6.649689000	5.057720000	25.939072000
H	-7.879567000	3.858279000	26.376341000
H	-6.802529000	3.556801000	24.998563000
C	-5.914695000	3.924768000	28.326279000
H	-5.694847000	4.993853000	28.279704000
H	-5.182108000	3.451971000	28.987565000
H	-6.909342000	3.792654000	28.764423000
C	0.337070000	13.015497000	22.246506000
C	-0.031253000	13.688285000	23.569973000
H	-0.300634000	14.737307000	23.411458000
H	0.809883000	13.650143000	24.268945000
H	-0.892516000	13.195415000	24.034220000
C	-0.861616000	13.006564000	21.297740000
H	-1.187435000	14.027506000	21.070967000
H	-1.701887000	12.469608000	21.749120000
H	-0.593852000	12.501765000	20.367278000
C	1.514850000	13.752933000	21.608663000
H	1.232175000	14.789357000	21.396107000
H	1.809697000	13.278306000	20.670839000
H	2.379815000	13.762433000	22.276314000
C	1.815362000	10.348544000	18.896551000
C	0.711481000	10.190482000	17.851662000
H	1.136198000	9.931263000	16.876360000
H	0.151833000	11.124752000	17.745676000
H	0.011198000	9.405018000	18.147180000
C	2.777161000	11.466366000	18.486628000
H	3.281835000	11.216538000	17.547033000
H	3.530772000	11.620853000	19.262333000
H	2.229840000	12.402925000	18.338031000
C	2.568047000	9.030513000	19.075596000
H	3.008971000	8.708153000	18.126685000
H	1.887573000	8.248542000	19.424929000
H	3.374709000	9.144351000	19.804899000
C	4.266191000	11.011801000	22.693922000
C	3.693777000	11.338117000	24.071577000
H	4.489208000	11.367507000	24.821693000
H	2.970695000	10.581760000	24.388056000
H	3.197987000	12.312742000	24.060537000
C	4.922718000	9.630352000	22.693830000
H	5.746832000	9.589287000	23.414050000
H	5.322516000	9.399584000	21.701682000
H	4.193427000	8.858995000	22.959237000
C	5.284999000	12.075028000	22.276252000
H	6.127871000	12.102121000	22.974498000
H	4.821330000	13.065743000	22.255996000

H	5.671867000	11.859005000	21.275778000
C	0.681000000	11.244480000	27.860095000
C	-0.637417000	11.978249000	27.610238000
H	-0.727188000	12.846020000	28.271333000
H	-1.490121000	11.319304000	27.793789000
H	-0.688740000	12.346883000	26.579659000
C	1.855667000	12.167982000	27.532883000
H	1.839061000	13.052300000	28.179283000
H	1.796591000	12.502160000	26.492476000
H	2.801654000	11.642137000	27.667673000
C	0.744224000	10.777120000	29.314531000
H	0.689566000	11.638179000	29.988939000
H	1.675289000	10.242974000	29.516031000
H	-0.089249000	10.106978000	29.542725000
C	4.398197000	8.727649000	27.775388000
C	5.561475000	9.627428000	27.354769000
H	6.506188000	9.253605000	27.762867000
H	5.408087000	10.647182000	27.720714000
H	5.644835000	9.660946000	26.264846000
C	4.292970000	8.682979000	29.301422000
H	5.197924000	8.246915000	29.738029000
H	3.430253000	8.085668000	29.604186000
H	4.176459000	9.694568000	29.703625000
C	4.587327000	7.325787000	27.200780000
H	5.516744000	6.879559000	27.569937000
H	4.637151000	7.368219000	26.109301000
H	3.757566000	6.674807000	27.488605000
C	0.413546000	6.700326000	28.459379000
C	0.269592000	6.518052000	29.971523000
H	-0.427662000	5.705890000	30.201247000
H	-0.104109000	7.437191000	30.432465000
H	1.238452000	6.280348000	30.421159000
C	0.969478000	5.425649000	27.821913000
H	0.279217000	4.588076000	27.964888000
H	1.929498000	5.158970000	28.274979000
H	1.120711000	5.576764000	26.748899000
C	-0.934717000	7.067327000	27.840305000
H	-1.673088000	6.283023000	28.034897000
H	-0.848066000	7.186316000	26.755940000
H	-1.308033000	8.002872000	28.266535000
C	1.668079000	1.450951000	21.403226000
C	1.155990000	1.796745000	20.004836000
H	1.145843000	0.909360000	19.362742000
H	1.793967000	2.558455000	19.552169000
H	0.135367000	2.187516000	20.061640000
C	0.733179000	0.446648000	22.077721000
H	0.676831000	-0.479572000	21.496930000
H	-0.281517000	0.850960000	22.157024000
H	1.092068000	0.199797000	23.081660000
C	3.078926000	0.867276000	21.329590000
H	3.069877000	-0.053888000	20.737429000
H	3.456048000	0.631475000	22.327972000
H	3.768892000	1.570989000	20.860064000
O	4.185996000	3.351105000	23.038894000
C	4.525991000	3.155024000	24.418054000
C	3.315023000	2.686185000	25.226370000
H	3.599090000	2.490003000	26.265553000
H	2.899724000	1.767343000	24.802645000
H	2.538095000	3.456731000	25.225764000
C	5.620332000	2.085969000	24.432796000
H	5.972581000	1.903554000	25.453278000
H	6.472170000	2.407233000	23.826145000
H	5.245448000	1.143673000	24.022512000
C	5.063713000	4.472518000	24.974712000

H	5.375358000	4.360770000	26.018350000
H	4.291801000	5.244760000	24.925018000
H	5.928117000	4.805571000	24.391980000
C	4.365712000	4.842882000	20.170967000
C	5.515523000	3.834693000	20.108570000
H	6.405341000	4.293652000	19.664420000
H	5.234863000	2.975466000	19.490818000
H	5.763973000	3.478407000	21.110744000
C	4.765587000	6.063519000	20.999302000
H	5.627969000	6.565963000	20.548918000
H	5.038382000	5.768937000	22.016809000
H	3.942907000	6.783207000	21.048937000
C	3.958554000	5.266608000	18.759634000
H	4.794211000	5.750301000	18.243576000
H	3.120212000	5.967115000	18.797457000
H	3.652198000	4.393667000	18.175095000

Rb₂-2

U	6.554440000	9.041519000	8.631160000
U	7.427076000	11.667680000	5.389178000
Rb	5.119266000	8.750981000	4.736982000
Rb	8.001289000	12.452616000	9.330943000
Si	9.508247000	8.796639000	10.889156000
Si	4.716970000	11.381592000	11.056358000
Si	4.598403000	6.031196000	7.419164000
Si	3.968959000	12.475719000	3.897542000
Si	8.556004000	9.244701000	2.650648000
Si	9.541844000	14.595928000	6.563993000
O	8.538784000	8.716543000	9.581956000
O	10.999693000	8.067187000	10.655945000
O	9.669058000	10.443811000	11.245150000
O	8.914555000	8.091409000	12.282911000
O	5.591472000	10.391591000	10.099703000
O	5.350416000	12.925903000	10.775265000
O	4.902184000	11.164862000	12.700781000
O	3.070200000	11.302460000	10.787229000
O	5.569165000	7.340454000	7.484818000
O	3.390013000	5.957004000	8.571133000
O	3.809232000	6.177471000	5.927969000
O	5.392929000	4.561964000	7.557472000
O	5.434970000	12.062562000	4.477278000
O	3.024363000	13.433402000	4.890010000
O	3.134616000	11.011473000	3.752355000
O	4.014259000	13.308505000	2.447060000
O	8.197551000	10.144063000	3.961486000
O	7.212746000	8.236928000	2.433213000
O	8.722702000	10.076735000	1.212492000
O	9.977766000	8.372364000	2.799211000
O	8.814998000	13.143079000	6.419197000
O	8.887879000	15.833779000	5.655479000
O	11.171598000	14.602496000	6.176195000
O	9.294008000	15.022832000	8.184504000
O	6.890360000	10.480106000	7.076171000
C	11.844046000	8.020105000	9.499966000
C	11.362247000	6.892013000	8.586047000
H	11.379341000	5.937540000	9.121551000
H	12.007894000	6.799293000	7.705908000
H	10.338946000	7.088971000	8.255994000
C	11.829035000	9.358421000	8.762281000
H	10.827517000	9.571644000	8.376736000
H	12.525526000	9.344322000	7.917876000
H	12.122781000	10.166589000	9.437916000
C	13.249905000	7.717832000	10.022781000
H	13.590904000	8.515042000	10.690018000

H	13.962538000	7.628500000	9.196270000
H	13.252546000	6.778898000	10.584581000
C	10.213676000	11.035395000	12.443811000
C	11.475731000	10.307294000	12.909283000
H	11.258755000	9.264376000	13.148473000
H	11.876224000	10.789452000	13.807406000
H	12.247312000	10.327552000	12.134751000
C	10.568191000	12.477748000	12.076202000
H	11.258074000	12.501564000	11.226647000
H	11.043420000	12.986972000	12.920518000
H	9.669684000	13.049245000	11.820170000
C	9.146569000	11.019444000	13.539263000
H	9.504066000	11.538613000	14.435463000
H	8.894751000	9.989867000	13.799676000
H	8.234477000	11.514384000	13.192692000
C	8.951824000	6.726493000	12.732779000
C	10.307647000	6.449714000	13.386457000
H	11.112551000	6.602946000	12.664292000
H	10.354990000	5.420329000	13.757947000
H	10.463885000	7.123766000	14.234874000
C	7.833049000	6.601144000	13.767616000
H	7.985719000	7.314463000	14.583162000
H	7.809631000	5.592078000	14.192277000
H	6.861883000	6.807391000	13.309444000
C	8.705249000	5.760757000	11.573428000
H	7.750730000	5.981627000	11.087834000
H	8.675726000	4.727684000	11.936313000
H	9.501096000	5.838431000	10.828561000
C	5.095223000	14.136148000	11.519510000
C	5.298410000	15.282898000	10.529281000
H	6.301848000	15.248421000	10.094303000
H	5.179057000	16.252190000	11.023687000
H	4.572873000	15.219092000	9.712930000
C	6.108031000	14.219794000	12.664134000
H	5.982315000	13.366440000	13.334370000
H	5.977483000	15.145169000	13.235247000
H	7.132856000	14.207032000	12.276481000
C	3.671165000	14.187876000	12.073967000
H	2.936641000	14.116918000	11.268488000
H	3.514061000	15.134652000	12.601453000
H	3.493841000	13.369668000	12.774760000
C	4.331433000	10.181619000	13.580184000
C	5.266663000	10.115026000	14.787730000
H	6.266200000	9.798419000	14.478276000
H	4.889094000	9.406098000	15.531859000
H	5.347263000	11.099098000	15.259965000
C	2.937083000	10.644814000	14.007780000
H	2.997180000	11.608583000	14.523731000
H	2.482113000	9.920982000	14.692651000
H	2.293046000	10.757870000	13.132538000
C	4.260407000	8.821058000	12.889125000
H	3.578169000	8.858986000	12.034875000
H	3.896978000	8.054740000	13.581702000
H	5.251626000	8.528553000	12.532209000
C	2.325678000	11.268053000	9.557152000
C	1.028029000	12.032396000	9.828993000
H	0.506256000	11.599997000	10.688038000
H	0.363052000	11.988689000	8.960435000
H	1.234962000	13.083669000	10.049116000
C	2.010353000	9.808983000	9.229837000
H	1.400967000	9.735592000	8.322951000
H	1.454347000	9.347836000	10.051770000
H	2.928265000	9.236029000	9.071067000
C	3.101226000	11.926879000	8.418699000

