Supporting Information to Accompany "Shining Light on Dinitrogen Cleavage: Structural Features, Redox Chemistry, and Photochemistry of the Key Intermediate Bridging Dinitrogen Complex"

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Contents:

Synthetic Procedures

General Remarks

All manipulations were carried out under an atmosphere of purified nitrogen in a Vacuum Atmospheres Model MO-40M glovebox equipped with the QP-30 accessory, or by standard Schlenk techniques.[1,2] Inside the MO-40M glovebox the ambient temperature ranged from 18–22 °C. All glassware was oven-dried at a temperature above 150 °C for at least 12 hours and allowed to cool under dynamic vacuum prior to use. Celite, alumina, and 4 Å sieves were activated by heating to a temperature greater than 180 °C under a dynamic vacuum for 2 d (Celite) or 5 d (alumina and 4 Å sieves). Et_2O, *n*-hexane, *n*-pentane, and toluene were bubble degassed with nitrogen and forced, under positive pressure, through a column of activated alumina followed by a column of activated Q5.[3] CH_2Cl_2 was bubble degassed with nitrogen and forced, under positive pressure, through two columns of activated alumina.[3] THF was taken from an Aldrich Pure-Pac and under positive pressure passed through two columns of activated molecular sieves. THF was additionally stirred over sodium metal which was removed by filtration through activated alumina or Celite prior to use. MeCN was taken from an Aldrich Sure-Seal bottle, filtered through a column of activated alumina (4 x 3 cm), and degassed under a dynamic vacuum. $O(SiMe_3)_2$ was distilled from dark purple solutions of sodium benzophenone ketyl. MeCy was distilled from CaH_2. All solvents were stored over 4 Å sieves. C_6D_6 was degassed by three freeze-pump-thaw cycles and stored over 4 Å sieves for 3 d prior to use. CD_2Cl_2 was refluxed over CaH_2 for 24 h then distilled and stored over 4 Å sieves. ^1H and ^{13}C NMR shifts are referenced against residual solvent resonances (for CD_2Cl_2 5.32 ppm and 54.00 ppm). All ^{15}N NMR spectra are externally referenced to neat $H_3CC^{15}N$ (δ = 245 ppm) in comparison to liquid NH_3 (δ = 0 ppm).[4] UV-Vis spectra were obtained on Cary 500i or HP8453 spectrophotometers in 1 cm quartz cells manufactured by Starna. Positive ion ESI-MS were obtained using a Bruker Daltonics APEXIV, 4.7 T Fourier Transform Ion Cyclotron Resonance Mass Spectrometer. Combustion analysis was preformed by Midwest Microlab, LLC (Indianapolis, IN). Literature procedures were used for the preparation of **1**[5-7], $[Cp_2Fe][B(Ar^F)_4]$[8], $K_2[C_8H_8]$[9], $[N(n\text{-}Bu)_4][B(C_6F_5)_4]$[10,11], and $K_3[Fe(O_4C_2)_3]$[12]. $[NH_4][(H_3N)_2Cr(NCS)_4]$ was purchased from TCI chemicals and treated with KNO_3 to afford $K[(H_3N)_2Cr(NCS)_4]$.[13]

Reduction of $2[B(Ar^F)_4]_2$ to 2

At –108 °C, to a stirred red solution of $\mathbf{2}[B(Ar^F)_2]_2$ (800 mg, 0.2663 mmol; 40 mL THF) was added a red solution of $K_2[C_8H_8]$ (50 mg, 0.2747 mmol, 1.03 equiv) in 10 mL THF dropwise. Upon completing addition the initially red solutions had turned bright purple. The purple solution was stirred for 5 min before the mixture the solvent was removed under a dynamic vacuum. To resulting resin was twice added 20 mL of *n*-hexane which was each time removed under a dynamic vacuum. The product was then extracted into toluene (60 mL), filtered through celite two times, and the solvent removed under a dynamic vacuum. The product **2** (290 mg, 0.227 mmol, 85.3%) was collected as a purple powder. A small amount of **3** was formed during manipulations, the amount was judged to be less than 5% by ^1H NMR.

Determination of Molecular Structure by X-ray Diffraction

General Remarks

X-ray diffraction data were collected using a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å), performing ϕ- and ω-scans. The structure was solved by direct methods using SHELXS[14] and refined against F^2 on all data by full-matrix least squares with SHELXL-97[15] All non-hydrogen atoms were refined anisotropically; all hydrogen atoms were included into the model at their geometrically calculated positions and refined using a riding model.

Disorders in the structures of **2** in $P2_1/n$, **3**, and $\mathbf{2}[B(Ar^F)_4]_2$ were refined with the help of similarity restraints on 1-2 and 1-3 distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters. The ratios were refined freely, while constraining the total occupancy of all components to unity. All bond distances and angles between atoms involved in a disorder given in this publication refer to the main component of the disorders. Further details for the X-ray structure solution for **3** will appear elsewhere.[16]

Crystal Growth of 2 in *P*2/*n*

As solid powders, **1** (circa 200 mg) was mixed with (circa 230 mg, 5 equiv) of mesitonitrile. To this mixture was added approximately 10 mL of MeCy to form a saturated solution. The purple solution was filtered and layered with an equal volume of $O(SiMe_3)_2$. The solution was stored at –35 °C for 4 to 7 d, and the solution was decanted away from colorless crystals, presumably mesityl nitrile. This was repeated three times before purple crystals formed. The purple crystals gave the structure of **2**.

Crystal Growth of 2 in $P2_1/n$

A saturated solution of **1** in n-pentane was filtered through glass wool and diluted to approximately 1.25 times its original volume. The solution was then layered with an equal volume of $O(SiMe_3)_2$ and stored at –35 °C for 3 to 4 weeks to afford purple crystals of **2**.

Crystal Growth of $2[B(Ar^F)_4]$

A red solution mixture was formed by stirring $\mathbf{2}[B(Ar^F)_4]_2$ in 3mL of THF. This mixture was filtered through glass wool to remove undissolved solids. The resulting solution was then diluted to a total volume of 5 mL. The solution was transferred into a 10 mL vial that was placed inside of a capped 20 mL vial. The 20 mL vial contained approximately 5 mL of *n*-pentane for the purpose of vapor diffusion. The 20 mL vial was tightly capped and stored at 22 °C for 2d. Crystals obtained via vapor diffusion were suitable for X-ray diffraction.

Crystal Growth of $2[B(Ar^F)_4]_2$

To 4 mL of THF was added more $\mathbf{2}[B(Ar^F)_4]_2$ then could be completely dissolved to form a darkly colored (nearly black) mixture. The mixture was filtered through glass wool to obtain a saturated solution which was diluted by the addition of an additional 4 mL of THF. To this solution was carefully added 4 mL of Et_2O/*n*-hexane (2:1), forming a colorless layer above the solution of $\mathbf{2}[B(Ar^F)_4]_2$. The two liquid phases were allowed to slowly mix (via diffusion) when this mixture was stored at –35 °C for 1 to 3 d to afforded crystals of $\mathbf{2}[B(Ar^F)_4]_2$.

Crystal Growth of 3

A saturated solution of **3** in 8 mL of Et_2O/*n*-hexane (2:1) was filtered through glass wool and diluted to a total volume of 12 mL. Storing this solution at –35 °C for 4 d afforded yellow crystals of **3**.

Thermal stability of 2 as single crystals

These experiments were carried out using crystals of **2** in $P2_1/n$ that contain *n*-pentane into the unit cell

By UV-Vis Spectroscopy

A piece of Whatman #1 filter paper was covered in Nujol oil and placed against the side of a quartz cuvette, and the UV-Vis spectrum was measured. This spectrum serves as a background for the experiment. The same piece of filter paper was cycled into the glove box and a small amount of **2** added to the surface. The compound was smeared across the surface of the filter paper with a metallic spatula, while care was taken not to crush the crystals. The crystals were coated in Nujol oil and UV-Vis spectrum monitored as a function of time. After 22 h, no net changes in the absorption were observed.

By Unit Cell Determination

Singles crystals of **2** were removed from the glovebox on a glass microscope slide covered with petroleum oil. One crystal was mounted and from that crystal both the unit cell and molecular structure of **2** were determined. The remaining singles crystals were allowed to stand overnight under petroleum oil. After 24 h, another crystal was mounted on the diffractometer and a unit cell search was performed. The metric parameters of the unit cell matched the unit cell parameters obtained 24 h earlier.

Computational Details

All density functional theory (DFT) calculations were carried out using the Amsterdam Density Functional (ADF) program package, version 2004.01.[17-19] The local exchange-correlation potential of Vosko et al.[20] (VWN) was augmented self-consistently with gradient-corrected functionals for electron exchange according to Becke[21] and for electron correlation according to Perdew.[22,23] This nonlocal density functional is termed BP86 in the literature and has been shown to give excellent results for both the geometries and energetics of transition-metal systems.[24] Relativistic effects were included using the zero-order regular approximation (ZORA).[25,26] The basis set used was the all-electron ADF ZORA/TZ2P (triple ζ with two polarization functions) basis. Crystallographically determined atomic coordinates were used as input, and the geometry optimization calculation constrained to crystallographic symmetry elements. Therefore, calculations were restricted to C_2 symmetry for **2** and to C_i symmetry for **2**$[B(Ar^F)_4]_2$. The orbital contour plot in Figure 4 is shown at an isosurface value of 0.03t.

Photochemical Reactions

General Remarks

Photochemical reactions were performed using a 1000 W, high-pressure Hg/Xe arc lamp (Oriel) as a broadband light source. The broadband light was passed through a water-jacket cooled, long wavelength pass filter (480 nm, Oriel) followed by an aperture and a culminating lens. The light was focused onto the sample through a Pyrex beaker used as a cooling bath.

Bulk Photolysis of 2

To a 250 mL Schlenk flask containing **2** (200 mg, 0.157 mmol) was added 200 mL Et_2O. The mixture was rapidly stirred at 20 °C to form a purple solution. The solution was then cooled to –78 °C in a dry-ice/EtOH bath before it was exposed to broadband light ($\lambda \geq 480$ nm). The solution was stirred during photolysis and remained purple in color for 10 min. Then the solution rapidly took on a yellow-orange hue and the reaction was judged to be complete. The solution was stripped of solvent under a dynamic vacuum yielding 196 mg (99% based on products, *vide infra*) of material. The solids were taken up in 50 mL Et_2O to form a homogenous solution. A 3 mL aliquot was taken from the solution, dried under a dynamic vacuum, and dissolved in C_6D_6 for ^{1}H NMR analysis. The ^{1}H NMR spectrum showed the production of both **1** and **3** during photolysis. A 20 mL aliquot taken from the Et_2O solution, was transferred into a 50 mL Schlenk flask, cooled to –78 °C, and exposed to NO gas (2.0 mL, 1 atm, 1.3 equiv based on **2**). The reaction was stirred at –78 °C for 10 min, then the cooling bath was removed and the reaction stirred for an additional 10 min, and then the solvent was removed under a dynamic vacuum. The residue was taken up in C_6D_6 for ^{1}H NMR analysis.

Two diamagnetic materials: **3** and $ONMo(N[t\text{-}Bu]Ar)_3$ were observed by ^{1}H NMR spectroscopy. No resonances attributable to **1** were located in the ^{1}H NMR after treatment with NO, as the reaction between **1** and NO has previously been shown to be both rapid and quantitative.[7,27] Integration of the *tert*-butyl resonances $ONMo(N[t\text{-}Bu]Ar)_3$ and **3** indicated a 56:44 ratio between the two products. This corresponds to a 56:44 ratio of **1**:**3** formed during photolysis.

Quantum Yield Determination for 2

Light from 1000 W arc lamp was passed through a 480 nm long wavelength pass filter followed by a 546 nm line filter. Samples were loaded into matched curvettes (Starna), placed in an immobile curvette holder, and stirred during irradiation. To ensure that thermal reactions were not competing with the photochemical process, the absorbance spectrum of the sample prior to irradiation was compared to a duplicate sample that was stored in the dark during irradiation. These manipulations were carried out under a red dark room lamp to minimize photolysis from ambient light. The quantum yield was calculated using the following equation:

$$\frac{N}{t} = \frac{V_{irr}\Delta A}{\phi \varepsilon t_{irr} l F}$$

where N/t is the number of moles of photons incident on the face of the cuvette per unit time, V_{irr} is the sample volume, ΔA is the change in absorbance of the sample at a given wavelength, ϕ is the quantum yield, ε is the molar extinction coefficient of the sample, t_{irr} is the time of irradiation, l is the pathlength of the sample, and F is the mean fraction of light absorbed. The intensity of the incident light was determined by chemical actinometry using both Reineke's salt and potassium ferrioxalate. The actinometry was staggered with respect to sample photolysis to confirm the stability of the photon flux. Both actinometric procedures are described.

Reineke's Salt Actinometry

A 0.05 M solution of $K[(H_3N)_2Cr(NCS)_4]$ in water was irradiated for 20 s at 20 °C. The absorbance of the solution at 545 nm was measured before and after irradiation to determine the

mean fraction of light absorbed. The number of moles of Reinecke salt reacted was determined by assaying the amount of Ferric thiocyanate formed. An aliquot of 1 mL of photolyzed sample was combined with 4 mL of an aqueous 0.1 M $Fe(NO_3)_3$ / 0.4 M $HClO_4$ solution. The solution was allowed to stand for 1 min before the absorbance of Fe^{3+} thiocyanate at 450 nm was recorded.[13,28] The procedure was then repeated with an unphotolyzed solution of the Reinecke salt to account for thermal reactivity. Three runs were averaged to determine the intensity of light incident on the sample.

Potassium Ferrioxalate Actinometry

The absorbance of a 0.15 M solution of $K_3[Fe(C_2O_4)_3]$ was measured at 550 nm measured before and after the solution was irradiated for 20 min at 20 °C, to determine the mean fraction of light absorbed. The number of moles of ferrous ion produced was then determined by quantifying the amount of $[Fe(phenanthroline)_3]^{2+}$ produced upon treatment with phenanthroline. This was accomplished by adding 1 mL of photolyzed sample, 0.5 mL of acetate buffer (600 mL of 1 M NaOAc and 360 mL 0.5 M H_2SO_4 diluted to a total volume of 1 L), and 2 mL of a 0.1 % aqueous phenanthroline solution to 10 mL of deionized water. After standing for 15 minutes the amount of $[Fe(phenanthroline)_3]^{2+}$ was determined by measuring the absorbance at 510 nm (ε = 11100 M^{-1} cm^{-1}).[12,28] The procedure was repeated with a sample of unphotolyzed ferrioxalate. Three runs were averaged to determine the intensity of light incident on the sample.

Photolysis of 2

The absorbance of Et_2O solutions of **2** was determined by measurement of the absorbance at 544 nm before these solutions were irradiated at –78 °C for 2 s intervals, and the absorbance at 544 nm was again measured after irradiation. The change in absorbance at 544 nm was used to determine the number of moles of **2** undergoing photolysis. Prior to irradiation, solutions of **2** ranged in concentration from 60 to 19 μM (ε = 41000 M^{-1} cm^{-1}). Varying the concentration within this range had a negligible effect upon the measured quantum yield. Samples of **2** stored in the dark at –78 °C showed no appreciable absorbance change during the timescale of the photolysis experiment, indicating thermal reactivity was negligible. Three runs were averaged to obtain quantum yields by the $K[(H_3N)_2Cr(NCS)_4]$ method Φ_p = 0.0505 (σ = 0.00689), and by the $K_3[Fe(C_2O_4)_3]$ method Φ_p = 0.0505 (σ = 0.0136).

Physical Measurements

Raman Spectroscopy

An Invictus solids state laser at 785 nm, manufactured by Kaiser Optics, or a Coherent Ar/ion laser at 514.5 nm was routed through fiber optic cables to a Hololab series 5000 Raman Microscope. The sample was placed, in a sealed container, under the objective of the microscope. The Raman scattering was observed via 180° reflectance through the objective of the Raman microscope. Each spectrum was collected for corrected for dark current and cosmic ray interference using the Hololab software. Solvent signals were subtracted using GRAMS software. Solutions of **2**$[B(Ar^F)_4]_2$ in CH_2Cl_2 were contained in 1 cm quartz cuvettes (Starna) and a single spectrum was acquired over 10 s using a 514.5 nm laser at a power of 9.7 mW. Solutions of **2**$[B(Ar^F)_4]$ in $CDCl_3$ were held in a 528-PP NMR tube (Wilmad); 8 spectra were collected, for 2 each, and averaged using a 785 nm laser at a power of 30 mW. Raman shifts are corrected to an external standard of cyclohexane (801.3 cm^{-1}), however these corrections were small (less than 1.5 cm^{-1}).

SQUID measurement of 2

A Quantum Design MPMS*XL* instrument was used for this measurement. A 137.5 mg sample of **2** was weighed into a gel cap (B&B pharmaceuticals), taking care to keep the sample chilled during the transfer process. The gel cap was then inserted into a straw (Quantum Design). The assembled gel cap and straw were placed into a Zip-lock bag before it was transported outside of the glovebox. The time between removing **2** from the freezer and loading it into the SQUID was kept as short as possible. The sample was loaded into the SQUID at 150 K and centered at a field of 50000 Oe. After centering, the sample was slowly cooled to 5 K at zero magnetic field. The SQUID measurement was performed at 3 fields 50000, 25000, and 5000 Oe. Because **2** is not thermally stable, data was collected between 5 and 250 K at all three fields before data was collected a higher temperatures (250-300 K) at 5000 Oe. Between measurements, **2** was cooled from 250 K to 5 K at 0 Oe. For every measurement, the long voltage was measured by averaging 3 scans of 64 data points over a 6 cm region of the straw. A correction made for the magnetic moment of the straw and gel cap was made by measuring their moment alone, and this negative number was subtracted from the observed long moment of the sample at each field. A diamagnetic correction of $-8.02(10^{-4})$ cm^3 mol was applied to the observed molar susceptibility. Contributions to the observed magnetic moment made by temperature independent paramagnetism (TIP) were fit and subtracted from the data using the JulX computer program.[29] JulX was also used to fit the data to magnetic models. The molar susceptibility (X_M) data are deposited in **Table S2**.

Susceptibility of 2 Measured by the Evans Method[30,31]

A stock solution of C_6D_6 containing a few drops of $O(SiMe_3)_2$ was prepared. This solution and **2** (70.1 mg, 0.055 mmol) were combined in a 10 mL volumetric flask. The resulting mixture was stirred for 3 min to ensure that a homogenous solution (55 mM of **2**) had been formed. An aliquant from this solution was then transferred to an NMR tube that contained a sealed capillary of the $C_6D_6/O(SiMe_3)_2$ stock solution. At this time the NMR tube was immediately transported to the NMR spectrometer. The difference in resonant frequency between the methyl protons of $O(SiMe_3)_2$ in the capillary and the solution containing **2** was measured by ^1H NMR spectroscopy. The separation between these two peaks was 23.05 Hz at 20 °C on a 600 MHz spectrometer. This measure value corresponds to a magnetic dipole moment of 2.40 μ_B when the diamagnetic correction of –0.008070 cm^3 mol, calculated from Pascal's constants, is applied.

SQUID measurement of 2$[B(Ar^F)_4]$

A Quantum Design MPMS*XL* instrument was used for this measurement. The sample was weighed into a gel cap. The gel cap was punctured and the puncture sealed with a small amount of M-grease. The gel cap loaded into a straw and the straw was placed into a Zip-lock bag before it was transported outside of the glovebox. The time between removing **2**$[B(Ar^F)_4]$ from the freezer and loading it into the SQUID was kept as short as possible. The sample was loaded into the SQUID at 150 K and centered at a field

of 5000 Oe. After centering, the sample was slowly cooled to 5 K at zero magnetic field. The SQUID measurement at a field of 5000 Oe was then performed from 5 K warming to 300 K. The long voltage was measured by averaging 3 scans of 64 data points over a 6 cm region of the straw. A correction made for the magnetic moment of the straw and gel cap was made by measuring their moment alone, and this negative number was subtracted from the observed long moment of the sample at each temperature. A diamagnetic correction of $-1.29(10^{-3})$ cm^3 mol was applied to the observed molar susceptibility. A Weiss constant was not determined because the plot of $1/\chi T$ vs. T was non-linear. The molar susceptibility (X_M) is deposited in **Table S3**.

Transient Absorbtion and Nanosecond Kinetics for photochemical decomposition of 2

Excitation (pump) light for nanosecond transient absorption experiments (525-560 nm) was provided by a tunable MOPO-OPO system that was pumped by the third harmonic ouptut of a Quanta Ray Lab–190 Nd:YAG nanosecond pulsed laser (Spectra-Physics). The signal (probe) light was provided by a Xe arc lamp (75 W, PTI), focused onto the sample, collinearly overlapped with the excitation beam, collimated after the sample, and focused onto the entrance slit of Triax 320 spectrometer. The signal light was dispersed by a 300 × 500 blazed grating and collected with either an intensified gated CCD camera (ICCD, CCD 30-11, Andor Technology, 1024 × 256 pixels, 26 μm^2) for transient absorbtion (TA) spectra or a photomultiplier tube (PMT) for TA kinetics at a single wavelength. PMT outputs were collected and averaged with a 1 GHz oscilloscope (LeCroy 9384CM).

To produce a TA spectrum, a series of four spectra were taken: I_F (pump on/probe off), I (pump on/probe on), I_B (pump off/probe off), and I_0 (pump off/probe on). Uniblitz shutters driven by delay generators (DG535, Stanford Research Systems) and T132 Uniblitz shutter drivers were used to block the pump and probe light in this sequence using a TTL trigger from the Q-switch of the laser. Transient spectra were corrected for fluorescence and background light using these spectra by the calculation: $\Delta OD = \log[(I_0 - I_B)/(I - I_F)]$. Spectra reported are the average of 1250 of the four-spectra sequences. The instrument control and data analysis were performed by custom software written in LabView. Kinetic runs were obtained by monitoring the signal beam at 530 nm. Data was obtained using stirred Et_2O solutions of **2** in sealed cuvettes at 20 °C. Freshly prepared solutions were used for each data collection.

Electrochemistry of 2[B(Ar^F)$_4$]$_2$

A Bioanalytic Systems CW-50 potentiostat, 1 mm diameter Pt disk working electrode, curly Pt wire counter electrode, and Ag wire pseudo-reference electrode were used for all measurements. All measurements are corrected to $Cp_2Fe^{0/+}$ by the addition of Cp_2Fe as an internal standard. Measurements were made in 0.1 M [(*n*-Bu)$_4$N][B(C$_6$F$_5$)$_4$] or 0.5 M [(*n*-Bu)$_4$N][PF$_6$] solutions in THF. Cyclic voltammograms of **2**[B(Ar^F)$_4$]$_2$ were performed at a range of scan rates from 50 to 1000 mV/s and concentrations ranging from 40 μM to 4 mM without change in the I_{pc}/I_{pa} ratio for either of the two Faradaic processes. Redox couples for the **2**/**2**$^+$/**2**$^{2+}$ system are deposited in **Table S1**.

Spectroelectrochemical 2e Oxidation of 2

A curvette was loaded with a 0.5 M THF solution of [(*n*-Bu)$_4$N][PF$_6$] was sealed with a silicone septum and fitted with electrodes: a Pt mesh working electrode, a Pt wire auxiliary electrode, and a Ag wire pseudo-reference electrode. The sealed cuvette was removed from the glovebox and placed under positive Ar pressure. The electrolyte solution was stirred and a –200 potential was applied across the cell. Then 50 μL of a 1.35 mM THF stock solution of **2** was injected into the cell. An immediate response in both current and absorbance was noted. UV-Vis spectra were acquired continuously in 0.5 s intervals until not further change in the absorbance was noted. Spectra are baseline corrected with respect to an average baseline between 750 nm and 850 nm where the absorbance is close to 0 for all three chromophores.