H	3.385716000	12.945540000	8.696179000
H	2.497897000	11.978034000	7.508693000
H	4.016255000	11.372708000	8.188009000
C	3.364032000	5.364111000	9.882224000
C	4.674796000	5.628613000	10.622320000
H	5.510440000	5.155099000	10.099976000
H	4.632028000	5.223957000	11.638781000
H	4.864283000	6.704586000	10.694115000
C	2.196034000	6.028187000	10.610959000
H	2.360538000	7.104814000	10.698093000
H	2.079450000	5.610873000	11.616351000
H	1.264400000	5.866772000	10.060061000
C	3.116793000	3.858479000	9.761080000
H	2.154839000	3.666027000	9.275107000
H	3.090401000	3.394242000	10.752884000
H	3.909436000	3.389768000	9.173917000
C	2.632108000	5.479420000	5.469360000
C	1.397850000	6.222048000	5.985144000
H	1.397881000	6.230103000	7.077185000
H	0.477467000	5.745480000	5.630999000
H	1.401235000	7.258936000	5.633410000
C	2.613905000	4.022235000	5.932347000
H	3.499026000	3.488070000	5.576907000
H	1.726377000	3.516939000	5.536994000
H	2.588097000	3.958289000	7.020938000
C	2.686539000	5.520419000	3.941778000
H	2.710741000	6.552850000	3.579436000
H	1.804406000	5.037316000	3.509615000
H	3.577702000	5.003002000	3.574644000
C	6.615901000	4.085258000	6.982361000
C	7.792419000	4.607012000	7.807946000
H	7.809360000	5.700001000	7.801671000
H	8.744022000	4.240759000	7.408440000
H	7.706664000	4.270922000	8.845518000
C	6.545435000	2.559062000	7.066286000
H	6.422485000	2.243043000	8.106498000
H	7.460023000	2.103489000	6.672990000
H	5.694438000	2.181573000	6.491484000
C	6.740223000	4.528448000	5.524811000
H	6.787676000	5.619284000	5.461123000
H	5.883182000	4.180814000	4.941284000
H	7.652686000	4.121875000	5.076973000
C	3.046360000	14.862145000	5.071327000
C	2.256535000	15.528908000	3.942220000
H	2.705364000	15.294898000	2.974932000
H	2.241765000	16.616221000	4.074269000
H	1.220678000	15.174114000	3.942589000
C	4.484188000	15.379265000	5.105763000
H	4.979982000	15.200330000	4.147390000
H	5.056245000	14.877264000	5.891846000
H	4.502168000	16.456219000	5.302141000
C	2.360292000	15.126398000	6.411268000
H	1.349031000	14.708274000	6.410987000
H	2.288594000	16.202327000	6.600865000
H	2.921417000	14.665552000	7.227657000
C	1.728281000	10.819338000	3.493641000
C	1.174346000	11.861400000	2.521136000
H	1.279525000	12.868842000	2.928523000
H	0.111087000	11.671533000	2.340182000
H	1.699102000	11.822322000	1.563238000
C	0.974813000	10.880993000	4.823754000
H	1.377207000	10.141422000	5.523811000
H	-0.090725000	10.672003000	4.679732000
H	1.084590000	11.873087000	5.267153000

C	1.605853000	9.426543000	2.875490000
H	1.975269000	8.664588000	3.569082000
H	2.182515000	9.364885000	1.947112000
H	0.561548000	9.189121000	2.649726000
C	4.825912000	13.145018000	1.277098000
C	5.053603000	11.666999000	0.965940000
H	5.594249000	11.176839000	1.780070000
H	5.650682000	11.552990000	0.056349000
H	4.097818000	11.155027000	0.818744000
C	4.053582000	13.815536000	0.138664000
H	3.088189000	13.323818000	-0.013334000
H	4.618996000	13.764915000	-0.797506000
H	3.866871000	14.867895000	0.373129000
C	6.157504000	13.860405000	1.502990000
H	5.985472000	14.911779000	1.753123000
H	6.781978000	13.819686000	0.605008000
H	6.701641000	13.390389000	2.327524000
C	6.924430000	7.371688000	1.313554000
C	5.896775000	6.360527000	1.822715000
H	4.975531000	6.864898000	2.132806000
H	6.293977000	5.799299000	2.673889000
H	5.630648000	5.648867000	1.034799000
C	6.321737000	8.200230000	0.177566000
H	5.418134000	8.713522000	0.520148000
H	6.052082000	7.557294000	-0.667393000
H	7.035549000	8.953403000	-0.160717000
C	8.173906000	6.632057000	0.833274000
H	8.935837000	7.331007000	0.482243000
H	7.914495000	5.961659000	0.007112000
H	8.606291000	6.033194000	1.639345000
C	9.862940000	10.742127000	0.642712000
C	9.297504000	11.718618000	-0.389087000
H	8.706718000	11.182622000	-1.138189000
H	10.104811000	12.250854000	-0.902691000
H	8.651303000	12.453836000	0.097859000
C	10.757246000	9.707927000	-0.045460000
H	11.124634000	8.980975000	0.682279000
H	11.614133000	10.194806000	-0.523625000
H	10.194735000	9.175429000	-0.819304000
C	10.642762000	11.502452000	1.715036000
H	9.995187000	12.224360000	2.220807000
H	11.479810000	12.047463000	1.265852000
H	11.045877000	10.811912000	2.460160000
C	10.560053000	7.720990000	3.936330000
C	11.535914000	6.688167000	3.368932000
H	11.005562000	5.954053000	2.755189000
H	12.053178000	6.157728000	4.175060000
H	12.286300000	7.178583000	2.741395000
C	11.311451000	8.759736000	4.768029000
H	12.071932000	9.256787000	4.157901000
H	11.809180000	8.289528000	5.621708000
H	10.616826000	9.514979000	5.144575000
C	9.487760000	7.031807000	4.778229000
H	8.789103000	7.768915000	5.186271000
H	9.940573000	6.494219000	5.616965000
H	8.927543000	6.314814000	4.172158000
C	9.216949000	16.346553000	4.353055000
C	7.989520000	17.139326000	3.903106000
H	7.114600000	16.486770000	3.842879000
H	8.158239000	17.589733000	2.919534000
H	7.770706000	17.939924000	4.616222000
C	9.501677000	15.209247000	3.372091000
H	10.368393000	14.628325000	3.697739000
H	9.710492000	15.607608000	2.373589000

H	8.636385000	14.543493000	3.296166000
C	10.430928000	17.272068000	4.463506000
H	10.221237000	18.094922000	5.154523000
H	10.675608000	17.704562000	3.487325000
H	11.298178000	16.717248000	4.828888000
C	12.206383000	13.641359000	6.418581000
C	12.171184000	12.592662000	5.306647000
H	11.206101000	12.079249000	5.301779000
H	12.961590000	11.847247000	5.443672000
H	12.314605000	13.067643000	4.331361000
C	13.521281000	14.422262000	6.371268000
H	13.628929000	14.923312000	5.404627000
H	14.377040000	13.753815000	6.511219000
H	13.544599000	15.184477000	7.155630000
C	12.033077000	12.978794000	7.785410000
H	12.010387000	13.731024000	8.579063000
H	12.859274000	12.289812000	7.985513000
H	11.101191000	12.406673000	7.813928000
C	9.525275000	16.297796000	8.820877000
C	10.857738000	16.910485000	8.387418000
H	11.690025000	16.241334000	8.622354000
H	11.021475000	17.858457000	8.910906000
H	10.870714000	17.105916000	7.313686000
C	9.564286000	16.010047000	10.322632000
H	8.618501000	15.573232000	10.659658000
H	9.723308000	16.932074000	10.890743000
H	10.376451000	15.316308000	10.560944000
C	8.369037000	17.243879000	8.490162000
H	8.320154000	17.415907000	7.413517000
H	8.496901000	18.203667000	9.002264000
H	7.416581000	16.810695000	8.808961000

Cs₂-2

U	4.349396000	12.111817000	37.718734000
U	8.122904000	12.786566000	35.775334000
Cs	6.690205000	14.647510000	39.284971000
Cs	6.024380000	9.725028000	34.729757000
Si	2.995118000	15.634282000	38.366544000
Si	5.700953000	11.250957000	41.195315000
Si	2.408879000	9.184358000	36.231498000
Si	9.694323000	15.945522000	37.366992000
Si	9.976277000	9.399289000	35.711291000
Si	7.015715000	12.681084000	32.090356000
O	6.270744000	12.367168000	36.767377000
O	3.447081000	14.133452000	37.916581000
O	3.599271000	16.675733000	37.208306000
O	3.714352000	16.090519000	39.825486000
O	1.350325000	15.831980000	38.602322000
O	4.957151000	11.706731000	39.817222000
O	7.086325000	12.217187000	41.291651000
O	4.877033000	11.586093000	42.612257000
O	6.044623000	9.617924000	41.266020000
O	3.439447000	10.413705000	36.532466000
O	1.933451000	8.286593000	37.556249000
O	0.971232000	9.646393000	35.504176000
O	3.278485000	8.120650000	35.247514000
O	8.948309000	14.547772000	36.979986000
O	9.110485000	17.301370000	36.582903000
O	11.346161000	15.983452000	37.108065000
O	9.312439000	16.218897000	38.996049000
O	9.175411000	10.818353000	35.762951000
O	10.485963000	8.786909000	37.182004000
O	11.357630000	9.420618000	34.768627000
O	8.849224000	8.269813000	35.146469000

O	7.399488000	12.783701000	33.671731000
O	8.289966000	12.671624000	31.011620000
O	6.288286000	11.162996000	31.903424000
O	6.015912000	13.916815000	31.566881000
C	3.666228000	18.108942000	37.157886000
C	2.394879000	18.764165000	37.700596000
H	1.517871000	18.443972000	37.131806000
H	2.473413000	19.853711000	37.621738000
H	2.231959000	18.509046000	38.750028000
C	3.838104000	18.461730000	35.679690000
H	4.742329000	17.993801000	35.281857000
H	3.920264000	19.545168000	35.544361000
H	2.981367000	18.104032000	35.100338000
C	4.887032000	18.572185000	37.954804000
H	5.794760000	18.111053000	37.554119000
H	4.780070000	18.287545000	39.004614000
H	5.003169000	19.659784000	37.896022000
C	3.187710000	16.059266000	41.167548000
C	4.392452000	16.243333000	42.093248000
H	5.072081000	15.387803000	42.027368000
H	4.069266000	16.322193000	43.136041000
H	4.938495000	17.156759000	41.835225000
C	2.209189000	17.219715000	41.359132000
H	1.366191000	17.119308000	40.672380000
H	2.709029000	18.175248000	41.169403000
H	1.826890000	17.234446000	42.385487000
C	2.507704000	14.720873000	41.453104000
H	1.649689000	14.583062000	40.791487000
H	2.150152000	14.693136000	42.487874000
H	3.205901000	13.891320000	41.307722000
C	0.241120000	15.351070000	37.827268000
C	-0.927410000	16.284167000	38.149282000
H	-1.132896000	16.278100000	39.224110000
H	-1.833736000	15.967896000	37.622783000
H	-0.693744000	17.310501000	37.851553000
C	-0.080869000	13.924957000	38.275969000
H	0.778115000	13.271856000	38.100308000
H	-0.943036000	13.527467000	37.729957000
H	-0.316703000	13.906668000	39.344587000
C	0.559199000	15.390358000	36.332093000
H	0.804221000	16.407583000	36.014968000
H	-0.300911000	15.045122000	35.749212000
H	1.411307000	14.744200000	36.102447000
C	8.001807000	12.360935000	42.398282000
C	9.343578000	12.763812000	41.783417000
H	9.258517000	13.695204000	41.215437000
H	9.703802000	11.983725000	41.106416000
H	10.095688000	12.916407000	42.564499000
C	7.478815000	13.462329000	43.323944000
H	7.405100000	14.416621000	42.790942000
H	8.152680000	13.608551000	44.174810000
H	6.486838000	13.196120000	43.695618000
C	8.169550000	11.056162000	43.177286000
H	8.890720000	11.198830000	43.989041000
H	8.536873000	10.259174000	42.526630000
H	7.221268000	10.733710000	43.611865000
C	3.828342000	10.867087000	43.282572000
C	3.206662000	11.861344000	44.264392000
H	2.409618000	11.384932000	44.844489000
H	2.784833000	12.715672000	43.728992000
H	3.965507000	12.231402000	44.960706000
C	4.426023000	9.682488000	44.045489000
H	4.932118000	9.003234000	43.356502000
H	3.641990000	9.132534000	44.577140000