Spectroelectrochemical Reduction of 2[B(Ar^F)$_4$]$_2$ at an optically transparent thin-layer electrode (OTTLE)

A solution of **2**$^{2+}$ was prepared by dissolving **2**[B(Ar^F)$_4$]$_2$ into a solution of 0.5 M [(*n*-Bu)$_4$N][PF$_6$]/THF. A UV-Vis spectrum of this solution was taken before electrodes were connected OTTLE and after the electrodes were connected, at a potential of –50 mV. No spectral change was noted between these two spectra of **2**$^{2+}$. The potential was then moved to –750 mV where changes in the visible region absorbance were observed. The OTTLE was held at –750 mV until no further spectral changes occurred. Returning the potential to –50 mV quantitatively regenerated the initial spectrum. All spectra had a background spectrum 0.5 M [(*n*-Bu)$_4$N][PF$_6$]/THF subtracted. The OTTLE design was adapted from literature descriptions (Figure S23).[32,33] The OTTLE contained both a KBr and a glass window. A 100 mesh Pt grid, Ag wire, and Pt wire were used to generate a potential difference across the cell.

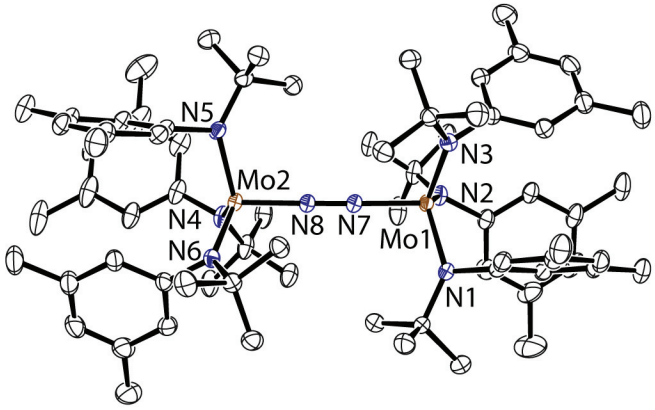

Figure S1. X-ray crystal structure of crystals of **2** grown from *n*-pentane. Crystal parameters, $P2_1/n$: a = 20.7 Å, b = 11.3 Å, c = 31.3 Å, β = 99.9°. A disordered *n*-pentane is contained in the unit cell.

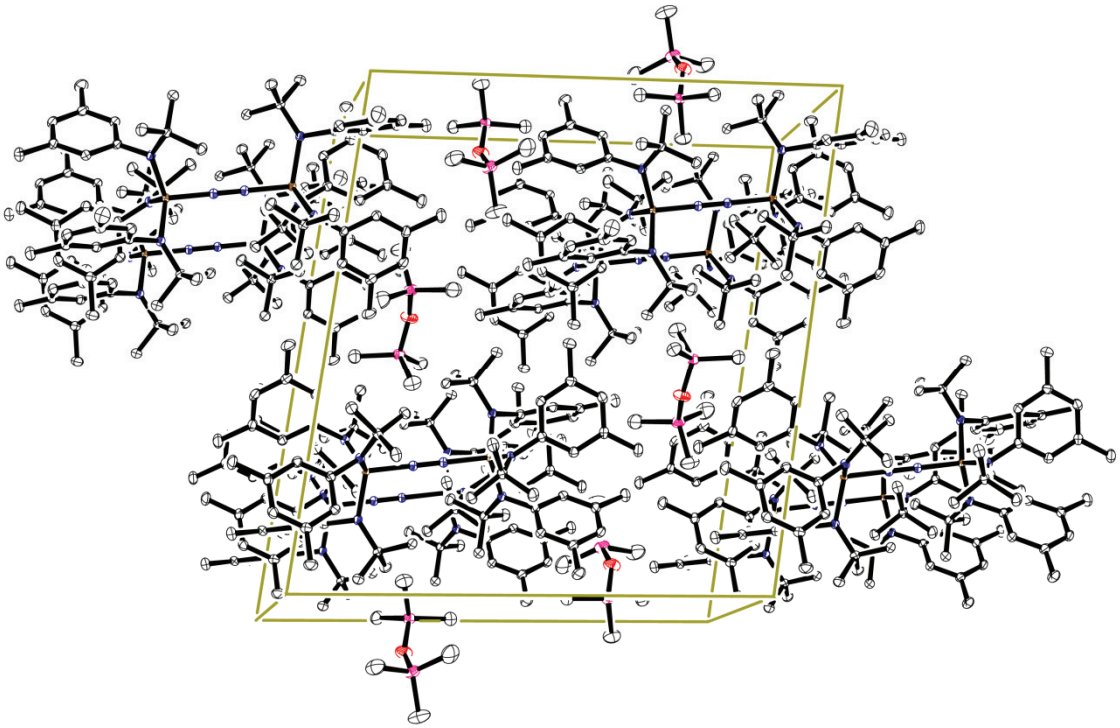

Figure S2. Packing Diagram for the crystal structure of crystals of **2** in $P2/n$ that contain $O(SiMe_3)_2$ in the unit cell.

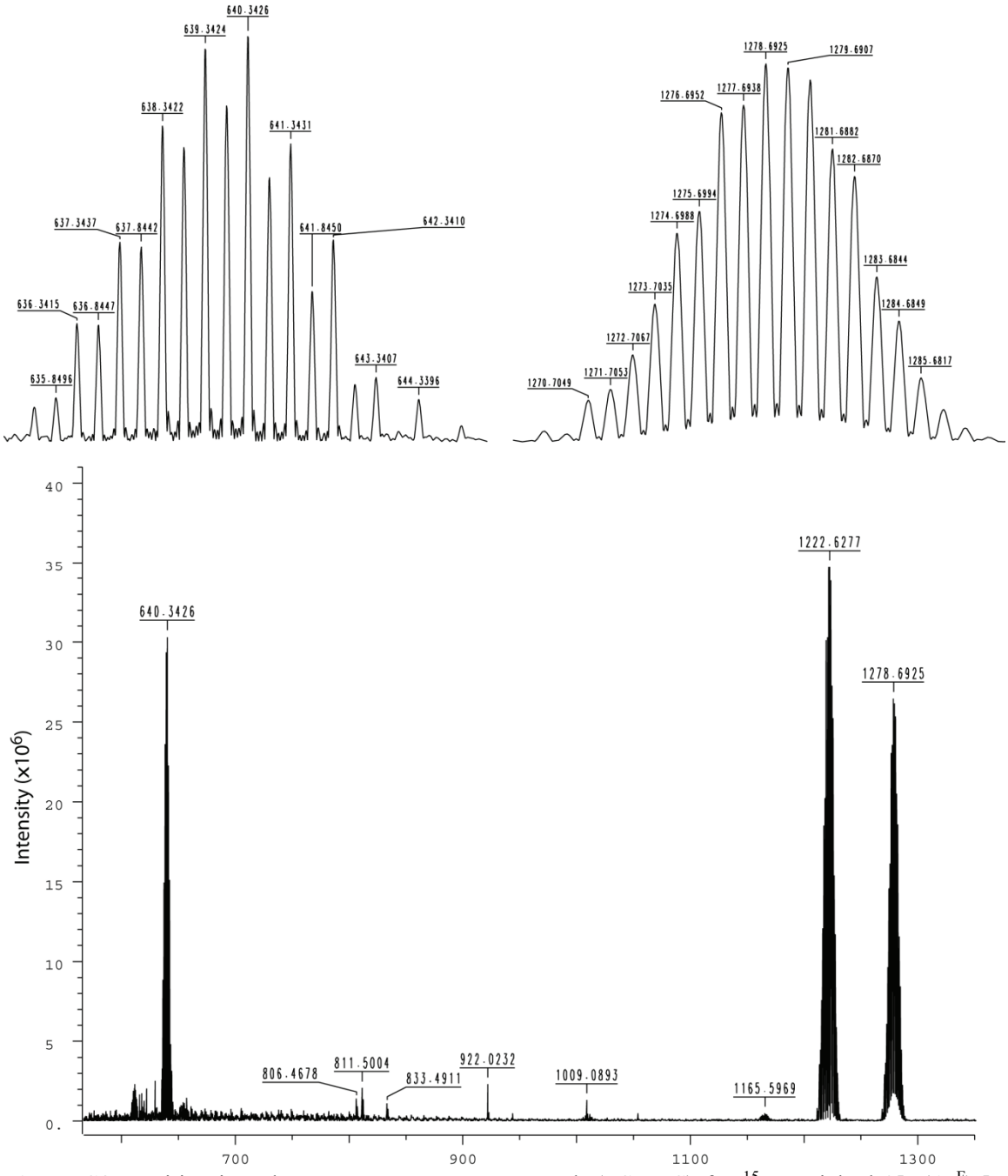

Figure S3. Positive-ion electrospray mass spectrograph (ESI-MS) for ^{15}N-enriched **2**[B(Ar^{F})$_4$]$_2$. Above are shown the isotope patterns for 2^{2+}, 640 amu; 2^{+}–(*t*-Bu), 1222 amu; and 2^{+}, 1278 amu.

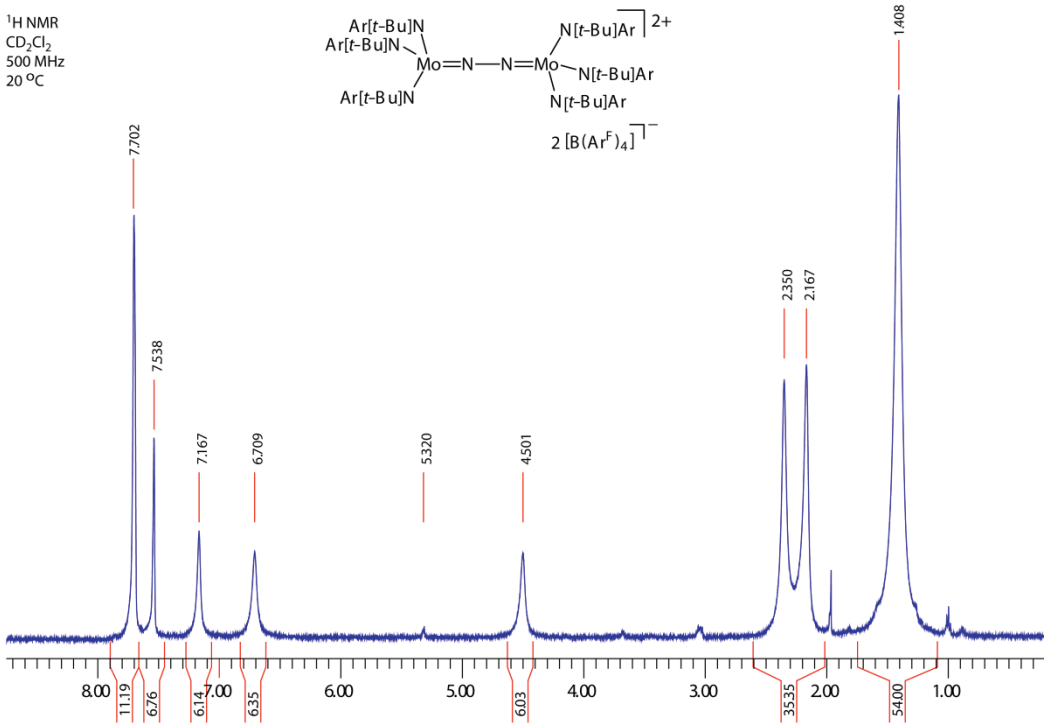

Figure S4. ^{1}H NMR spectrum of **2**[B(Ar^{F})$_4$]$_2$ (500 MHz, CD_2Cl_2, 20 °C).

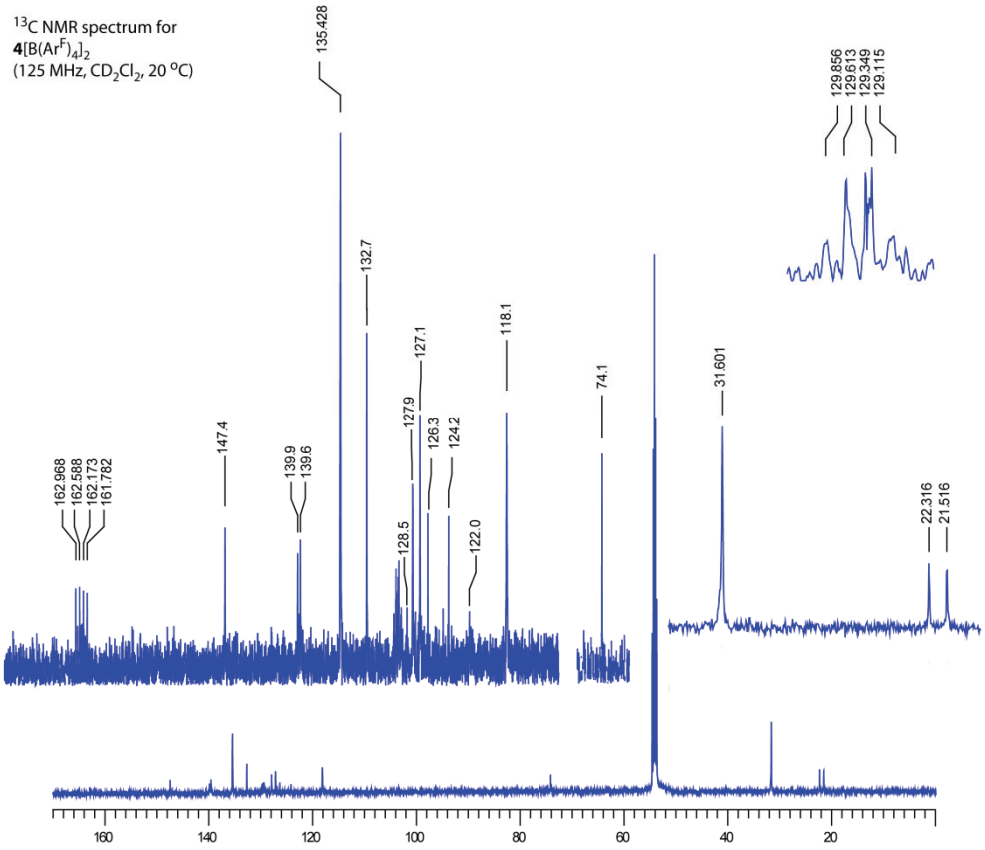

Figure S5. ^{13}C NMR spectrum of **2**[B(Ar^{F})$_4$]$_2$ (125 MHz, CD_2Cl_2, 20 °C). Detail shown in insets.

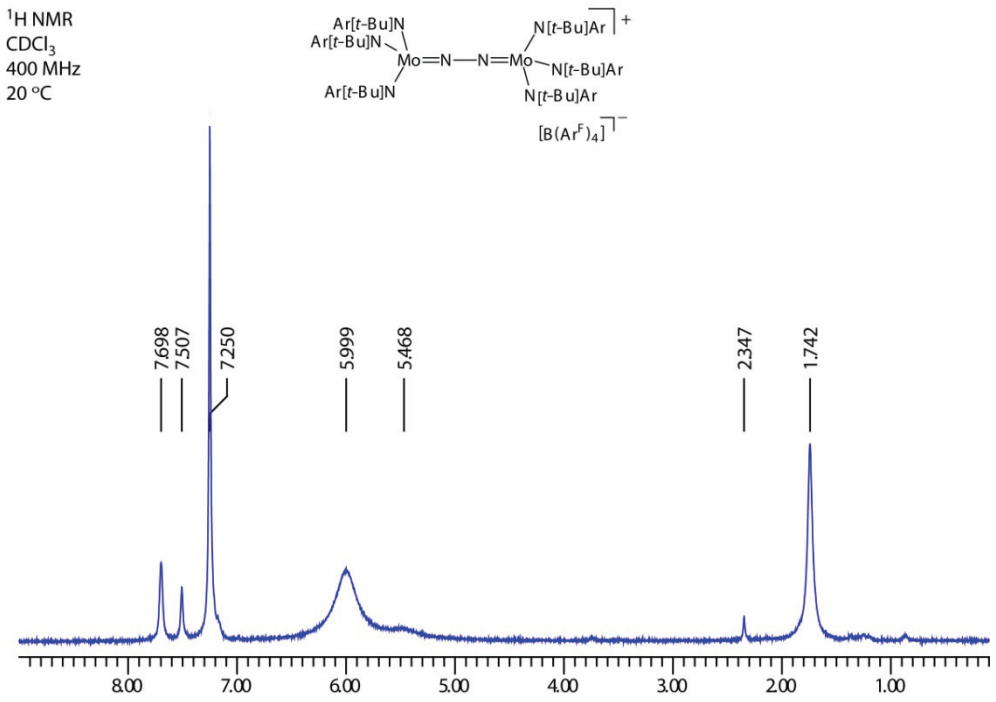

Figure S6. ^{1}H NMR spectrum of **2**[B(Ar^{F})$_4$] (400 MHz, $CDCl_3$, 20 °C).

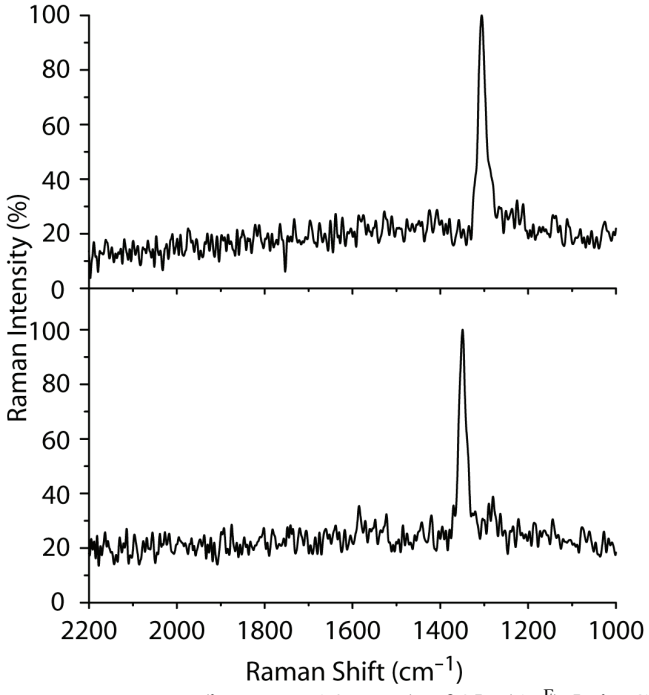

Figure S7. Resonance Raman spectra (λ_{excite} = 514.5 nm) of **2**$[B(Ar^F)_4]_2$ in CH_2Cl_2.

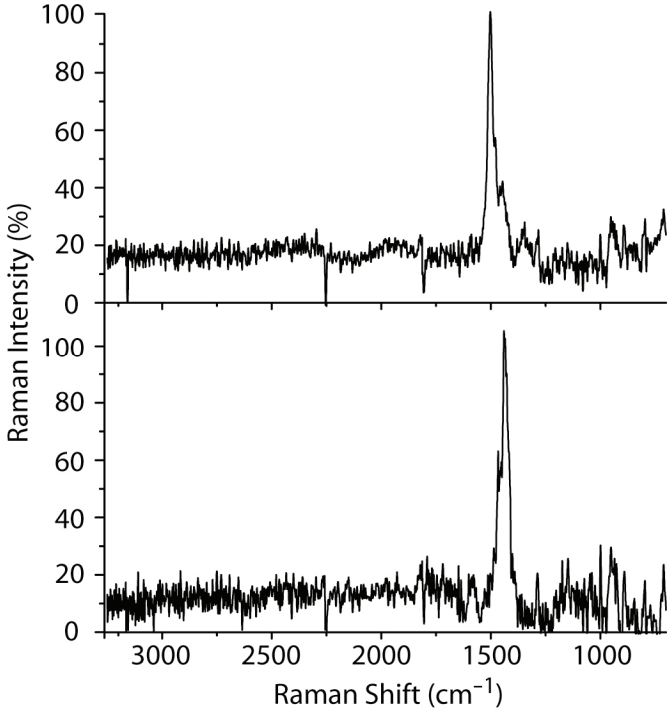

Figure S8. Raman spectra (λ_{excite} = 785 nm) of $\mathbf{2}^+$ in $CDCl_3$. In the spectrum shown, $\mathbf{2}^+$ was generated by addition of **2** to $CDCl_3$.

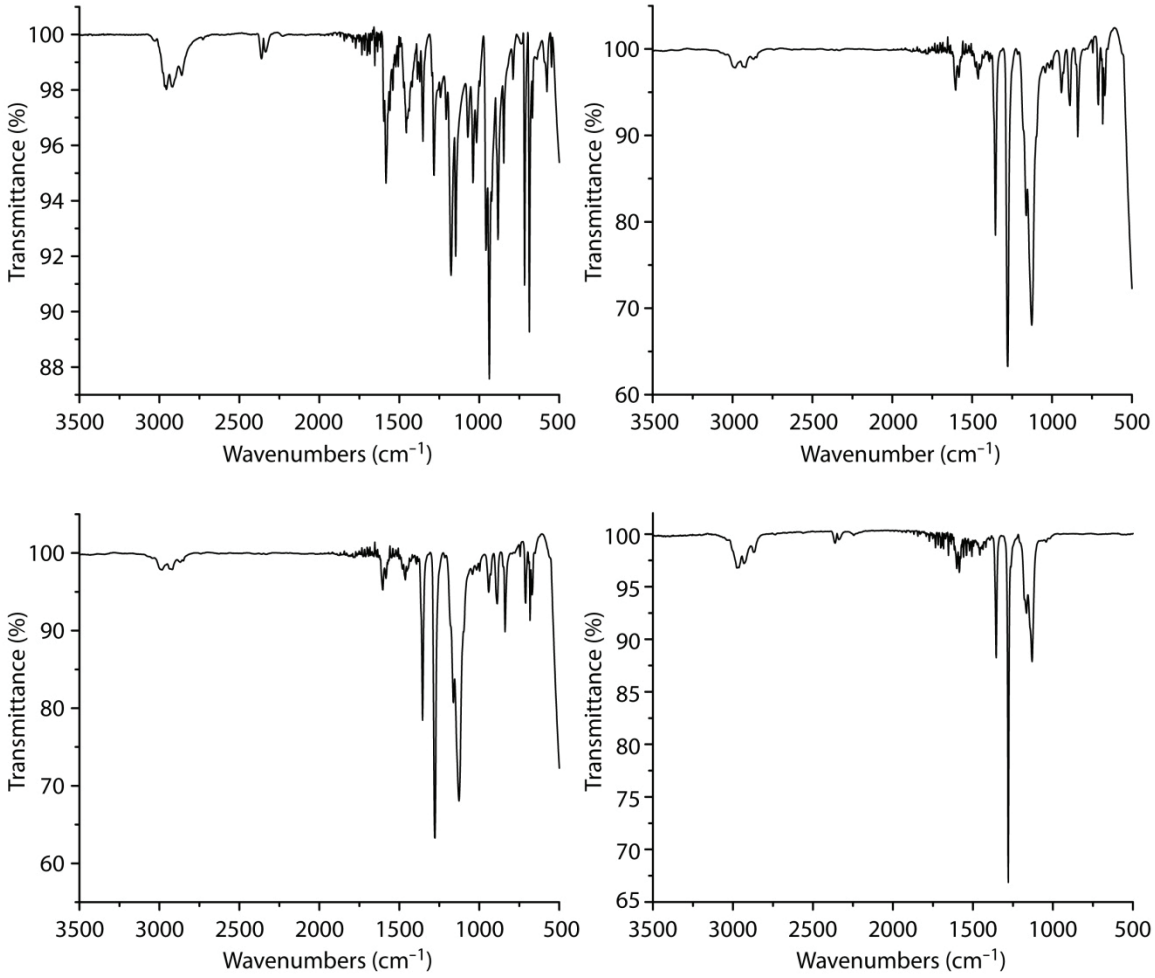

Figure S9. Infrared spectra as thin films (KBr) of **2** (top-left), **2**[$B(Ar^F)_4]_2$ (top-right), **2**[$B(Ar^F)_4$] (bottom-left); and **2**[$B(Ar^F)_4$] in $CDCl_3$ (bottom-right). Note that the Raman active ν_{NN} is not detected in the infrared spectrum for any of these three molecules.