H	5.153189000	10.033599000	44.784956000
C	2.783630000	10.390081000	42.275084000
H	2.380367000	11.236836000	41.712877000
H	1.956079000	9.884715000	42.783807000
H	3.229910000	9.684905000	41.568214000
C	6.569614000	8.734232000	40.260180000
C	7.325079000	7.641777000	41.020131000
H	8.165463000	8.066933000	41.576482000
H	7.716792000	6.889124000	40.328463000
H	6.659354000	7.145808000	41.733053000
C	5.395530000	8.121106000	39.497882000
H	4.729098000	7.595132000	40.188359000
H	5.747633000	7.399756000	38.752827000
H	4.814400000	8.890890000	38.983010000
C	7.514665000	9.471693000	39.313698000
H	6.986299000	10.238695000	38.738122000
H	7.986528000	8.780566000	38.610346000
H	8.308822000	9.966922000	39.878922000
C	0.867609000	8.489459000	38.500441000
C	0.769747000	9.963427000	38.893745000
H	1.720208000	10.313211000	39.308877000
H	-0.006110000	10.110423000	39.652310000
H	0.514861000	10.576470000	38.024554000
C	-0.452935000	8.008903000	37.893367000
H	-1.274357000	8.147396000	38.604691000
H	-0.396139000	6.943240000	37.648767000
H	-0.676587000	8.565590000	36.980925000
C	1.227624000	7.634226000	39.715253000
H	1.329589000	6.584750000	39.422502000
H	0.450208000	7.704315000	40.482886000
H	2.175346000	7.963800000	40.148112000
C	0.687107000	10.496347000	34.387853000
C	1.719727000	10.312522000	33.275546000
H	2.713053000	10.609288000	33.624466000
H	1.463970000	10.934919000	32.411673000
H	1.761582000	9.269283000	32.951789000
C	0.668665000	11.948744000	34.861560000
H	-0.058307000	12.073249000	35.668849000
H	0.396270000	12.625056000	34.044458000
H	1.653577000	12.239415000	35.237194000
C	-0.700680000	10.082886000	33.892398000
H	-0.698216000	9.036995000	33.571122000
H	-1.014876000	10.704804000	33.047856000
H	-1.437060000	10.191596000	34.694234000
C	2.999060000	6.737547000	34.950055000
C	1.499191000	6.473843000	34.809881000
H	1.327362000	5.422350000	34.556461000
H	1.064930000	7.092211000	34.019667000
H	0.979141000	6.692590000	35.743832000
C	3.592615000	5.873964000	36.064967000
H	4.667914000	6.058951000	36.157641000
H	3.446691000	4.808859000	35.854657000
H	3.117237000	6.117092000	37.017675000
C	3.692520000	6.444412000	33.618439000
H	4.771284000	6.614448000	33.694243000
H	3.295501000	7.086966000	32.826893000
H	3.541135000	5.400991000	33.324153000
C	9.481137000	17.904787000	35.332908000
C	9.796096000	16.839494000	34.284804000
H	10.651511000	16.232926000	34.595203000
H	10.038253000	17.305627000	33.324278000
H	8.933729000	16.183821000	34.134711000
C	10.691998000	18.813207000	35.557954000
H	11.540090000	18.227657000	35.920765000

H	10.455603000	19.585381000	36.297300000
H	10.980889000	19.312337000	34.626714000
C	8.270997000	18.731479000	34.896917000
H	8.475770000	19.254222000	33.956897000
H	8.023255000	19.476627000	35.658996000
H	7.400607000	18.085246000	34.752378000
C	12.386412000	15.043325000	37.409173000
C	13.667650000	15.867767000	37.554153000
H	13.862484000	16.430296000	36.636076000
H	14.527098000	15.218361000	37.749923000
H	13.578051000	16.581265000	38.378298000
C	12.519339000	14.074613000	36.234750000
H	11.600839000	13.494979000	36.110829000
H	13.347046000	13.376017000	36.395131000
H	12.708513000	14.625353000	35.308270000
C	12.090756000	14.284960000	38.703333000
H	11.985536000	14.975917000	39.543941000
H	12.902785000	13.587060000	38.930633000
H	11.163981000	13.711189000	38.611490000
C	9.525512000	17.400260000	39.797261000
C	10.873051000	18.059734000	39.502581000
H	11.697688000	17.370840000	39.701528000
H	11.001406000	18.939346000	40.142187000
H	10.936513000	18.380049000	38.461130000
C	8.387691000	18.390088000	39.539695000
H	7.419704000	17.942846000	39.788643000
H	8.371455000	18.678801000	38.487096000
H	8.507712000	19.287660000	40.155792000
C	9.497717000	16.928499000	41.252606000
H	10.286398000	16.192792000	41.434601000
H	8.535265000	16.467039000	41.498765000
H	9.645815000	17.771518000	41.935193000
C	11.676800000	9.040866000	37.946099000
C	12.839450000	8.231712000	37.366054000
H	12.613479000	7.160991000	37.402625000
H	13.753580000	8.403366000	37.944732000
H	13.018126000	8.516182000	36.327149000
C	11.370416000	8.566831000	39.367227000
H	10.539317000	9.135730000	39.791543000
H	12.245593000	8.693143000	40.012988000
H	11.094775000	7.507885000	39.364670000
C	12.004910000	10.532827000	37.946817000
H	12.227942000	10.879252000	36.934023000
H	12.877219000	10.734308000	38.577628000
H	11.159019000	11.108140000	38.333414000
C	11.614838000	9.954404000	33.461878000
C	12.812283000	9.167982000	32.923294000
H	13.669686000	9.272099000	33.595147000
H	13.103342000	9.531377000	31.932384000
H	12.568842000	8.104391000	32.843784000
C	11.976382000	11.432987000	33.600384000
H	11.128006000	11.996728000	33.998571000
H	12.252166000	11.860999000	32.631145000
H	12.823829000	11.553313000	34.281753000
C	10.407397000	9.778425000	32.542584000
H	10.136864000	8.721882000	32.459709000
H	10.631363000	10.155464000	31.540387000
H	9.544092000	10.334269000	32.918220000
C	8.954271000	6.831873000	35.142376000
C	8.510153000	6.304374000	36.508252000
H	8.525398000	5.209342000	36.528969000
H	7.489997000	6.635166000	36.730047000
H	9.173896000	6.685997000	37.286752000
C	10.373345000	6.358439000	34.824404000

H	10.407317000	5.263806000	34.818184000
H	11.082193000	6.720264000	35.571145000
H	10.695426000	6.716900000	33.843403000
C	8.001132000	6.344211000	34.049508000
H	6.968654000	6.627981000	34.278579000
H	8.030055000	5.253260000	33.966226000
H	8.274833000	6.772220000	33.080197000
C	9.024528000	13.739609000	30.392748000
C	10.336154000	13.115855000	29.913736000
H	10.899850000	12.718070000	30.762038000
H	10.955706000	13.859628000	29.402115000
H	10.137305000	12.295495000	29.217225000
C	9.306272000	14.853901000	31.397850000
H	8.371823000	15.306677000	31.739595000
H	9.918969000	15.638843000	30.941963000
H	9.842105000	14.460192000	32.266282000
C	8.229498000	14.276599000	29.200354000
H	8.056833000	13.481341000	28.467856000
H	8.778195000	15.082721000	28.701281000
H	7.262975000	14.660550000	29.534078000
C	6.003101000	10.461530000	30.674336000
C	7.276021000	9.767698000	30.185538000
H	8.046639000	10.507580000	29.963435000
H	7.073343000	9.177804000	29.284893000
H	7.660464000	9.093780000	30.957721000
C	5.455354000	11.405062000	29.602885000
H	4.544852000	11.900638000	29.950289000
H	5.217262000	10.841960000	28.694236000
H	6.187444000	12.173745000	29.348744000
C	4.941515000	9.416184000	31.021655000
H	5.325196000	8.693698000	31.749804000
H	4.647459000	8.853958000	30.129459000
H	4.048744000	9.893391000	31.436136000
C	4.928260000	14.573831000	32.234137000
C	5.488335000	15.646770000	33.167603000
H	6.115091000	15.189916000	33.938401000
H	4.678306000	16.189541000	33.663323000
H	6.092643000	16.363810000	32.602895000
C	4.081723000	13.571810000	33.019603000
H	3.694111000	12.792186000	32.357657000
H	3.234663000	14.075420000	33.495527000
H	4.679342000	13.101946000	33.807006000
C	4.093172000	15.218629000	31.126175000
H	4.704790000	15.915959000	30.545642000
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H	3.705262000	14.455940000	30.444133000

Cs₂-2 (AF)

U	-2.040684000	-0.745371000	-0.128098000
U	1.966948000	0.777332000	-0.135530000
Cs	-1.598295000	2.994871000	0.405165000
Cs	1.438357000	-3.030541000	0.091598000
Si	-3.985406000	1.588532000	-2.447906000
Si	-3.037023000	0.723875000	3.268781000
Si	-2.214822000	-4.557406000	-0.227252000
Si	1.771556000	4.635037000	-0.283395000
Si	3.826000000	-0.984434000	2.740286000
Si	3.549057000	-1.319543000	-2.963176000
O	-0.010621000	-0.045247000	-0.112254000
O	-3.184118000	0.436448000	-1.618260000
O	-2.905226000	2.203783000	-3.564431000
O	-4.418279000	2.887583000	-1.459351000
O	-5.409979000	1.074462000	-3.159614000
O	-2.761054000	0.222821000	1.740278000

O	-2.181615000	2.175976000	3.394813000
O	-4.616091000	1.147062000	3.622752000
O	-2.620120000	-0.392052000	4.438056000
O	-1.797730000	-2.988227000	-0.379921000
O	-3.299726000	-4.913840000	0.990764000
O	-2.891404000	-5.234730000	-1.602926000
O	-0.780635000	-5.345677000	0.199085000
O	1.640569000	3.035065000	0.004890000
O	1.662747000	5.079503000	-1.891751000
O	3.180654000	5.351719000	0.262450000
O	0.400102000	5.338180000	0.423745000
O	2.949777000	-0.228546000	1.590823000
O	3.420637000	-0.630099000	4.322838000
O	5.470954000	-0.689740000	2.659421000
O	3.470132000	-2.630045000	2.563904000
O	2.835891000	-0.411283000	-1.810856000
O	5.207803000	-1.179444000	-3.108014000
O	3.298998000	-2.925561000	-2.484362000
O	2.960852000	-1.035576000	-4.503593000
C	-2.988172000	3.336970000	-4.441428000
C	-4.381658000	3.492816000	-5.053422000
H	-4.664146000	2.597516000	-5.613420000
H	-4.392617000	4.343866000	-5.742780000
H	-5.137877000	3.666837000	-4.285010000
C	-1.965525000	3.077509000	-5.548698000
H	-0.966835000	2.960794000	-5.119940000
H	-1.942545000	3.909225000	-6.260428000
H	-2.216085000	2.161918000	-6.093333000
C	-2.606955000	4.593857000	-3.656958000
H	-1.601814000	4.486164000	-3.238075000
H	-3.315149000	4.754048000	-2.840008000
H	-2.612373000	5.476959000	-4.304974000
C	-5.668139000	3.179174000	-0.803199000
C	-5.355785000	4.265693000	0.228269000
H	-4.697802000	3.882166000	1.014455000
H	-6.274194000	4.613091000	0.712097000
H	-4.878023000	5.124963000	-0.253962000
C	-6.669411000	3.714440000	-1.828717000
H	-6.859083000	2.962881000	-2.597912000
H	-6.279273000	4.619264000	-2.306259000
H	-7.618175000	3.968658000	-1.343968000
C	-6.217201000	1.935906000	-0.104408000
H	-6.430747000	1.152950000	-0.835366000
H	-7.147903000	2.177198000	0.420081000
H	-5.498490000	1.553985000	0.626437000
C	-5.707430000	-0.141863000	-3.862835000
C	-6.927793000	0.169220000	-4.731151000
H	-7.761151000	0.508354000	-4.108339000
H	-7.248759000	-0.719977000	-5.283395000
H	-6.695144000	0.959219000	-5.451185000
C	-6.048064000	-1.226930000	-2.840026000
H	-5.191146000	-1.416484000	-2.188573000
H	-6.321887000	-2.162534000	-3.339077000
H	-6.892532000	-0.912844000	-2.218525000
C	-4.528581000	-0.573408000	-4.736394000
H	-4.280537000	0.202895000	-5.465285000
H	-4.773152000	-1.491095000	-5.281155000
H	-3.643364000	-0.764300000	-4.123053000
C	-2.219108000	3.166043000	4.442774000
C	-0.864321000	3.875121000	4.395927000
H	-0.688283000	4.330720000	3.416729000
H	-0.054523000	3.165894000	4.590533000
H	-0.817033000	4.668076000	5.149692000
C	-3.353995000	4.148545000	4.142863000