For **2** (film, KBr): 2956.1, 2918.0, 2860.2, 1596.6, 1583.0 (s), 1456.6, 1352.0, 1283.4 (s), 1176.4 (s), 1147.3 (s), 1071.32, 1038.9, 1016.8, 957.7 (s), 937.2 (s), 882.7 (s), 846.7, 788.5, 716.6 (s), 686.8 (s), 677.2, 576.7 cm^{-1}.

For **2**[$B(Ar^F)_4]_2$ (film, KBr): 2983.8, 2919.9, 2868.7, 1603.4, 1583.2, 1462.2, 1354.3 (s), 1277.6 (s), 1161.7 (s), 1126.7 (s), 940.9, 887.9, 838.6, 710.5, 682.5, 669.3 cm^{-1}.

For **2**[$B(Ar^F)_4$] (film, KBr): 2974.21, 2924.6, 2866.0, 1600.67, 1584.56, 1353.2 (s), 1276.7 (s), 1162.4 (s), 1126.4 (s), 1041.0, 1016.8, 998.2, 940.7, 885.5, 838.2, 713.1, 681.9, 669.3 cm^{-1}.

For **2**[$B(Ar^F)_4$] ($CDCl_3$, KBr): 2973.3, 2930.4, 2870.2, 1354.6 (s), 1279.0 (s), 1165.4 (s), 1130.4 (s) cm^{-1}.

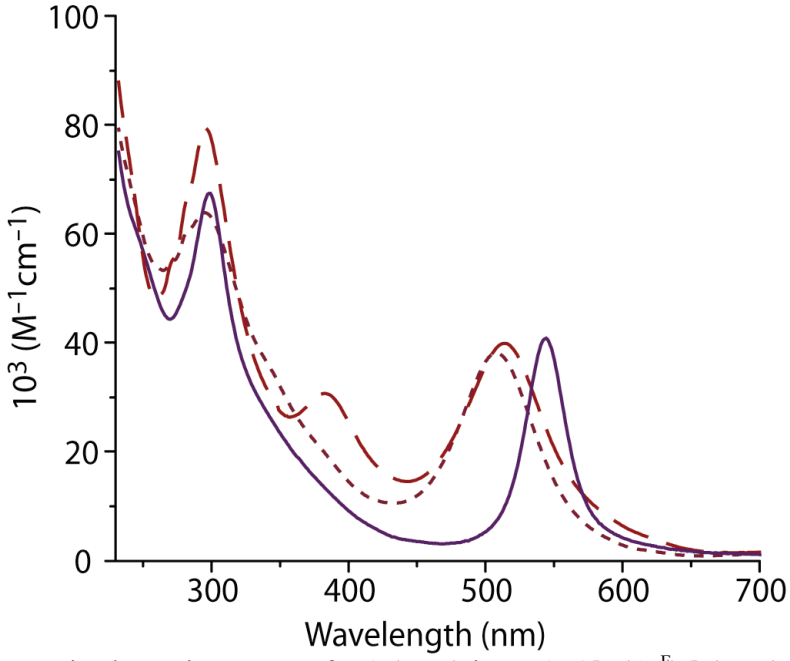

Figure S10. Electronic absorption spectra for **2** (——) in Et_2O, **2**[$B(Ar^F)_4$] (- - -) in CH_2Cl_2, and **2** [$B(Ar^F)_4]_2$ (—) in CH_2Cl_2 are shown 20 °C.

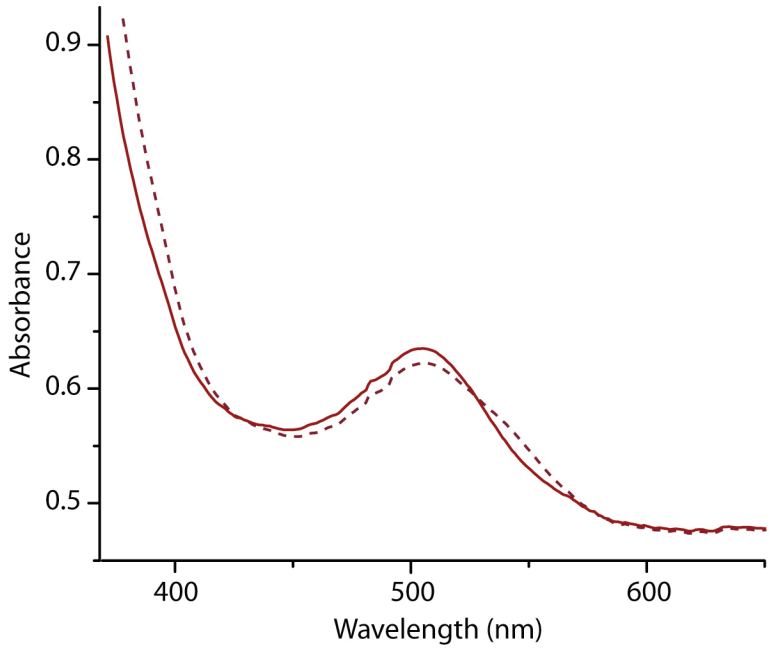

Figure S11. UV-Vis spectrum of $\mathbf{2}^{2+}$ (——) taken in an optically transparent thin-layer electrode at a potential difference of –50 mV, and of electrochemically generated $\mathbf{2}^{+}$ (- - -) holding the solution at a potential of –750 mV. This experiment was carried out in 0.5 M [$(n\text{-}Bu)_4N$][PF_6]/THF at 20 °C.

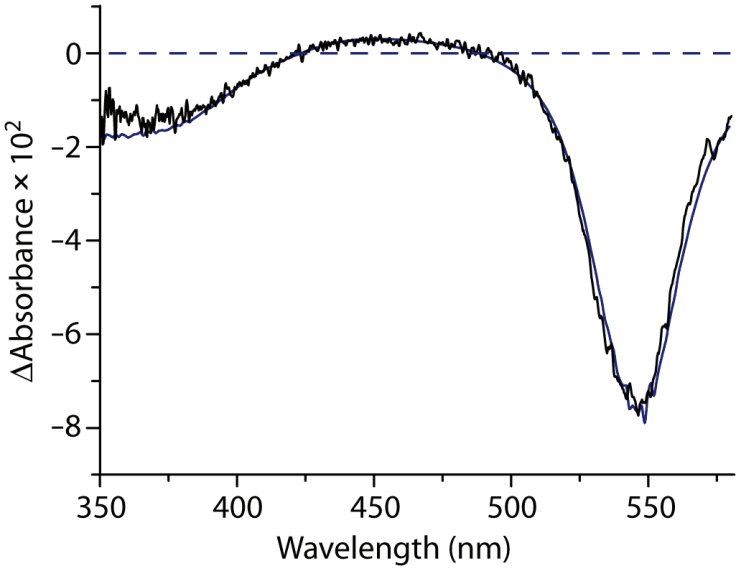

Figure S12. (black) Transient absorbance UV-Vis spectrum observed at of **2** following excitation with a 10 ns laser pulse. (blue) The spectrum that results from digital subtraction the spectrum of **2** from the spectrum of the mixture of products formed during exhaustive photolysis at 546 nm. These spectra are shown in figure 11 of the main text.

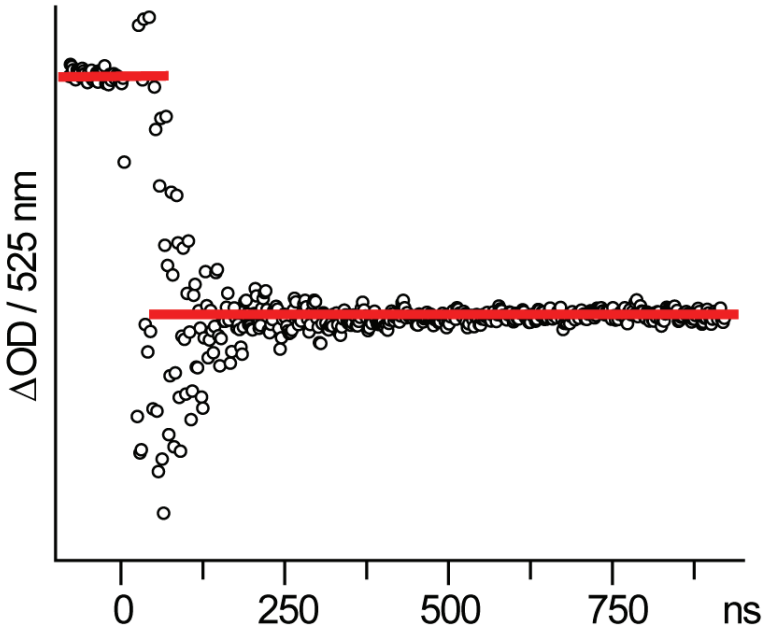

Figure S13. The kinetics of photochemical NN bond cleavage of **2** are shown on a ns timescale. The data points correspond to changes in absorbance measured at 530 nm with time. The line to guide-the-eye is a step function indicating that the photochemical process is faster than the resolved timescale.

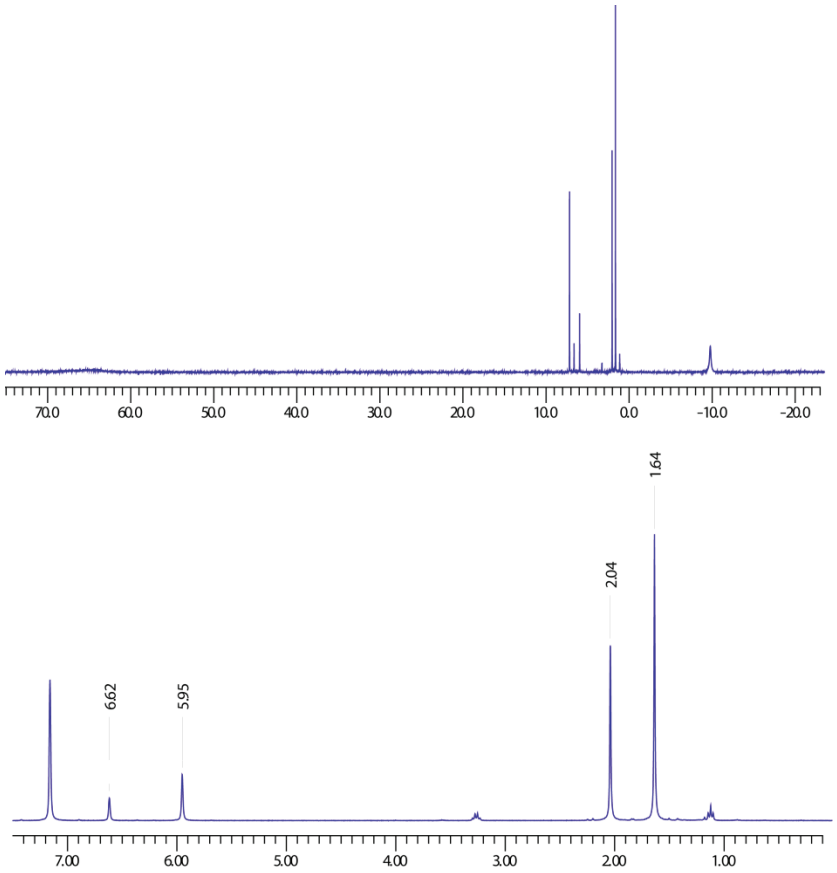

Figure S14. ^{1}H NMR spectrum (300 MHz, C_6D_6, 20 °C) of the product obtained after photolysis of **2**. (Top) The full spectrum shows **1** at 65 and –10 ppm, and (below) the resonances for **3** are clearly shown.