H	-3.198460000	4.635818000	3.174144000
H	-3.403801000	4.933048000	4.905532000
H	-4.308404000	3.618193000	4.114290000
C	-2.421139000	2.535126000	5.820623000
H	-2.420672000	3.314769000	6.589743000
H	-1.618525000	1.829570000	6.048682000
H	-3.372718000	2.001992000	5.872118000
C	-5.736444000	0.342883000	4.029047000
C	-6.974213000	1.208913000	3.790928000
H	-7.881614000	0.682186000	4.103900000
H	-7.066966000	1.462993000	2.732074000
H	-6.901366000	2.139002000	4.363145000
C	-5.613363000	0.005844000	5.517132000
H	-4.696737000	-0.556885000	5.704804000
H	-6.471231000	-0.589404000	5.848286000
H	-5.588488000	0.923599000	6.113682000
C	-5.805887000	-0.931281000	3.189426000
H	-5.864757000	-0.685584000	2.125356000
H	-6.684978000	-1.526450000	3.457542000
H	-4.915144000	-1.543317000	3.356666000
C	-1.448692000	-1.212786000	4.584869000
C	-1.266157000	-1.411857000	6.091125000
H	-1.083811000	-0.454734000	6.588012000
H	-0.417372000	-2.072613000	6.293788000
H	-2.165211000	-1.857446000	6.527781000
C	-1.716360000	-2.558337000	3.910924000
H	-2.609128000	-3.027548000	4.334965000
H	-0.872027000	-3.240461000	4.056239000
H	-1.875228000	-2.434757000	2.835583000
C	-0.219472000	-0.536432000	3.983242000
H	-0.320288000	-0.424100000	2.899128000
H	0.687870000	-1.112108000	4.183096000
H	-0.085124000	0.460651000	4.411415000
C	-4.737581000	-4.908669000	1.009306000
C	-5.283525000	-3.690999000	0.263705000
H	-4.902336000	-2.764551000	0.704980000
H	-6.377098000	-3.665886000	0.314179000
H	-4.992458000	-3.725403000	-0.789933000
C	-5.262583000	-6.200418000	0.377199000
H	-6.357768000	-6.214806000	0.388578000
H	-4.909124000	-7.071772000	0.937958000
H	-4.917981000	-6.284984000	-0.655536000
C	-5.127369000	-4.853109000	2.486519000
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H	-6.215852000	-4.874001000	2.602135000
H	-4.746045000	-3.939640000	2.949765000
C	-2.515746000	-5.154627000	-2.982981000
C	-0.995363000	-5.127084000	-3.141372000
H	-0.582074000	-4.229025000	-2.673005000
H	-0.721258000	-5.114486000	-4.201563000
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C	-3.137322000	-3.896953000	-3.588833000
H	-4.224931000	-3.920442000	-3.474534000
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C	-3.094419000	-6.406003000	-3.646845000
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H	-4.178811000	-6.441759000	-3.506178000
C	-0.607938000	-6.666518000	0.750270000
C	-1.609116000	-7.666433000	0.170331000
H	-1.421409000	-8.663854000	0.581747000
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H	-2.632270000	-7.379134000	0.417203000

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C	0.811221000	-7.098150000	0.375993000
H	1.550685000	-6.396793000	0.775289000
H	0.927951000	-7.142306000	-0.711012000
H	1.036202000	-8.087362000	0.787207000
C	2.670581000	5.175183000	-2.910973000
C	3.678839000	4.035348000	-2.786568000
H	4.202160000	4.087377000	-1.827645000
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C	3.373272000	6.529812000	-2.793242000
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C	1.923649000	5.078699000	-4.241747000
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H	1.179189000	5.876952000	-4.319635000
H	1.406775000	4.118038000	-4.320057000
C	3.883067000	5.245752000	1.508726000
C	4.666205000	6.551744000	1.661512000
H	5.341975000	6.691226000	0.812319000
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C	4.848751000	4.064624000	1.422868000
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C	2.913377000	5.065615000	2.676788000
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C	1.037554000	7.716111000	0.272106000
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H	1.706803000	7.547919000	-0.573574000
C	-0.920515000	6.794943000	-0.992095000
H	-1.762459000	6.094970000	-0.974435000
H	-0.298879000	6.562433000	-1.858741000
H	-1.330601000	7.804168000	-1.105610000
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H	5.954981000	-0.044072000	4.983989000
C	2.808354000	0.503430000	6.310179000
H	1.825143000	0.750779000	5.901814000
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H	4.188799000	2.569993000	5.119145000
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C	6.390456000	-0.691934000	1.558122000
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H	8.018309000	-0.243794000	2.919882000
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H	6.627831000	1.457778000	1.673927000
C	6.018643000	-1.756123000	0.527641000
H	6.009644000	-2.749169000	0.985980000
H	6.737492000	-1.763179000	-0.296268000
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C	3.738916000	-4.985820000	2.625498000
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H	3.989486000	-5.861628000	3.232158000
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C	6.029802000	-0.265207000	-3.850899000
C	7.426552000	-0.373085000	-3.237078000
H	7.404718000	-0.078602000	-2.184203000
H	8.133482000	0.275697000	-3.764328000
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H	4.503576000	1.243519000	-4.152671000
H	6.160413000	1.865967000	-4.237232000
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C	6.068358000	-0.689633000	-5.321099000
H	6.476643000	-1.701054000	-5.416212000
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H	5.061419000	-0.678069000	-5.743830000
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H	5.946256000	-3.422067000	-2.613511000
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C	3.337894000	5.859943000	3.213231000
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H	7.415182000	9.216815000	-0.810382000
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H	10.943471000	10.450650000	-0.971497000
C	11.174133000	11.333263000	1.621153000
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H	12.245199000	11.139846000	1.737278000
H	10.785280000	11.640458000	2.595932000
C	7.933355000	13.627821000	0.112863000
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C	12.110657000	10.653745000	7.212602000
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H	12.773120000	9.899474000	7.649873000
H	11.250582000	10.144056000	6.769761000
C	13.982249000	12.289596000	6.845058000
H	14.531656000	12.875228000	6.100497000
H	14.693392000	11.625357000	7.348109000
H	13.558420000	12.970746000	7.587501000
C	11.589554000	15.484479000	4.528351000
C	12.371038000	14.826273000	3.389519000
H	12.847973000	13.909985000	3.742818000
H	13.138763000	15.505095000	3.002293000
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C	10.860945000	16.731516000	4.020289000
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H	11.575574000	17.487475000	3.679787000
H	10.249402000	17.169772000	4.815261000
C	12.525854000	15.868545000	5.673961000
H	11.969447000	16.335358000	6.490921000
H	13.279797000	16.579236000	5.319425000
H	13.040892000	14.991072000	6.069654000
C	10.194644000	14.252828000	8.626546000
C	9.137199000	15.200885000	8.062567000
H	9.607286000	16.001612000	7.483382000
H	8.563481000	15.657915000	8.874885000
H	8.433633000	14.665109000	7.419627000
C	11.149955000	15.012444000	9.549499000
H	11.930137000	14.342284000	9.922822000
H	10.611206000	15.426512000	10.407874000
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C	9.541508000	13.092765000	9.375785000
H	8.897375000	12.503189000	8.717585000
H	8.939476000	13.468214000	10.210179000
H	10.308424000	12.428391000	9.785188000
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H	3.844631000	11.166451000	4.581347000
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C	3.709787000	13.377611000	2.929861000
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C	5.629986000	16.616303000	4.887705000
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C	4.139597000	16.898614000	5.077211000
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C	6.439445000	17.216195000	6.038408000

H	6.132693000	16.768922000	6.985760000
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C	4.520260000	14.042950000	8.450484000
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H	3.286218000	15.826823000	8.493649000
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C	5.365476000	14.476148000	9.647912000
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C	4.352332000	12.525470000	8.438300000
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K₄-(N)₂

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C	-7.636259000	1.905456000	-1.317350000
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C	-4.851240000	0.273673000	-3.724721000
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H	4.232528000	-6.348951000	-0.583478000
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C	4.855035000	-3.253827000	3.382790000
H	4.708156000	-4.317466000	3.597151000
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H	7.274542000	-4.528915000	3.910624000
H	8.319526000	-3.237180000	3.285419000
H	7.256581000	-2.923192000	4.669397000
C	5.072839000	1.030410000	4.462438000
C	5.462951000	2.431627000	3.985015000
H	6.242235000	2.370298000	3.223721000
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C	3.916276000	1.132629000	5.461646000
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H	7.092824000	0.212215000	4.443491000
H	6.597027000	0.909329000	5.997035000
H	5.963226000	-0.665319000	5.481635000
C	7.687780000	0.809958000	0.906782000
C	8.636659000	0.649378000	2.096612000
H	8.475468000	-0.316498000	2.579325000
H	9.678793000	0.705999000	1.764010000
H	8.473758000	1.445115000	2.830131000
C	7.892851000	2.188891000	0.271826000
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H	7.260880000	2.315472000	-0.614633000
H	7.646950000	2.980484000	0.986320000
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C	0.388700000	-0.905462000	-4.911055000
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C	1.693330000	6.125963000	0.987893000
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H	2.372055000	4.298539000	0.048599000
H	1.772916000	5.528079000	-1.092082000
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H	0.479979000	5.512240000	-3.322847000
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C	-2.739795000	6.336527000	1.862701000
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H	-4.772253000	5.854862000	1.273340000
H	-4.284148000	5.154804000	2.832342000

Rb₂-N₂

U	12.608767000	2.069006000	31.269746000
U	12.015814000	-0.799697000	29.641841000
Rb	13.202815000	5.184848000	33.257757000
Rb	11.321678000	-3.887405000	27.640780000
Si	12.175106000	2.177512000	35.068644000
Si	15.980179000	3.874405000	31.381353000
Si	10.669976000	5.320213000	30.638999000
Si	11.672343000	-0.732561000	25.829672000
Si	8.888237000	-2.945649000	30.196890000
Si	14.331852000	-3.843497000	29.612123000
O	11.052816000	0.913062000	30.426016000
O	12.162709000	2.293450000	33.433964000
O	10.735247000	1.669744000	35.739259000
O	13.347808000	1.195724000	35.723321000
O	12.582794000	3.731898000	35.606437000
O	14.520099000	3.164553000	31.600324000
O	17.306312000	2.949984000	31.777976000
O	15.882347000	5.261470000	32.356794000
O	16.276949000	4.455073000	29.850469000
O	11.706548000	4.065801000	30.827162000
O	9.096322000	5.042603000	31.104301000
O	10.585633000	5.932947000	29.089241000
O	11.218380000	6.497020000	31.730349000
O	11.582534000	-0.826283000	27.463252000
O	13.161618000	-0.339026000	25.199894000
O	10.594298000	0.334279000	25.136572000
O	11.397999000	-2.315304000	25.287836000

O	10.357983000	-2.234244000	30.063044000
O	7.590029000	-2.044970000	29.673280000
O	8.942477000	-4.250672000	29.114520000
O	8.494429000	-3.459109000	31.734081000
O	13.310669000	-2.588483000	29.355240000
O	13.687640000	-5.072508000	28.632397000
O	14.315422000	-4.477776000	31.150069000
O	15.932940000	-3.563200000	29.250680000
N	13.445114000	0.087157000	31.123283000
N	13.596718000	0.652088000	29.842025000
C	9.376194000	2.038557000	35.454870000
C	9.269564000	3.508447000	35.047895000
H	9.663452000	4.159095000	35.834031000
H	8.223461000	3.778027000	34.871707000
H	9.821952000	3.696147000	34.122767000
C	8.599550000	1.786693000	36.748771000
H	8.709017000	0.743309000	37.059349000
H	7.534094000	1.996137000	36.609067000
H	8.973655000	2.424106000	37.555482000
C	8.855740000	1.135038000	34.339948000
H	9.424597000	1.289569000	33.419699000
H	7.799859000	1.339191000	34.135956000
H	8.950146000	0.084895000	34.631897000
C	13.365616000	-0.226512000	35.943219000
C	12.693174000	-0.524818000	37.285137000
H	13.219051000	-0.013459000	38.098140000
H	12.709359000	-1.599795000	37.494405000
H	11.654580000	-0.185403000	37.271022000
C	14.842281000	-0.617683000	35.989103000
H	15.324668000	-0.391194000	35.034819000
H	14.951630000	-1.688267000	36.190586000
H	15.358868000	-0.064109000	36.779594000
C	12.654519000	-0.957528000	34.807888000
H	11.595954000	-0.684454000	34.780217000
H	12.721184000	-2.039480000	34.956258000
H	13.108197000	-0.714657000	33.842760000
C	12.998699000	4.151717000	36.922960000
C	12.720008000	5.656093000	36.992253000
H	13.311993000	6.203916000	36.249847000
H	12.987331000	6.052493000	37.976770000
H	11.659770000	5.861481000	36.814954000
C	14.496798000	3.882335000	37.078480000
H	14.695261000	2.813397000	36.981709000
H	14.854124000	4.227168000	38.054857000
H	15.064869000	4.407785000	36.303686000
C	12.210112000	3.436224000	38.019821000
H	11.139199000	3.631682000	37.921959000
H	12.536114000	3.788748000	39.004067000
H	12.368146000	2.357126000	37.971100000
C	17.548723000	2.025397000	32.851945000
C	17.050305000	0.644532000	32.431025000
H	15.973939000	0.648922000	32.238431000
H	17.263641000	-0.093054000	33.211912000
H	17.558229000	0.324305000	31.516483000
C	16.860021000	2.482213000	34.137664000
H	17.180644000	3.492269000	34.410069000
H	17.110369000	1.808949000	34.963471000
H	15.772843000	2.474379000	34.021525000
C	19.067262000	2.007242000	33.039311000
H	19.559593000	1.716171000	32.106493000
H	19.353039000	1.292756000	33.818056000
H	19.435199000	2.997199000	33.325623000
C	16.738047000	6.418860000	32.394896000
C	18.213581000	6.032717000	32.292099000

H	18.491941000	5.345929000	33.095644000
H	18.841702000	6.926599000	32.368596000
H	18.424650000	5.545715000	31.338381000
C	16.479033000	7.086376000	33.749108000
H	15.433951000	7.405943000	33.836027000
H	17.103710000	7.977314000	33.867077000
H	16.704564000	6.397269000	34.569033000
C	16.348075000	7.365846000	31.257443000
H	16.479485000	6.867975000	30.294986000
H	16.960789000	8.273560000	31.279633000
H	15.297531000	7.661889000	31.348615000
C	16.931985000	3.866625000	28.711166000
C	16.348224000	4.584706000	27.494205000
H	15.270642000	4.410360000	27.433656000
H	16.813712000	4.225235000	26.570678000
H	16.518149000	5.663506000	27.568680000
C	16.667022000	2.365358000	28.632220000
H	17.132793000	1.850746000	29.475595000
H	17.086901000	1.957351000	27.706910000
H	15.597037000	2.142466000	28.653580000
C	18.434591000	4.136967000	28.817078000
H	18.630790000	5.213192000	28.865665000
H	18.961118000	3.734899000	27.944718000
H	18.839119000	3.662754000	29.715149000
C	7.982222000	4.484716000	30.384693000
C	7.050450000	3.910073000	31.451243000
H	7.557991000	3.121240000	32.012640000
H	6.150282000	3.488600000	30.992086000
H	6.744871000	4.692598000	32.153080000
C	8.447645000	3.390658000	29.429069000
H	9.091929000	3.814590000	28.654047000
H	7.586855000	2.926332000	28.938320000
H	9.006659000	2.612994000	29.956791000
C	7.284514000	5.609387000	29.616609000
H	6.937983000	6.387216000	30.305082000
H	6.414535000	5.224405000	29.073688000
H	7.974935000	6.057685000	28.897555000
C	11.613987000	6.214641000	28.126502000
C	11.929992000	4.929665000	27.364567000
H	12.322806000	4.171144000	28.046029000
H	12.672671000	5.113245000	26.581569000
H	11.025218000	4.535147000	26.892926000
C	11.017594000	7.260243000	27.182449000
H	10.096863000	6.880430000	26.729584000
H	11.721692000	7.506641000	26.381213000
H	10.776716000	8.178495000	27.726278000
C	12.874185000	6.760094000	28.798970000
H	12.645185000	7.655956000	29.382947000
H	13.621576000	7.024641000	28.044126000
H	13.320337000	6.012142000	29.460560000
C	10.554403000	7.695898000	32.180215000
C	11.662511000	8.617104000	32.699375000
H	12.182391000	8.167937000	33.553625000
H	11.246684000	9.571606000	33.036929000
H	12.395537000	8.819633000	31.912493000
C	9.805524000	8.390082000	31.042545000
H	10.489104000	8.663580000	30.234776000
H	9.326788000	9.302731000	31.412853000
H	9.032312000	7.738537000	30.631438000
C	9.591579000	7.333720000	33.313131000
H	8.830507000	6.641295000	32.948948000
H	9.102875000	8.230356000	33.709283000
H	10.130045000	6.849979000	34.135258000
C	13.782263000	0.945879000	25.009160000

C	15.284961000	0.673138000	24.951313000
H	15.628691000	0.240010000	25.894184000
H	15.839055000	1.599958000	24.771148000
H	15.514619000	-0.027534000	24.142295000
C	13.452569000	1.876005000	26.172596000
H	12.377593000	2.073905000	26.212480000
H	13.968908000	2.832802000	26.051134000
H	13.765852000	1.434241000	27.122547000
C	13.296489000	1.538359000	23.684547000
H	13.552165000	0.874964000	22.851781000
H	13.768328000	2.509664000	23.500831000
H	12.212329000	1.672338000	23.705589000
C	9.193909000	0.556399000	25.367061000
C	9.048032000	1.612409000	26.459645000
H	9.475435000	1.258403000	27.401134000
H	7.993278000	1.854379000	26.625094000
H	9.566531000	2.530613000	26.167929000
C	8.633694000	1.083350000	24.044342000
H	9.172265000	1.984972000	23.737716000
H	7.572137000	1.331503000	24.144782000
H	8.739825000	0.336195000	23.252274000
C	8.480507000	-0.734416000	25.770413000
H	8.616990000	-1.507298000	25.008729000
H	7.407406000	-0.553217000	25.887758000
H	8.860661000	-1.109282000	26.725042000
C	11.632796000	-2.867310000	23.974789000
C	13.108567000	-3.253784000	23.855949000
H	13.737270000	-2.369084000	23.972904000
H	13.311793000	-3.713161000	22.882577000
H	13.381818000	-3.973695000	24.634760000
C	10.748538000	-4.114006000	23.879687000
H	11.033717000	-4.859637000	24.630908000
H	10.851105000	-4.586473000	22.897773000
H	9.695911000	-3.853456000	24.027363000
C	11.245786000	-1.882295000	22.871584000
H	10.189843000	-1.609921000	22.945731000
H	11.416897000	-2.335051000	21.889298000
H	11.840572000	-0.969360000	22.938964000
C	6.783792000	-1.065079000	30.352062000
C	7.625485000	-0.247693000	31.327172000
H	8.004085000	-0.885025000	32.130856000
H	7.016744000	0.541342000	31.779409000
H	8.477124000	0.218202000	30.823591000
C	6.214751000	-0.169314000	29.252222000
H	7.024783000	0.335214000	28.719010000
H	5.549922000	0.589787000	29.677090000
H	5.643385000	-0.763876000	28.532430000
C	5.653838000	-1.787276000	31.089403000
H	5.040691000	-2.359633000	30.385416000
H	5.003565000	-1.067919000	31.598835000
H	6.066589000	-2.472644000	31.834130000
C	7.859440000	-5.070643000	28.629883000
C	7.183453000	-4.354977000	27.458403000
H	6.768919000	-3.402410000	27.793118000
H	6.380034000	-4.970028000	27.039150000
H	7.907383000	-4.153327000	26.661379000
C	6.842071000	-5.375357000	29.729447000
H	7.315016000	-5.898043000	30.564680000
H	6.043584000	-6.011092000	29.332585000
H	6.392878000	-4.456316000	30.110356000
C	8.501598000	-6.377527000	28.154730000
H	9.199762000	-6.199462000	27.328545000
H	7.738419000	-7.072907000	27.791373000
H	9.045484000	-6.860027000	28.972510000

C	9.269577000	-4.138278000	32.735163000
C	10.033677000	-3.094041000	33.545730000
H	10.733581000	-2.552037000	32.905335000
H	10.596907000	-3.565865000	34.357214000
H	9.338470000	-2.372998000	33.985765000
C	8.253781000	-4.859897000	33.623333000
H	7.538723000	-4.144741000	34.040882000
H	8.755404000	-5.370757000	34.451564000
H	7.695212000	-5.603484000	33.047002000
C	10.236317000	-5.142842000	32.107720000
H	9.695306000	-5.871021000	31.496610000
H	10.777799000	-5.685775000	32.889067000
H	10.976041000	-4.636762000	31.480811000
C	13.984561000	-6.481558000	28.612911000
C	13.479323000	-6.995745000	27.261158000
H	12.395038000	-6.862005000	27.168933000
H	13.685894000	-8.064874000	27.151043000
H	13.969891000	-6.464664000	26.439301000
C	13.231055000	-7.169642000	29.753519000
H	13.563968000	-6.774118000	30.714842000
H	13.398737000	-8.251919000	29.731601000
H	12.154605000	-6.989002000	29.664731000
C	15.486592000	-6.741976000	28.726955000
H	16.028739000	-6.261135000	27.908400000
H	15.684863000	-7.818276000	28.685981000
H	15.879329000	-6.356536000	29.669636000
C	15.127298000	-4.210129000	32.308333000
C	14.272158000	-4.624775000	33.505989000
H	13.360426000	-4.022846000	33.545766000
H	14.823328000	-4.487901000	34.442096000
H	13.985964000	-5.678230000	33.425147000
C	16.388927000	-5.073032000	32.232839000
H	16.127062000	-6.135083000	32.181319000
H	17.014242000	-4.919890000	33.118995000
H	16.972570000	-4.809784000	31.346839000
C	15.496066000	-2.731669000	32.394219000
H	16.145078000	-2.450368000	31.561808000
H	16.030313000	-2.530551000	33.328518000
H	14.608987000	-2.093830000	32.358292000
C	16.557419000	-2.832314000	28.181084000
C	17.945506000	-3.454675000	28.016298000
H	18.496850000	-3.403604000	28.959944000
H	18.519836000	-2.922394000	27.251152000
H	17.867962000	-4.505661000	27.721390000
C	16.677109000	-1.367807000	28.597174000
H	15.694354000	-0.923707000	28.777955000
H	17.185856000	-0.788244000	27.819561000
H	17.263017000	-1.284856000	29.517499000
C	15.759776000	-2.964982000	26.883984000
H	15.618100000	-4.018704000	26.625785000
H	16.289515000	-2.478037000	26.059282000
H	14.780462000	-2.487862000	26.976866000

Rb₄-(N)₂

U	9.364198000	5.714048000	5.549837000
U	10.309783000	2.591506000	6.147826000
Rb	10.485182000	5.152367000	9.291328000
Rb	6.586164000	4.701472000	8.043859000
Rb	8.476068000	8.532393000	8.259247000
Rb	8.391307000	2.883157000	2.942331000
Si	11.586815000	0.837235000	2.915152000
Si	12.229169000	1.741201000	9.337248000
Si	7.025038000	0.820032000	6.231075000
Si	6.644364000	7.075204000	10.799144000

Si	11.859902000	8.171916000	7.311939000
Si	7.350740000	6.402965000	2.349795000
O	11.022348000	1.548564000	4.264159000
O	10.380836000	1.087172000	1.743837000
O	13.071719000	1.388558000	2.372606000
O	11.775866000	-0.821740000	2.986756000
O	7.964610000	6.687465000	6.266428000
O	11.666618000	2.420745000	7.970978000
O	13.879359000	1.441962000	9.338020000
O	11.545991000	0.282849000	9.790085000
O	11.808561000	2.821827000	10.577481000
O	8.609806000	1.128621000	6.121577000
O	6.658552000	-0.814993000	6.152591000
O	6.242399000	1.361806000	7.627679000
O	6.275944000	1.665855000	4.968649000
O	7.925080000	6.438140000	10.091792000
O	6.399372000	6.825795000	12.451967000
O	5.281471000	6.499245000	9.946598000
O	6.545901000	8.769876000	10.588942000
O	10.764073000	7.080362000	6.852421000
O	12.255188000	7.722573000	8.896819000
O	11.170355000	9.714560000	7.472123000
O	13.196315000	8.404395000	6.344065000
O	8.294891000	5.723211000	3.477059000
O	5.977901000	7.201038000	2.870070000
O	8.134759000	7.523701000	1.372075000
O	6.762011000	5.097938000	1.436084000
N	9.059510000	4.079798000	6.832848000
N	10.650280000	4.564542000	4.921121000
C	10.232699000	0.466221000	0.452149000
C	9.300680000	1.381166000	-0.346341000
H	9.148177000	0.993274000	-1.358545000
H	8.315715000	1.447660000	0.128782000
H	9.723048000	2.388231000	-0.425473000
C	11.571135000	0.344306000	-0.277283000
H	11.419682000	-0.108432000	-1.263012000
H	12.028779000	1.327177000	-0.417350000
H	12.267508000	-0.280328000	0.284773000
C	9.589076000	-0.910981000	0.626482000
H	9.428829000	-1.389790000	-0.345788000
H	10.229273000	-1.548002000	1.239570000
H	8.619679000	-0.816720000	1.125870000
C	14.302615000	3.068880000	3.578212000
H	14.799741000	4.041878000	3.503363000
H	13.557401000	3.125108000	4.375078000
H	15.053946000	2.319340000	3.845507000
C	13.630254000	2.703828000	2.254727000
C	12.559638000	3.735695000	1.902051000
H	13.021650000	4.710602000	1.713490000
H	12.021919000	3.434274000	0.998160000
H	11.850723000	3.860352000	2.727783000
C	14.674650000	2.608197000	1.139634000
H	15.198480000	3.561430000	1.013424000
H	15.413600000	1.836488000	1.376720000
H	14.201274000	2.345981000	0.188755000
C	12.885980000	-1.631392000	3.402496000
C	13.680168000	-0.954311000	4.519056000
H	14.467037000	-1.620896000	4.888158000
H	14.146283000	-0.036309000	4.153866000
H	13.021700000	-0.702501000	5.353564000
C	13.784690000	-1.891865000	2.191385000
H	14.627506000	-2.536635000	2.463607000
H	13.219283000	-2.388742000	1.396251000
H	14.176488000	-0.946692000	1.807060000