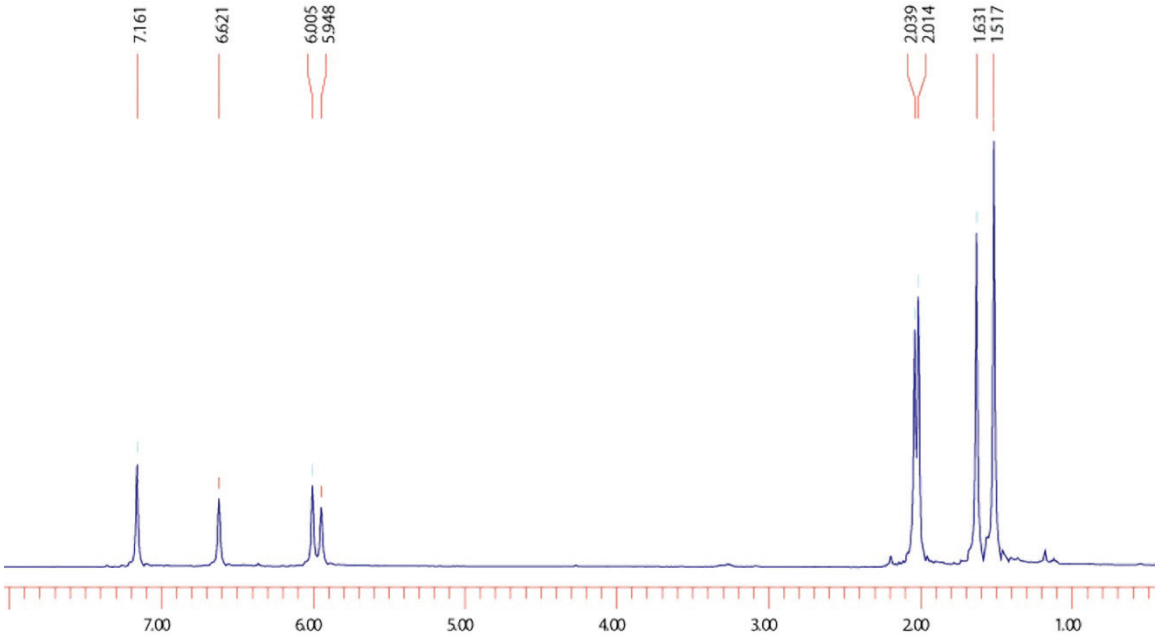

Figure S15. Treatment of the mixture of **1** and **3** formed during photolysis with NO affords both **3** and the diamagnetic ONMo(N[*t*-Bu]Ar)$_3$.

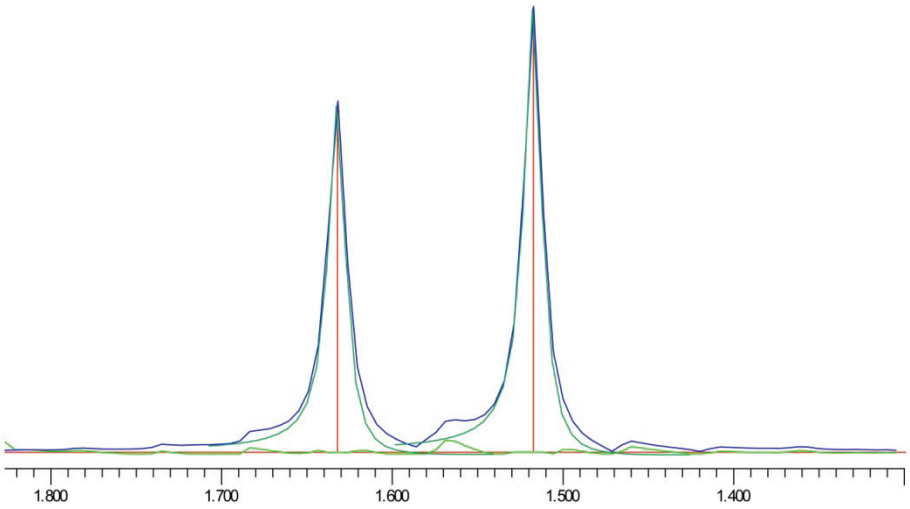

Figure S16. A Monte-Carlo simulation of the *t*-Bu resonances gives highly accurate integrals.[34] Experimental ^{1}H NMR spectrum (blue) and the simulation of the line shape shown in (green). Data fitting indicated that 44.212% of the total area is contained under the resonance centered at 1.64 ppm corresponding to **3**, and 55.788% is contained under the reasonance at 1.52 ppm corresponding to ONMo(N[*t*-Bu]Ar)$_3$. The relative error for total fit was 0.5%.

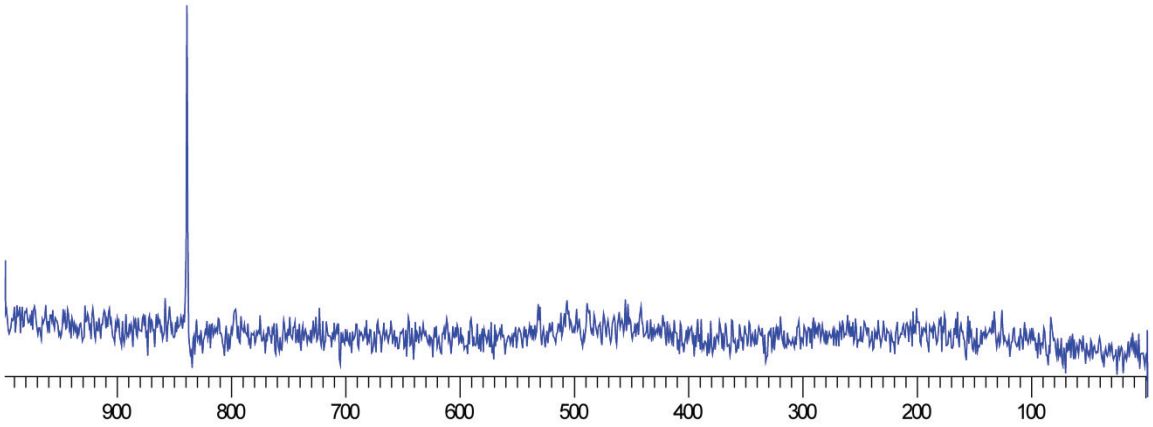

Figure S17. ^{15}N NMR spectrum of the products after photolysis ($\lambda > 480$ nm) of ^{15}N-labeled **2**.

Table S1. Electrochemical potentials measured from [2][B(Ar^{F})$_4$]$_2$ (data in mV vs. $Cp_2Fe^{+/0}$).[35,36]

Electrolyte Solution	$\mathbf{2}^{2+}/\mathbf{2}^{+}$	$\mathbf{2}^{+}/\mathbf{2}$	$\mathbf{2} \rightarrow 2$ [NNMo(N[*t*-Bu]Ar)$_3$]$^-$
0.1 M [N(*n*-Bu)$_4$][B(C$_6$F$_5$)$_4$] in THF	–320	–1260	not measured
0.5 M [N(*n*-Bu)$_4$][PF$_6$] in THF	–332	–1140	–2250
2.0 M [N(*n*-Bu)$_4$][PF$_6$] in MeCN	–377	–1190	–2530

Table S2. SQUID data for **2**.

Field (Oe)	Temperature (K)	X_M ($cm^3\ mol^{-1}$)	$1/X_M$ ($cm^{-3}\ mol$)	$X_M \times T$ ($cm^3\ mol^{-1}\ K$)	μ_{eff} (μ_B)
50000	5	0.02355	42.47	0.11774	0.97
50000	6	0.02352	42.53	0.14109	1.06
50000	7	0.02348	42.59	0.16436	1.15
50000	8	0.02345	42.64	0.18763	1.22
50000	9	0.02343	42.69	0.21084	1.30
50000	10	0.02340	42.73	0.23380	1.37
50000	12	0.02329	42.94	0.27920	1.49
50000	14	0.02305	43.38	0.32299	1.61
50000	16	0.02273	44.00	0.36365	1.71
50000	18	0.02229	44.87	0.40114	1.79
50000	20	0.02176	45.96	0.43516	1.87
50000	23	0.02083	48.00	0.47917	1.96
50000	26	0.01982	50.44	0.51541	2.03
50000	29	0.01879	53.22	0.54513	2.09
50000	32	0.01778	56.24	0.56913	2.13
50000	35	0.01682	59.46	0.58882	2.17
50000	38	0.01592	62.83	0.60499	2.20
50000	41	0.01510	66.24	0.61927	2.23
50000	44	0.01434	69.74	0.63116	2.25
50000	47	0.01362	73.40	0.64056	2.26
50000	50	0.01294	77.26	0.64768	2.28
50000	55	0.01210	82.68	0.66596	2.31
50000	60	0.01116	89.59	0.67037	2.32
50000	65	0.01042	95.99	0.67786	2.33
50000	70	0.00975	102.59	0.68312	2.34
50000	75	0.00915	109.24	0.68736	2.34
50000	80	0.00863	115.88	0.69142	2.35
50000	85	0.00815	122.65	0.69416	2.36
50000	90	0.00772	129.46	0.69627	2.36
50000	95	0.00733	136.35	0.69760	2.36
50000	100	0.00697	143.39	0.69810	2.36
50000	110	0.00646	154.89	0.71120	2.38
50000	120	0.00585	170.82	0.70320	2.37
50000	130	0.00542	184.43	0.70557	2.38
50000	140	0.00505	198.20	0.70710	2.38
50000	150	0.00472	211.96	0.70830	2.38
50000	160	0.00444	225.40	0.71044	2.38
50000	170	0.00418	239.06	0.71187	2.39
50000	180	0.00395	252.92	0.71201	2.39
50000	190	0.00375	266.41	0.71372	2.39
50000	200	0.00357	279.92	0.71487	2.39
50000	210	0.00341	293.42	0.71615	2.39
50000	220	0.00326	306.86	0.71739	2.40
50000	230	0.00312	320.40	0.71817	2.40
50000	240	0.00300	333.86	0.71914	2.40
50000	250	0.00288	347.42	0.72000	2.40