C	12.275500000	-2.941049000	3.904534000
H	13.057001000	-3.645645000	4.207766000
H	11.624107000	-2.751327000	4.762191000
H	11.677301000	-3.407932000	3.115788000
C	14.980097000	2.220469000	8.854496000
C	14.808406000	3.693413000	9.228482000
H	15.679543000	4.274702000	8.908604000
H	13.923869000	4.110459000	8.738723000
H	14.694901000	3.804750000	10.310624000
C	15.080028000	2.059750000	7.337404000
H	15.933036000	2.619934000	6.939661000
H	15.210998000	1.005524000	7.075254000
H	14.168102000	2.423245000	6.858472000
C	16.224068000	1.644555000	9.534341000
H	17.127533000	2.165144000	9.200453000
H	16.148078000	1.742319000	10.621498000
H	16.328713000	0.582456000	9.293432000
C	11.909288000	-1.071831000	9.470718000
C	12.289758000	-1.192202000	7.997005000
H	12.515029000	-2.232171000	7.739089000
H	11.467367000	-0.853281000	7.359745000
H	13.175096000	-0.587991000	7.782399000
C	13.072304000	-1.515659000	10.361673000
H	12.784240000	-1.470983000	11.417058000
H	13.355396000	-2.549097000	10.134002000
H	13.938760000	-0.869811000	10.204522000
C	10.671118000	-1.916058000	9.770892000
H	10.374164000	-1.797180000	10.817585000
H	9.835560000	-1.607550000	9.138641000
H	10.873335000	-2.976605000	9.588700000
C	11.798949000	2.590793000	12.000666000
C	11.847646000	3.973715000	12.653679000
H	11.850155000	3.885296000	13.744874000
H	12.752321000	4.509880000	12.351541000
H	10.972840000	4.571505000	12.376752000
C	10.499369000	1.875155000	12.376663000
H	10.441671000	1.715800000	13.459043000
H	9.634295000	2.474210000	12.073919000
H	10.444317000	0.910105000	11.869465000
C	13.012684000	1.777728000	12.452458000
H	12.987491000	1.639487000	13.538622000
H	13.020521000	0.794476000	11.980341000
H	13.943654000	2.289417000	12.193398000
C	7.290495000	-1.848455000	5.377768000
C	7.622876000	-1.353405000	3.969850000
H	8.049714000	-2.164368000	3.371893000
H	6.719444000	-0.993574000	3.467141000
H	8.358490000	-0.545153000	4.010826000
C	8.562772000	-2.299776000	6.095094000
H	9.060716000	-3.099983000	5.537917000
H	9.251636000	-1.457083000	6.190784000
H	8.323614000	-2.678100000	7.094062000
C	6.278604000	-2.993777000	5.313955000
H	6.693743000	-3.847781000	4.768951000
H	6.013793000	-3.324734000	6.322844000
H	5.362888000	-2.673032000	4.808006000
C	6.109498000	0.673909000	8.889393000
C	5.784210000	1.748979000	9.926526000
H	5.576663000	1.295509000	10.900552000
H	6.626965000	2.434759000	10.057856000
H	4.896619000	2.315878000	9.624620000
C	7.409613000	-0.032663000	9.266907000
H	7.322292000	-0.493245000	10.256528000
H	7.635665000	-0.819063000	8.543363000

H	8.246733000	0.670917000	9.287048000
C	4.950831000	-0.322730000	8.805909000
H	4.821316000	-0.841803000	9.761703000
H	4.015229000	0.197240000	8.573545000
H	5.145612000	-1.062103000	8.026718000
C	4.871038000	1.823121000	4.697711000
C	4.349991000	3.028108000	5.486302000
H	4.423866000	2.821657000	6.557606000
H	4.935802000	3.920102000	5.239982000
H	3.301900000	3.232322000	5.242459000
C	4.063656000	0.572558000	5.047419000
H	4.422449000	-0.293894000	4.486806000
H	4.135107000	0.339511000	6.111391000
H	3.008792000	0.732215000	4.799477000
C	4.765781000	2.094783000	3.197477000
H	5.181217000	1.254969000	2.629936000
H	3.721099000	2.221769000	2.896317000
H	5.302385000	3.010009000	2.930351000
C	6.947723000	5.801141000	13.292536000
C	8.402216000	6.146379000	13.620477000
H	8.855799000	5.377930000	14.255290000
H	8.976060000	6.224048000	12.692470000
H	8.460599000	7.102505000	14.150232000
C	6.874936000	4.433830000	12.609325000
H	7.287652000	3.653508000	13.257221000
H	5.839210000	4.170263000	12.376888000
H	7.448012000	4.460190000	11.677821000
C	6.101111000	5.805793000	14.566395000
H	6.471673000	5.066124000	15.283708000
H	6.130868000	6.791663000	15.040346000
H	5.057941000	5.569614000	14.335376000
C	3.869272000	6.624051000	10.160607000
C	3.498773000	7.938350000	10.845181000
H	3.924745000	7.978899000	11.850304000
H	3.875163000	8.790424000	10.274611000
H	2.410172000	8.023753000	10.930922000
C	3.222822000	6.566018000	8.772763000
H	2.133375000	6.647407000	8.843558000
H	3.589778000	7.384788000	8.146130000
H	3.451697000	5.618053000	8.272661000
C	3.393641000	5.445416000	11.014677000
H	3.857389000	5.488704000	12.003300000
H	2.305857000	5.466684000	11.141949000
H	3.663106000	4.493050000	10.546161000
C	6.868614000	9.868531000	11.452315000
C	5.876587000	9.965162000	12.614742000
H	5.882639000	9.038657000	13.191929000
H	6.144426000	10.797284000	13.274908000
H	4.863411000	10.140402000	12.243285000
C	6.755630000	11.126912000	10.584936000
H	6.929787000	12.028374000	11.181093000
H	7.492686000	11.120404000	9.773533000
H	5.757776000	11.193048000	10.141032000
C	8.293530000	9.731841000	11.993461000
H	8.388203000	8.824410000	12.593560000
H	9.022341000	9.683488000	11.178164000
H	8.555869000	10.589523000	12.622066000
C	13.428434000	7.340475000	10.919350000
H	14.022807000	7.778153000	11.727838000
H	12.537317000	6.888934000	11.366946000
H	14.018834000	6.550569000	10.445560000
C	13.035061000	8.407076000	9.896315000
C	14.294141000	9.036263000	9.300206000
H	14.876057000	9.526023000	10.088001000

H	14.924135000	8.274143000	8.834235000
H	14.046333000	9.782304000	8.542255000
C	12.167094000	9.474285000	10.566493000
H	12.723428000	9.988194000	11.357521000
H	11.835457000	10.210773000	9.831306000
H	11.285515000	9.011043000	11.020975000
C	11.186252000	10.842171000	6.575967000
C	12.554126000	11.525165000	6.632915000
H	12.574136000	12.403803000	5.979485000
H	12.772634000	11.855758000	7.653573000
H	13.333480000	10.830855000	6.313112000
C	10.856212000	10.403207000	5.149182000
H	10.811672000	11.268437000	4.479439000
H	11.619845000	9.717763000	4.775167000
H	9.886340000	9.897011000	5.113381000
C	10.111140000	11.802374000	7.092919000
H	10.109917000	12.729584000	6.511640000
H	9.111347000	11.361609000	7.006766000
H	10.294617000	12.055396000	8.141931000
C	14.033024000	7.465188000	5.639327000
C	15.415324000	8.116241000	5.567101000
H	16.111588000	7.481225000	5.010046000
H	15.354934000	9.085602000	5.062690000
H	15.821770000	8.276775000	6.569686000
C	13.465958000	7.269048000	4.234314000
H	14.135432000	6.642281000	3.636186000
H	12.493942000	6.770421000	4.275692000
H	13.359642000	8.233577000	3.727961000
C	14.100975000	6.130804000	6.377762000
H	14.784511000	5.446386000	5.866213000
H	14.462164000	6.272949000	7.400138000
H	13.114213000	5.658028000	6.405280000
C	5.757357000	8.551322000	3.294711000
C	4.553357000	8.494236000	4.237564000
H	4.278169000	9.496302000	4.583887000
H	3.690065000	8.056653000	3.726838000
H	4.787915000	7.873744000	5.107836000
C	6.975353000	9.108800000	4.033252000
H	6.755332000	10.108989000	4.425219000
H	7.244381000	8.444281000	4.860337000
H	7.826880000	9.189373000	3.352075000
C	5.438530000	9.404437000	2.064345000
H	5.224363000	10.439915000	2.351161000
H	6.289141000	9.399232000	1.377878000
H	4.563481000	9.007260000	1.539891000
C	9.465213000	7.533763000	0.840897000
C	10.402258000	8.162503000	1.873568000
H	10.059009000	9.167630000	2.136572000
H	10.429366000	7.551701000	2.779762000
H	11.422657000	8.238268000	1.483473000
C	9.409049000	8.406312000	-0.415316000
H	9.042395000	9.406616000	-0.165320000
H	10.401923000	8.504063000	-0.866647000
H	8.732733000	7.971147000	-1.156557000
C	9.940698000	6.122947000	0.490037000
H	9.261967000	5.651817000	-0.226600000
H	10.941054000	6.155064000	0.046604000
H	9.988668000	5.507491000	1.392482000
C	5.800500000	5.100730000	0.361160000
C	4.385064000	5.264003000	0.921396000
H	4.294572000	6.214670000	1.449160000
H	3.649296000	5.231867000	0.110394000
H	4.151905000	4.460881000	1.624871000
C	6.088474000	6.208873000	-0.653792000

H	6.023730000	7.196099000	-0.191807000
H	7.089298000	6.096687000	-1.079394000
H	5.362185000	6.161066000	-1.472250000
C	5.943607000	3.737962000	-0.320808000
H	5.233758000	3.641476000	-1.148701000
H	6.954906000	3.613592000	-0.720662000
H	5.745465000	2.927456000	0.388135000

Cs₂-N₂

U	12.602854000	2.077560000	31.277788000
U	12.010934000	-0.805843000	29.642331000
Cs	13.233169000	5.329276000	33.364762000
Cs	11.306908000	-4.042188000	27.555894000
Si	12.161739000	2.112052000	35.086386000
Si	16.003827000	3.844521000	31.342331000
Si	10.631918000	5.312874000	30.604549000
Si	11.701385000	-0.689400000	25.816257000
Si	8.841337000	-2.905820000	30.211181000
Si	14.373254000	-3.829185000	29.680825000
O	11.054804000	0.917598000	30.418297000
O	12.174118000	2.273671000	33.453888000
O	10.712495000	1.583914000	35.721163000
O	13.327496000	1.114744000	35.730199000
O	12.554205000	3.643264000	35.695689000
O	14.519583000	3.188404000	31.581002000
O	17.299520000	2.869688000	31.719913000
O	15.992664000	5.235571000	32.315174000
O	16.300284000	4.414475000	29.807071000
O	11.678286000	4.072958000	30.842145000
O	9.061222000	5.039282000	31.084766000
O	10.537009000	5.863020000	29.031788000
O	11.160238000	6.548755000	31.637481000
O	11.622317000	-0.826010000	27.448775000
O	13.188067000	-0.283196000	25.187455000
O	10.621326000	0.400621000	25.161709000
O	11.420099000	-2.248381000	25.213588000
O	10.321363000	-2.219645000	30.039692000
O	7.547768000	-1.993529000	29.695608000
O	8.836903000	-4.234878000	29.159396000
O	8.468374000	-3.388819000	31.764053000
O	13.303862000	-2.614972000	29.412617000
O	13.796820000	-5.099127000	28.712017000
O	14.376999000	-4.458651000	31.220763000
O	15.963875000	-3.488816000	29.322647000
N	13.435698000	0.089306000	31.136435000
N	13.597894000	0.642680000	29.858881000
C	9.359501000	1.983780000	35.452546000
C	9.275241000	3.464083000	35.078706000
H	9.686553000	4.090353000	35.875377000
H	8.232512000	3.754678000	34.915971000
H	9.824549000	3.662454000	34.153776000
C	8.581773000	1.715192000	36.742582000
H	8.676363000	0.663701000	37.029746000
H	7.519264000	1.943314000	36.609666000
H	8.966213000	2.328865000	37.562657000
C	8.820557000	1.115125000	34.319798000
H	9.388882000	1.281689000	33.401344000
H	7.767377000	1.340141000	34.124279000
H	8.899915000	0.057333000	34.587060000
C	13.348979000	-0.310257000	35.921648000
C	12.665182000	-0.640605000	37.250355000
H	13.183610000	-0.149237000	38.080307000
H	12.680130000	-1.720344000	37.433737000
H	11.626384000	-0.301672000	37.235113000

C	14.826787000	-0.696311000	35.974107000
H	15.318130000	-0.444308000	35.030974000
H	14.939103000	-1.770895000	36.150969000
H	15.332229000	-0.159598000	36.783326000
C	12.649497000	-1.016659000	34.765036000
H	11.589320000	-0.749930000	34.740919000
H	12.723971000	-2.101392000	34.884229000
H	13.105103000	-0.743256000	33.809179000
C	12.959542000	4.004582000	37.032873000
C	12.674762000	5.503486000	37.171769000
H	13.281696000	6.091626000	36.474354000
H	12.916566000	5.848171000	38.182041000
H	11.618289000	5.715315000	36.980131000
C	14.457656000	3.733533000	37.187759000
H	14.660235000	2.670193000	37.048708000
H	14.806903000	4.039866000	38.179870000
H	15.029620000	4.291736000	36.439094000
C	12.164977000	3.241221000	38.092825000
H	11.094711000	3.441067000	37.997092000
H	12.484748000	3.552100000	39.093125000
H	12.323026000	2.165458000	37.999927000
C	17.544503000	1.979330000	32.821471000
C	17.042376000	0.588882000	32.440592000
H	15.964805000	0.590018000	32.254582000
H	17.260028000	-0.128282000	33.238938000
H	17.544008000	0.245200000	31.531221000
C	16.859527000	2.471415000	34.096438000
H	17.180567000	3.488426000	34.340925000
H	17.111276000	1.819221000	34.938616000
H	15.772043000	2.460815000	33.982224000
C	19.063556000	1.961365000	33.005890000
H	19.552587000	1.647249000	32.078849000
H	19.349153000	1.264153000	33.800248000
H	19.435910000	2.956179000	33.268469000
C	16.882016000	6.367543000	32.314893000
C	18.341006000	5.938435000	32.160923000
H	18.631309000	5.256950000	32.964820000
H	18.996638000	6.814944000	32.198226000
H	18.500231000	5.430954000	31.208294000
C	16.695261000	7.049873000	33.673899000
H	15.668233000	7.412783000	33.795310000
H	17.359750000	7.914702000	33.766434000
H	16.919936000	6.354704000	34.488875000
C	16.476860000	7.320941000	31.187910000
H	16.557254000	6.815571000	30.223896000
H	17.115589000	8.210886000	31.182706000
H	15.439465000	7.647777000	31.317488000
C	16.932295000	3.819838000	28.659366000
C	16.346788000	4.552868000	27.452163000
H	15.264834000	4.403310000	27.408499000
H	16.789888000	4.185475000	26.520768000
H	16.541649000	5.627535000	27.526191000
C	16.642607000	2.324007000	28.581975000
H	17.112282000	1.801867000	29.418470000
H	17.041201000	1.910720000	27.649847000
H	15.569761000	2.119264000	28.620409000
C	18.440938000	4.062834000	28.745809000
H	18.658699000	5.134944000	28.793338000
H	18.947763000	3.652905000	27.865438000
H	18.849242000	3.578283000	29.636722000
C	7.946672000	4.450424000	30.392590000
C	7.029073000	3.901975000	31.485034000
H	7.549301000	3.137459000	32.067880000
H	6.128941000	3.457169000	31.048288000

H	6.722032000	4.704467000	32.163421000
C	8.415178000	3.333387000	29.466599000
H	9.041025000	3.742279000	28.668986000
H	7.555213000	2.839244000	29.004711000
H	8.995237000	2.582940000	30.010405000
C	7.230394000	5.542529000	29.594920000
H	6.873724000	6.335631000	30.260494000
H	6.364308000	5.128848000	29.067072000
H	7.911439000	5.978782000	28.859620000
C	11.557403000	6.166258000	28.068078000
C	11.919562000	4.881095000	27.328899000
H	12.338210000	4.148370000	28.023052000
H	12.655563000	5.076828000	26.542673000
H	11.029398000	4.446913000	26.864754000
C	10.927885000	7.173971000	27.104270000
H	10.020398000	6.755540000	26.658807000
H	11.623943000	7.428021000	26.298357000
H	10.656733000	8.094324000	27.630025000
C	12.797546000	6.766485000	28.731632000
H	12.537909000	7.662622000	29.301807000
H	13.534679000	7.043929000	27.971190000
H	13.269595000	6.045347000	29.405027000
C	10.467913000	7.743928000	32.051099000
C	11.554497000	8.728417000	32.494774000
H	12.113546000	8.341591000	33.354105000
H	11.111151000	9.682455000	32.796879000
H	12.258828000	8.918282000	31.679191000
C	9.663984000	8.361611000	30.906787000
H	10.314081000	8.609170000	30.063918000
H	9.175951000	9.280915000	31.247520000
H	8.893940000	7.673133000	30.555123000
C	9.549831000	7.400653000	33.226439000
H	8.811384000	6.658879000	32.916776000
H	9.032437000	8.294842000	33.590432000
H	10.128368000	6.983292000	34.057932000
C	13.810759000	1.002383000	25.017470000
C	15.313018000	0.728128000	24.954585000
H	15.655263000	0.275372000	25.888711000
H	15.869382000	1.657014000	24.793043000
H	15.541533000	0.043060000	24.131900000
C	13.479867000	1.912309000	26.195262000
H	12.404778000	2.108722000	26.235187000
H	13.996480000	2.870650000	26.091505000
H	13.790298000	1.453794000	27.137998000
C	13.326173000	1.618660000	23.703196000
H	13.582022000	0.970529000	22.858530000
H	13.798556000	2.592903000	23.537155000
H	12.242057000	1.753366000	23.726447000
C	9.216279000	0.596332000	25.387266000
C	9.049653000	1.626201000	26.500875000
H	9.476527000	1.258058000	27.437179000
H	7.991149000	1.851591000	26.665238000
H	9.558090000	2.556634000	26.231560000
C	8.654998000	1.143822000	24.073318000
H	9.182943000	2.058734000	23.788354000
H	7.589839000	1.375965000	24.174103000
H	8.774373000	0.415415000	23.265876000
C	8.518210000	-0.712131000	25.760011000
H	8.670343000	-1.468247000	24.984758000
H	7.442152000	-0.547256000	25.874717000
H	8.897965000	-1.100163000	26.709608000
C	11.661192000	-2.753696000	23.882963000
C	13.136544000	-3.140583000	23.757544000
H	13.767313000	-2.263037000	23.910306000

H	13.343005000	-3.564785000	22.768924000
H	13.403623000	-3.889911000	24.510335000
C	10.774253000	-3.993891000	23.734803000
H	11.061572000	-4.775953000	24.446582000
H	10.870411000	-4.417944000	22.730372000
H	9.722923000	-3.739083000	23.900666000
C	11.281326000	-1.730709000	22.812367000
H	10.224585000	-1.462244000	22.888858000
H	11.458759000	-2.149726000	21.816236000
H	11.874734000	-0.820551000	22.914617000
C	6.759703000	-0.995215000	30.366637000
C	7.621388000	-0.175497000	31.320827000
H	7.994984000	-0.806543000	32.131711000
H	7.030003000	0.631309000	31.764148000
H	8.477173000	0.266620000	30.803423000
C	6.188813000	-0.111181000	29.258354000
H	6.998808000	0.372602000	28.706413000
H	5.538723000	0.663737000	29.677516000
H	5.601193000	-0.710973000	28.556079000
C	5.628476000	-1.690464000	31.127972000
H	4.995816000	-2.261445000	30.440300000
H	4.996793000	-0.954262000	31.636699000
H	6.040494000	-2.372424000	31.876283000
C	7.723046000	-5.024603000	28.696384000
C	7.078318000	-4.314740000	27.503774000
H	6.701165000	-3.338171000	27.812548000
H	6.252283000	-4.908546000	27.097852000
H	7.811550000	-4.162251000	26.704233000
C	6.692562000	-5.258506000	29.800962000
H	7.144717000	-5.771902000	30.653134000
H	5.872628000	-5.877069000	29.420875000
H	6.276293000	-4.312593000	30.151151000
C	8.311129000	-6.370311000	28.260002000
H	9.010410000	-6.248034000	27.425268000
H	7.518921000	-7.046664000	27.923927000
H	8.841583000	-6.846588000	29.090185000
C	9.240069000	-4.095393000	32.748000000
C	10.020884000	-3.072558000	33.568695000
H	10.720435000	-2.527360000	32.930740000
H	10.586586000	-3.561692000	34.368028000
H	9.336264000	-2.351615000	34.025031000
C	8.222523000	-4.818982000	33.632635000
H	7.515376000	-4.102713000	34.061511000
H	8.723874000	-5.343160000	34.452724000
H	7.655026000	-5.551812000	33.051296000
C	10.192630000	-5.100960000	32.100118000
H	9.640976000	-5.814286000	31.481204000
H	10.733293000	-5.660063000	32.870637000
H	10.933502000	-4.592275000	31.476356000
C	14.157186000	-6.493265000	28.715928000
C	13.698756000	-7.049850000	27.363788000
H	12.609345000	-6.989884000	27.259244000
H	13.977126000	-8.103714000	27.264951000
H	14.161670000	-6.493881000	26.542230000
C	13.417140000	-7.200761000	29.853670000
H	13.723175000	-6.786038000	30.815697000
H	13.625371000	-8.276186000	29.841750000
H	12.335788000	-7.061243000	29.750328000
C	15.667525000	-6.684260000	28.853835000
H	16.197065000	-6.198506000	28.030030000
H	15.913839000	-7.751399000	28.839494000
H	16.031428000	-6.259480000	29.790723000
C	15.174883000	-4.169243000	32.382057000
C	14.327619000	-4.614051000	33.574569000

H	13.393009000	-4.047919000	33.605170000
H	14.865329000	-4.454863000	34.514918000
H	14.082217000	-5.677826000	33.493597000
C	16.464461000	-4.990628000	32.313146000
H	16.238606000	-6.060754000	32.258553000
H	17.078036000	-4.818378000	33.204016000
H	17.045791000	-4.706338000	31.432073000
C	15.497102000	-2.680898000	32.469202000
H	16.141824000	-2.380750000	31.640091000
H	16.018358000	-2.461595000	33.406437000
H	14.590474000	-2.072145000	32.425799000
C	16.564325000	-2.772222000	28.230284000
C	17.954631000	-3.385428000	28.048861000
H	18.520544000	-3.320866000	28.982995000
H	18.512145000	-2.855451000	27.269761000
H	17.882087000	-4.439620000	27.764675000
C	16.681348000	-1.302100000	28.624356000
H	15.699030000	-0.861282000	28.815595000
H	17.174179000	-0.730050000	27.831286000
H	17.281335000	-1.204365000	29.534005000
C	15.745753000	-2.926263000	26.948260000
H	15.609052000	-3.983793000	26.703002000
H	16.257328000	-2.442878000	26.110125000
H	14.763956000	-2.456295000	27.053171000