25000	5	0.02375	42.11	0.11874	0.97
25000	6	0.02371	42.18	0.14224	1.07
25000	7	0.02366	42.26	0.16564	1.15
25000	8	0.02364	42.31	0.18909	1.23
25000	9	0.02360	42.37	0.21242	1.30
25000	10	0.02355	42.45	0.23555	1.37
25000	12	0.02343	42.68	0.28118	1.50
25000	14	0.02323	43.06	0.32516	1.61
25000	16	0.02287	43.72	0.36593	1.71
25000	18	0.02242	44.60	0.40356	1.80
25000	20	0.02187	45.73	0.43737	1.87
25000	23	0.02091	47.81	0.48103	1.96
25000	26	0.01988	50.30	0.51708	2.03
25000	29	0.01883	53.10	0.54610	2.09
25000	32	0.01780	56.17	0.56984	2.13
25000	35	0.01683	59.42	0.58921	2.17
25000	38	0.01592	62.81	0.60519	2.20
25000	41	0.01508	66.31	0.61846	2.22
25000	44	0.01431	69.90	0.62974	2.24
25000	47	0.01357	73.71	0.63808	2.26
25000	50	0.01291	77.44	0.64577	2.27
25000	55	0.01208	82.78	0.66512	2.31
25000	60	0.01117	89.53	0.67093	2.32
25000	65	0.01042	96.01	0.67771	2.33
25000	70	0.00974	102.65	0.68293	2.34
25000	75	0.00915	109.33	0.68700	2.34
25000	80	0.00861	116.13	0.68992	2.35
25000	85	0.00813	122.95	0.69246	2.35
25000	90	0.00770	129.88	0.69382	2.36
25000	95	0.00731	136.88	0.69513	2.36
25000	100	0.00694	144.14	0.69440	2.36
25000	110	0.00642	155.71	0.70749	2.38
25000	120	0.00582	171.93	0.69862	2.36
25000	130	0.00538	185.83	0.70031	2.37
25000	140	0.00501	199.76	0.70159	2.37
25000	150	0.00468	213.66	0.70260	2.37
25000	160	0.00440	227.40	0.70432	2.37
25000	170	0.00415	241.21	0.70535	2.38
25000	180	0.00392	255.36	0.70507	2.37
25000	190	0.00372	269.00	0.70689	2.38
25000	200	0.00353	282.93	0.70741	2.38
25000	210	0.00337	296.70	0.70837	2.38
25000	220	0.00322	310.48	0.70897	2.38
25000	230	0.00308	324.17	0.70981	2.38
25000	240	0.00296	337.87	0.71078	2.38
25000	250	0.00284	351.96	0.71054	2.38
5000	5	0.02404	41.60	0.12019	0.98
5000	6	0.02396	41.74	0.14376	1.07
5000	7	0.02390	41.84	0.16731	1.16
5000	8	0.02385	41.93	0.19080	1.24

5000	9	0.02380	42.01	0.21422	1.31
5000	10	0.02375	42.10	0.23751	1.38
5000	12	0.02362	42.33	0.28324	1.51
5000	14	0.02339	42.76	0.32739	1.62
5000	16	0.02302	43.45	0.36828	1.72
5000	18	0.02255	44.34	0.40595	1.80
5000	20	0.02199	45.48	0.43975	1.88
5000	23	0.02103	47.56	0.48360	1.97
5000	26	0.01998	50.04	0.51958	2.04
5000	29	0.01891	52.87	0.54871	2.09
5000	32	0.01788	55.92	0.57244	2.14
5000	35	0.01690	59.18	0.59180	2.18
5000	38	0.01599	62.53	0.60783	2.20
5000	41	0.01515	65.99	0.62148	2.23
5000	44	0.01439	69.49	0.63351	2.25
5000	47	0.01369	73.03	0.64402	2.27
5000	50	0.01299	76.97	0.65016	2.28
5000	55	0.01216	82.21	0.66962	2.31
5000	60	0.01122	89.10	0.67421	2.32
5000	65	0.01046	95.60	0.68076	2.33
5000	70	0.00979	102.19	0.68578	2.34
5000	75	0.00919	108.86	0.68989	2.35
5000	80	0.00865	115.64	0.69287	2.35
5000	85	0.00817	122.42	0.69524	2.36
5000	90	0.00774	129.26	0.69725	2.36
5000	95	0.00734	136.22	0.69834	2.36
5000	100	0.00698	143.27	0.69903	2.36
5000	110	0.00641	155.91	0.70680	2.38
5000	120	0.00584	171.14	0.70192	2.37
5000	130	0.00541	184.86	0.70390	2.37
5000	140	0.00503	198.73	0.70524	2.37
5000	150	0.00470	212.65	0.70597	2.38
5000	160	0.00442	226.47	0.70711	2.38
5000	170	0.00416	240.28	0.70825	2.38
5000	180	0.00394	254.07	0.70906	2.38
5000	190	0.00373	268.04	0.70937	2.38
5000	200	0.00354	282.21	0.70897	2.38
5000	210	0.00338	295.76	0.71059	2.38
5000	220	0.00323	309.80	0.71052	2.38
5000	230	0.00309	323.78	0.71076	2.38
5000	240	0.00296	337.83	0.71077	2.38
5000	250	0.00284	352.08	0.71047	2.38
5000	260	0.00273	366.21	0.71025	2.38
5000	270	0.00263	380.71	0.70956	2.38
5000	280	0.00253	395.48	0.70823	2.38
5000	290	0.00243	411.13	0.70554	2.38
5000	300	0.00233	429.98	0.69795	2.36

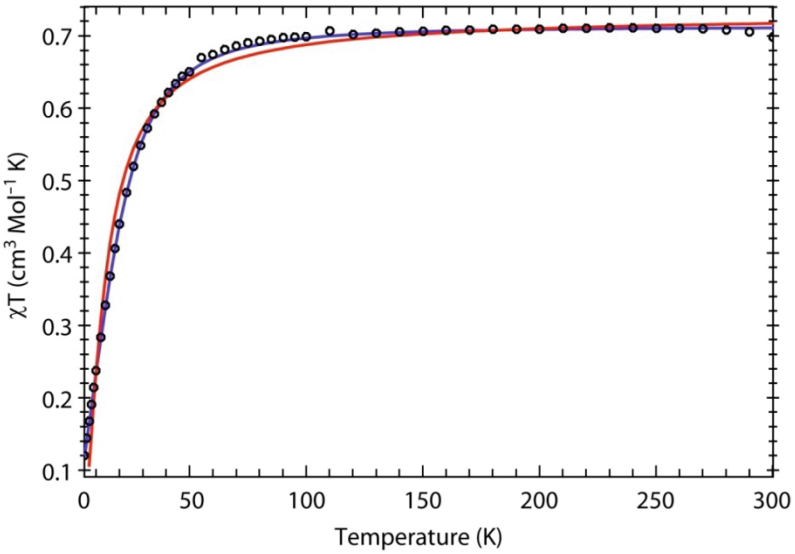

Figure S18. The molar susceptibility data acquired for **2** at 0.5 T were fit to two magnetic models. Both a $S = 1$ triplet with zero-field splitting (blue) and a Bleaney-Bowers model (red) are shown. Note that the $S = 1$ description of the magnetic data provides a better fit for the data between 10 and 100 K. The fit parameters are (blue) $g = 1.69$, $D = 42$ cm^{-1}, TIP = 423 (10^{-6}) emu (subtracted) and (red) $g = 1.98$, $2J = -15.6$ cm^{-1}, TIP = 443 (10^{-6}) emu (subtracted).

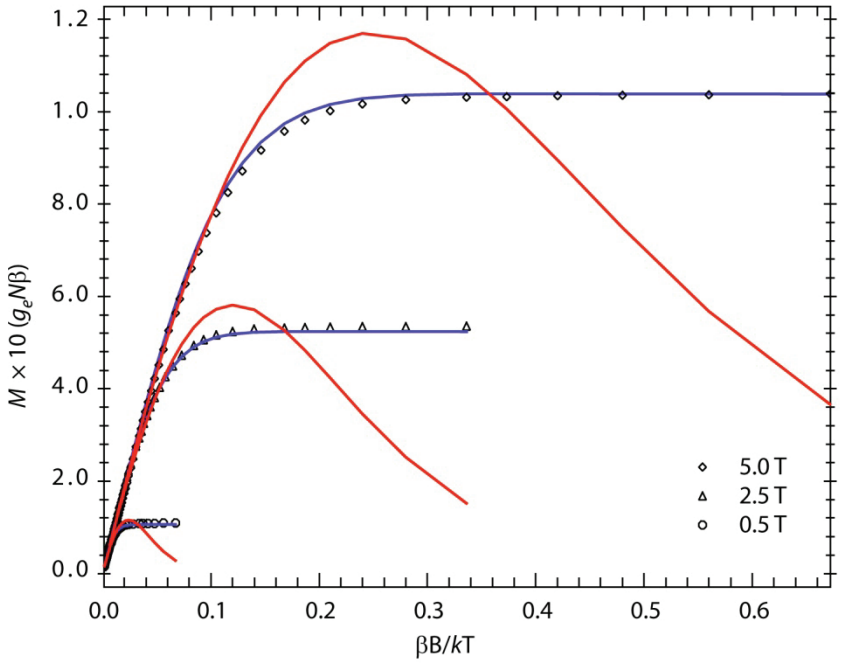

Figure S19. Variable-field–variable temperature molar magnetization data of **2** were fit to both a $S = 1$ triplet with zero-field splitting (blue) and to the Bleaney-Bowers equation (red). Notice that only the $S = 1$ description accounts for the field dependence of the molar magnetization. Data are shown over a temperature range of 5–50 K at fields of 0.5, 2.5, and 5.0 T. The fit parameters are (blue) $g = 1.69$, $D = 42$ cm^{-1}, TIP = 334 (10^{-6}) emu (subtracted) and (red) $g = 1.95$, $2J = -15.5$ cm^{-1}, TIP = 420 (10^{-6}) emu (subtracted).

Table S2. SQUID data for **2**[B(Ar^F)$_4$] measured at 5000 Oe.

Temperature (K)	X_M ($cm^3\ mol^{-1}$)	$1/X_M$ ($cm^{-3}\ mol$)	$X_M \times T$ ($cm^3\ mol^{-1}\ K$)	μ_{eff} (μ_B)
5	0.03344	29.90646	0.16705	1.15581
6	0.02805	35.6468	0.16842	1.16054
7	0.02418	41.36404	0.16912	1.16294
8	0.02122	47.12103	0.16963	1.16469
9	0.01897	52.71615	0.17062	1.1681
10	0.01716	58.26148	0.17146	1.17097
12	0.01448	69.04422	0.17376	1.1788
14	0.01259	79.43723	0.17633	1.18747
16	0.01112	89.95505	0.17782	1.19249
18	0.01005	99.52636	0.18083	1.20255
20	0.00915	109.2667	0.18301	1.20975
23	0.00811	123.2652	0.1866	1.22157
26	0.00731	136.878	0.18996	1.23253
29	0.00666	150.0712	0.19327	1.2432
32	0.00614	162.8128	0.19658	1.2538
35	0.00571	175.1675	0.19984	1.26417
38	0.00538	186	0.20435	1.27835
41	0.00505	197.9537	0.20713	1.28701
44	0.00478	209.1516	0.21043	1.29723
47	0.00459	217.9258	0.21573	1.31345
50	0.00441	226.6237	0.2207	1.32851
55	0.00405	246.6945	0.22309	1.33568
60	0.00382	261.5141	0.22959	1.35501
65	0.00362	276.1523	0.23557	1.37253
70	0.00344	290.609	0.24109	1.38854
75	0.00328	305.1629	0.24586	1.4022
80	0.00314	318.2171	0.25168	1.4187
85	0.00302	331.5379	0.25667	1.4327
90	0.0029	344.5799	0.26152	1.44615
95	0.0028	356.835	0.26658	1.46008
100	0.00271	369.3386	0.27073	1.47139
110	0.00256	391.287	0.28137	1.50003
120	0.00243	411.0713	0.29219	1.5286
130	0.00233	429.9571	0.30261	1.55563
140	0.00224	447.0264	0.31326	1.58277
150	0.00216	462.5414	0.32456	1.61105
160	0.00209	478.0486	0.33494	1.63663
170	0.00204	491.3699	0.34621	1.66393
180	0.00198	504.6169	0.35693	1.6895
190	0.00193	516.8001	0.36786	1.71517
200	0.00189	528.1896	0.37857	1.73996
210	0.00185	539.1173	0.38971	1.76537
220	0.00182	548.4974	0.40128	1.79139
230	0.00179	558.4456	0.41203	1.81522
240	0.00176	567.3344	0.42305	1.83933
250	0.00174	575.2747	0.43474	1.86456

260	0.00172	582.6822	0.44636	1.88932
270	0.0017	589.5113	0.45815	1.91411
280	0.00168	596.6002	0.46944	1.93755
290	0.00166	601.5265	0.48224	1.96379
300	0.00158	633.0658	0.47399	1.98725