Cs₄-(N)₂

U	9.455055000	5.771052000	5.511042000
U	10.264963000	2.604713000	6.120316000
Cs	10.400037000	5.219423000	9.392470000
Cs	6.363669000	4.819796000	7.833637000
Cs	8.399854000	8.816010000	8.217617000
Cs	8.270253000	2.825370000	2.888641000
Si	11.672458000	0.819059000	2.958034000
Si	12.112067000	1.648657000	9.373598000
Si	6.968232000	0.724352000	6.146692000
Si	6.477304000	7.229953000	10.813440000
Si	11.959307000	8.263551000	7.213046000
Si	7.406196000	6.524914000	2.378743000
O	11.079021000	1.552121000	4.283987000
O	10.471295000	0.980823000	1.767147000
O	13.139191000	1.408455000	2.406369000
O	11.925221000	-0.828842000	3.087349000
O	8.062956000	6.782318000	6.194263000
O	11.473458000	2.311690000	8.031950000
O	13.768606000	1.392145000	9.308528000
O	11.490555000	0.172623000	9.856208000
O	11.722058000	2.711226000	10.636613000
O	8.498147000	1.216936000	5.946305000
O	6.771807000	-0.940627000	6.146580000
O	6.190843000	1.235480000	7.553548000
O	6.089128000	1.430691000	4.884084000
O	7.741961000	6.602281000	10.069415000
O	6.201721000	6.821720000	12.431833000
O	5.102730000	6.808094000	9.898475000
O	6.447703000	8.937489000	10.778548000
O	10.858950000	7.180331000	6.746123000
O	12.301379000	7.851262000	8.819630000
O	11.325228000	9.833516000	7.312071000
O	13.330463000	8.430724000	6.278801000
O	8.419955000	5.816062000	3.425125000
O	6.121552000	7.388626000	3.012228000
O	8.144505000	7.598015000	1.315673000
O	6.682433000	5.241894000	1.538428000
N	9.039775000	4.134958000	6.771387000

N	10.722280000	4.576919000	4.930463000
C	10.366980000	0.325632000	0.489059000
C	9.399227000	1.173727000	-0.342001000
H	9.279380000	0.752494000	-1.345266000
H	8.406472000	1.202237000	0.121003000
H	9.771897000	2.198272000	-0.443832000
C	11.716181000	0.254073000	-0.227203000
H	11.596800000	-0.232169000	-1.201427000
H	12.123275000	1.255318000	-0.391032000
H	12.439816000	-0.317449000	0.356324000
C	9.790675000	-1.077922000	0.687314000
H	9.666956000	-1.585712000	-0.275592000
H	10.454211000	-1.667999000	1.322279000
H	8.811607000	-1.020510000	1.172725000
C	14.332515000	3.157434000	3.549619000
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H	13.601409000	3.220864000	4.358911000
H	15.105990000	2.432987000	3.823330000
C	13.648726000	2.739394000	2.247580000
C	12.536343000	3.725056000	1.890792000
H	12.960541000	4.709655000	1.667003000
H	11.990787000	3.379897000	1.007226000
H	11.841892000	3.847711000	2.728756000
C	14.677858000	2.656012000	1.117024000
H	15.160277000	3.626169000	0.958565000
H	15.451592000	1.921054000	1.359921000
H	14.200417000	2.350962000	0.181177000
C	13.073192000	-1.580961000	3.508166000
C	13.825299000	-0.862365000	4.627700000
H	14.641562000	-1.488421000	5.004115000
H	14.248683000	0.075914000	4.262333000
H	13.148789000	-0.641566000	5.456529000
C	13.991873000	-1.800295000	2.303685000
H	14.864461000	-2.400388000	2.584308000
H	13.458020000	-2.328860000	1.507104000
H	14.338011000	-0.838228000	1.917704000
C	12.528177000	-2.919175000	4.010393000
H	13.344243000	-3.583603000	4.313572000
H	11.868952000	-2.762987000	4.868764000
H	11.954035000	-3.415501000	3.221707000
C	14.838227000	2.200860000	8.807355000
C	14.665646000	3.660148000	9.232494000
H	15.520186000	4.258286000	8.899566000
H	13.762215000	4.085991000	8.786684000
H	14.590043000	3.739142000	10.320677000
C	14.885697000	2.088052000	7.283706000
H	15.720783000	2.666822000	6.874933000
H	15.014030000	1.043832000	6.984061000
H	13.956664000	2.458942000	6.844215000
C	16.114817000	1.622398000	9.422423000
H	16.998256000	2.167400000	9.074063000
H	16.076473000	1.683384000	10.514279000
H	16.225705000	0.570424000	9.142974000
C	11.876303000	-1.171325000	9.521510000
C	12.216672000	-1.278376000	8.037082000
H	12.454910000	-2.312627000	7.767854000
H	11.371431000	-0.950706000	7.424943000
H	13.084382000	-0.656275000	7.803374000
C	13.077155000	-1.587827000	10.374953000
H	12.821109000	-1.553723000	11.438986000
H	13.380660000	-2.612562000	10.134753000
H	13.920803000	-0.918453000	10.193375000
C	10.670159000	-2.048082000	9.857877000
H	10.402774000	-1.938063000	10.913510000

H	9.806792000	-1.761098000	9.253387000
H	10.894541000	-3.102802000	9.667714000
C	11.768787000	2.482524000	12.057665000
C	11.816721000	3.868197000	12.707389000
H	11.872560000	3.782232000	13.797305000
H	12.694186000	4.424137000	12.361963000
H	10.917270000	4.446254000	12.470244000
C	10.496197000	1.744700000	12.480958000
H	10.478591000	1.587576000	13.565125000
H	9.611061000	2.327064000	12.204618000
H	10.443022000	0.777605000	11.977306000
C	13.011986000	1.691427000	12.466207000
H	13.032878000	1.561019000	13.553474000
H	13.015908000	0.704947000	12.000717000
H	13.923108000	2.215488000	12.165292000
C	7.434640000	-1.944150000	5.360495000
C	7.606596000	-1.484841000	3.912588000
H	8.069877000	-2.276957000	3.316376000
H	6.638239000	-1.238435000	3.465923000
H	8.257910000	-0.607506000	3.865679000
C	8.797065000	-2.244871000	5.984013000
H	9.316937000	-3.027617000	5.422378000
H	9.415259000	-1.344085000	5.980112000
H	8.676577000	-2.587691000	7.016359000
C	6.534979000	-3.179841000	5.423617000
H	6.982977000	-4.014047000	4.874017000
H	6.387865000	-3.490833000	6.462338000
H	5.553664000	-2.966595000	4.988860000
C	6.143504000	0.584465000	8.839181000
C	5.760267000	1.669052000	9.845304000
H	5.614375000	1.239710000	10.841302000
H	6.550498000	2.421821000	9.921978000
H	4.825639000	2.156251000	9.546637000
C	7.504275000	-0.004166000	9.203821000
H	7.480031000	-0.433001000	10.210929000
H	7.772668000	-0.796243000	8.501189000
H	8.283166000	0.762701000	9.176613000
C	5.067602000	-0.503825000	8.820153000
H	5.003319000	-0.998128000	9.795606000
H	4.087753000	-0.068759000	8.595717000
H	5.303564000	-1.252397000	8.061212000
C	4.671201000	1.439698000	4.648812000
C	4.064641000	2.637567000	5.385386000
H	4.208842000	2.512679000	6.462023000
H	4.548127000	3.564626000	5.058786000
H	2.991593000	2.723354000	5.182688000
C	3.991584000	0.145901000	5.098204000
H	4.416668000	-0.718856000	4.583393000
H	4.108990000	-0.007949000	6.172254000
H	2.921086000	0.191693000	4.870937000
C	4.501088000	1.607157000	3.138170000
H	4.961587000	0.767823000	2.606891000
H	3.442221000	1.646731000	2.863324000
H	4.969682000	2.536616000	2.801624000
C	6.688424000	5.684390000	13.155671000
C	8.140490000	5.937329000	13.569692000
H	8.545570000	5.086610000	14.127987000
H	8.752004000	6.098666000	12.676982000
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C	6.601879000	4.414669000	12.306119000
H	6.987313000	3.550368000	12.857248000
H	5.565545000	4.205040000	12.025868000
H	7.191484000	4.550320000	11.394225000
C	5.798970000	5.560597000	14.393877000

H	6.119352000	4.724015000	15.023730000
H	5.843391000	6.477853000	14.988987000
H	4.757478000	5.393897000	14.102293000
C	3.697162000	6.970394000	10.120626000
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H	3.822369000	7.995996000	12.025618000
H	3.789982000	9.076713000	10.620835000
H	2.300250000	8.262537000	11.152864000
C	3.071861000	7.204847000	8.741878000
H	1.985025000	7.316164000	8.815293000
H	3.482108000	8.111764000	8.287320000
H	3.278424000	6.361835000	8.073248000
C	3.149597000	5.677458000	10.733192000
H	3.591113000	5.510026000	11.719026000
H	2.061121000	5.725794000	10.846541000
H	3.387009000	4.817742000	10.097216000
C	6.860804000	9.915100000	11.741789000
C	5.889379000	9.955285000	12.924989000
H	5.847256000	8.977769000	13.408788000
H	6.210846000	10.703052000	13.658179000
H	4.883727000	10.220909000	12.587500000
C	6.826341000	11.262853000	11.012898000
H	7.063654000	12.082751000	11.698400000
H	7.556034000	11.292926000	10.195765000
H	5.831920000	11.439898000	10.592211000
C	8.279199000	9.625417000	12.239093000
H	8.316705000	8.656496000	12.741374000
H	8.991328000	9.609664000	11.407871000
H	8.608513000	10.393883000	12.946685000
C	13.443980000	7.488572000	10.864185000
H	14.043330000	7.931454000	11.666334000
H	12.546821000	7.056017000	11.319570000
H	14.024164000	6.683058000	10.404051000
C	13.069227000	8.543277000	9.820357000
C	14.341206000	9.159224000	9.236968000
H	14.918036000	9.647802000	10.029287000
H	14.968894000	8.389293000	8.780921000
H	14.107168000	9.903515000	8.473330000
C	12.195368000	9.624349000	10.461170000
H	12.741601000	10.152223000	11.250225000
H	11.876296000	10.347255000	9.706918000
H	11.306717000	9.171402000	10.913289000
C	11.399244000	10.930342000	6.381924000
C	12.784061000	11.576413000	6.458109000
H	12.849957000	12.430145000	5.775062000
H	12.980886000	11.937955000	7.472774000
H	13.552048000	10.849176000	6.187515000
C	11.098317000	10.457774000	4.959374000
H	11.085122000	11.305734000	4.266247000
H	11.859955000	9.750774000	4.623799000
H	10.121730000	9.966158000	4.913990000
C	10.338504000	11.937763000	6.835438000
H	10.389437000	12.849855000	6.232708000
H	9.329276000	11.526411000	6.723520000
H	10.493198000	12.211021000	7.884236000
C	14.139737000	7.454452000	5.596897000
C	15.527737000	8.086050000	5.474822000
H	16.211954000	7.415788000	4.944700000
H	15.471420000	9.028566000	4.921298000
H	15.945334000	8.295428000	6.464065000
C	13.546387000	7.204602000	4.210805000
H	14.205146000	6.556541000	3.623934000
H	12.575567000	6.707230000	4.287841000
H	13.430623000	8.149069000	3.669844000

C	14.206316000	6.153101000	6.391926000
H	14.866068000	5.434840000	5.895809000
H	14.591908000	6.335835000	7.398989000
H	13.212536000	5.701136000	6.463432000
C	5.983722000	8.755608000	3.414655000
C	4.910534000	8.757260000	4.505967000
H	4.702829000	9.775985000	4.851490000
H	3.978961000	8.326379000	4.126073000
H	5.246517000	8.156649000	5.356492000
C	7.295743000	9.310300000	3.971940000
H	7.150140000	10.333449000	4.338294000
H	7.643370000	8.675577000	4.792961000
H	8.060280000	9.331394000	3.191163000
C	5.526644000	9.577645000	2.207062000
H	5.367341000	10.625661000	2.484181000
H	6.284277000	9.535998000	1.419950000
H	4.585811000	9.183297000	1.809670000
C	9.414745000	7.520220000	0.655819000
C	10.500504000	8.034014000	1.603274000
H	10.270042000	9.053207000	1.928448000
H	10.569254000	7.390412000	2.483816000
H	11.478055000	8.044693000	1.109446000
C	9.304548000	8.435827000	-0.565390000
H	9.048792000	9.453014000	-0.253173000
H	10.250992000	8.470138000	-1.114991000
H	8.522566000	8.081451000	-1.243406000
C	9.729551000	6.087140000	0.222316000
H	8.943815000	5.697178000	-0.431121000
H	10.680340000	6.050188000	-0.319568000
H	9.813971000	5.441166000	1.100702000
C	5.591296000	5.271111000	0.599916000
C	4.267031000	5.350136000	1.364163000
H	4.235212000	6.264507000	1.959474000
H	3.418760000	5.341540000	0.670929000
H	4.162418000	4.497685000	2.041381000
C	5.707111000	6.445800000	-0.373125000
H	5.666099000	7.400324000	0.155156000
H	6.649120000	6.402868000	-0.925977000
H	4.883382000	6.414801000	-1.094355000
C	5.678980000	3.955352000	-0.178333000
H	4.874573000	3.885536000	-0.917692000
H	6.636145000	3.884567000	-0.704953000
H	5.587709000	3.097966000	0.496530000

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