Table S3. Optimized Geometry of **2** in Cartesian Coordinates (Å)

N	0.611428	-0.000329	0.007226
Mo	2.496313	0.007269	-0.004429
N	3.043555	-0.284814	1.912730
C	2.446310	0.114322	3.232398
C	1.322305	1.117608	2.976811
H	0.576044	0.737429	2.279721
H	1.731947	2.042840	2.550717
H	0.826808	1.366349	3.922575
C	3.460500	0.828304	4.155278
H	3.869528	1.722931	3.667788
H	2.934921	1.144660	5.069384
H	4.292256	0.177097	4.450952
C	1.942212	-1.146947	3.967377
H	1.387812	-0.874916	4.878266
H	2.791285	-1.776073	4.268428
H	1.286550	-1.741196	3.321961
C	4.290948	-0.991555	2.033806
C	5.503518	-0.294106	2.149382
C	6.718234	-0.964152	2.326612
C	6.716001	-2.364096	2.355121
C	5.526642	-3.094195	2.230563
C	4.323281	-2.394499	2.085041
H	3.384133	-2.939634	2.000321
H	5.486124	0.794510	2.113380
C	7.994672	-0.181244	2.524485
H	7.878669	0.847788	2.164432
H	8.261893	-0.130539	3.590754
H	8.843250	-0.641354	2.000547
H	7.660825	-2.899722	2.479054
C	5.547168	-4.604990	2.223632
H	4.623267	-5.022551	2.642458
H	5.643969	-4.993115	1.198128
H	6.393662	-4.996469	2.801686
N	3.021568	-1.491186	-1.232675
C	2.442149	-2.847319	-1.511442
C	1.314124	-3.110336	-0.513601
H	0.530557	-2.354071	-0.568853
H	1.703955	-3.107967	0.512996
H	0.868117	-4.092901	-0.711649
C	3.487134	-3.967221	-1.311761
H	3.003120	-4.940192	-1.486432
H	4.331501	-3.877209	-2.006955
H	3.875149	-3.955725	-0.284702
C	1.929747	-2.915407	-2.966550
H	1.268646	-2.069872	-3.186598
H	1.373461	-3.848637	-3.140489
H	2.771026	-2.890054	-3.672128
C	4.255899	-1.215245	-1.920400
C	5.489991	-1.486536	-1.315141

C	6.699998	-1.234299	-1.974829
C	6.661735	-0.703581	-3.267710
C	5.444332	-0.428081	-3.908843
C	4.254158	-0.689144	-3.224718
H	3.297944	-0.477288	-3.700849
C	5.417915	0.155943	-5.301867
H	4.665947	-0.340232	-5.929092
H	6.392674	0.055701	-5.794536
H	5.165816	1.226875	-5.281313
H	7.599010	-0.503113	-3.792648
C	8.008050	-1.535274	-1.285719
H	8.087667	-2.602130	-1.034221
H	8.081722	-0.981861	-0.339868
H	8.867773	-1.266830	-1.911663
H	5.498357	-1.910228	-0.311000
N	3.052250	1.794842	-0.740737
C	2.504054	2.673655	-1.827268
C	1.390826	1.913248	-2.549593
H	0.607271	1.582594	-1.866185
H	1.798914	1.021444	-3.042654
H	0.939995	2.555907	-3.316165
C	3.569296	3.022227	-2.890906
H	4.401873	3.600965	-2.471773
H	3.096323	3.628834	-3.678311
H	3.970942	2.109838	-3.350707
C	1.986763	3.992760	-1.215029
H	1.297204	3.794867	-0.387558
H	2.824470	4.589864	-0.829001
H	1.463291	4.596109	-1.971773
C	4.232268	2.308014	-0.099111
C	5.509821	2.072071	-0.630163
C	6.659790	2.588324	-0.020990
C	6.520959	3.338536	1.153082
C	5.260432	3.595563	1.710056
C	4.130152	3.080342	1.069251
H	3.139793	3.263922	1.483809
H	5.599316	1.467684	-1.532535
H	7.413535	3.730248	1.648112
C	5.120852	4.432327	2.960149
H	4.212944	4.171247	3.517536
H	5.057189	5.502711	2.714174
H	5.980658	4.300596	3.629348
C	8.018953	2.353176	-0.636459
H	8.783905	2.162062	0.127866
H	7.995514	1.499049	-1.323006
H	8.347140	3.231615	-1.211896
N	-0.611428	0.000329	0.007226
Mo	-2.496313	-0.007269	-0.004429
N	-3.043555	0.284814	1.912730
C	-2.446310	-0.114322	3.232398
C	-1.322305	-1.117608	2.976811
H	-0.576044	-0.737429	2.279721
H	-1.731947	-2.042840	2.550717
H	-0.826808	-1.366349	3.922575
C	-3.460500	-0.828304	4.155278
H	-3.869528	-1.722931	3.667788
H	-2.934921	-1.144660	5.069384

H	-4.292256	-0.177097	4.450952
C	-1.942212	1.146947	3.967377
H	-1.387812	0.874916	4.878266
H	-2.791285	1.776073	4.268428
H	-1.286550	1.741196	3.321961
C	-4.290948	0.991555	2.033806
C	-5.503518	0.294106	2.149382
C	-6.718234	0.964152	2.326612
C	-6.716001	2.364096	2.355121
C	-5.526642	3.094195	2.230563
C	-4.323281	2.394499	2.085041
H	-3.384133	2.939634	2.000321
H	-5.486124	-0.794510	2.113380
C	-7.994672	0.181244	2.524485
H	-7.878669	-0.847788	2.164432
H	-8.261893	0.130539	3.590754
H	-8.843250	0.641354	2.000547
H	-7.660825	2.899722	2.479054
C	-5.547168	4.604990	2.223632
H	-4.623267	5.022551	2.642458
H	-5.643969	4.993115	1.198128
H	-6.393662	4.996469	2.801686
N	-3.021568	1.491186	-1.232675
C	-2.442149	2.847319	-1.511442
C	-1.314124	3.110336	-0.513601
H	-0.530557	2.354071	-0.568853
H	-1.703955	3.107967	0.512996
H	-0.868117	4.092901	-0.711649
C	-3.487134	3.967221	-1.311761
H	-3.003120	4.940192	-1.486432
H	-4.331501	3.877209	-2.006955
H	-3.875149	3.955725	-0.284702
C	-1.929747	2.915407	-2.966550
H	-1.268646	2.069872	-3.186598
H	-1.373461	3.848637	-3.140489
H	-2.771026	2.890054	-3.672128
C	-4.255899	1.215245	-1.920400
C	-5.489991	1.486536	-1.315141
C	-6.699998	1.234299	-1.974829
C	-6.661735	0.703581	-3.267710
C	-5.444332	0.428081	-3.908843
C	-4.254158	0.689144	-3.224718
H	-3.297944	0.477288	-3.700849
C	-5.417915	-0.155943	-5.301867
H	-4.665947	0.340232	-5.929092
H	-6.392674	-0.055701	-5.794536
H	-5.165816	-1.226875	-5.281313
H	-7.599010	0.503113	-3.792648
C	-8.008050	1.535274	-1.285719
H	-8.087667	2.602130	-1.034221
H	-8.081722	0.981861	-0.339868
H	-8.867773	1.266830	-1.911663
H	-5.498357	1.910228	-0.311000
N	-3.052250	-1.794842	-0.740737
C	-2.504054	-2.673655	-1.827268
C	-1.390826	-1.913248	-2.549593
H	-0.607271	-1.582594	-1.866185

H	-1.798914	-1.021444	-3.042654
H	-0.939995	-2.555907	-3.316165
C	-3.569296	-3.022227	-2.890906
H	-4.401873	-3.600965	-2.471773
H	-3.096323	-3.628834	-3.678311
H	-3.970942	-2.109838	-3.350707
C	-1.986763	-3.992760	-1.215029
H	-1.297204	-3.794867	-0.387558
H	-2.824470	-4.589864	-0.829001
H	-1.463291	-4.596109	-1.971773
C	-4.232268	-2.308014	-0.099111
C	-5.509821	-2.072071	-0.630163
C	-6.659790	-2.588324	-0.020990
C	-6.520959	-3.338536	1.153082
C	-5.260432	-3.595563	1.710056
C	-4.130152	-3.080342	1.069251
H	-3.139793	-3.263922	1.483809
H	-5.599316	-1.467684	-1.532535
H	-7.413535	-3.730248	1.648112
C	-5.120852	-4.432327	2.960149
H	-4.212944	-4.171247	3.517536
H	-5.057189	-5.502711	2.714174
H	-5.980658	-4.300596	3.629348
C	-8.018953	-2.353176	-0.636459
H	-8.783905	-2.162062	0.127866
H	-7.995514	-1.499049	-1.323006
H	-8.347140	-3.231615	-1.211896

Table S4. Optimized geometry of 2^{2+} in Cartesian Coordinates (Å)

H	-5.117071	-2.573540	-6.280621
H	-3.492220	-2.801338	-5.600842
C	-4.549006	-2.659106	-5.346569
H	-6.840829	-1.239951	-4.950699
H	-4.895478	-3.572741	-4.841261
H	-2.137273	0.922544	-4.939367
H	-7.847048	1.374090	-4.490490
H	-0.794059	2.065688	-4.751319
C	-4.749751	-1.445295	-4.472066
C	-6.007756	-0.833385	-4.372395
H	3.728076	-1.146734	-4.397715
H	5.848468	1.721787	-4.095752
C	-1.375563	1.285934	-4.239128
H	-3.757960	2.662167	-4.063333
H	5.521211	3.449406	-3.913680
H	7.178903	2.840140	-3.748246
H	-0.698531	0.459094	-3.990256
H	-2.408000	3.799140	-3.875440
C	-7.579631	0.950860	-3.512333
C	6.128744	2.619999	-3.527378
H	-2.697105	-1.347324	-3.813894
C	-6.224136	0.289639	-3.564836
C	-3.689043	-0.903808	-3.739099
H	-8.366225	0.230450	-3.250548
H	1.518424	-0.449423	-3.866745
H	2.075038	-2.919608	-3.684153
C	-2.983023	3.009802	-3.371070

C	4.050723	-1.016043	-3.355230
H	4.386453	0.020011	-3.224087
H	4.899183	-1.685997	-3.176419
H	-7.595884	1.764105	-2.778465
C	-2.014385	1.880239	-2.972541
C	-3.880210	0.213906	-2.915278
C	-5.148787	0.799878	-2.827164
C	1.708739	-0.391712	-2.787740
H	-3.468615	3.444136	-2.488786
C	2.425487	-2.794424	-2.649655
H	-7.619238	-2.527633	-2.224567
H	3.260352	-3.487827	-2.494019
H	-0.457935	3.314886	-2.587477
H	-3.463646	-3.524609	-2.505187
H	1.959116	0.651261	-2.550493
C	2.859481	-1.335343	-2.433076
H	-5.292037	1.673233	-2.192247
C	5.907683	2.424220	-2.047401
H	0.786012	-0.659304	-2.265288
H	3.773076	2.137645	-2.225604
H	-1.244166	-2.171214	-2.301224
N	-2.761860	0.800333	-2.205378
C	-0.929038	2.467722	-2.073639
H	1.606255	-3.067030	-1.973988
H	7.975063	2.706234	-1.520672
H	-4.610299	5.358865	-1.644051
H	-2.648602	-4.935382	-1.785612
H	-5.328001	-1.918153	-1.776608
H	-0.153491	1.729512	-1.847564
H	-0.608893	-3.743135	-1.790061
H	-6.313365	5.643982	-1.235761
C	-7.957464	-2.410263	-1.188897
H	-8.577811	-1.503621	-1.141493
C	-3.214617	-4.020960	-1.558695
C	4.622535	2.180099	-1.544825
H	8.839218	-1.825393	-1.144200
H	-8.607722	-3.257704	-0.938184
C	6.972977	2.495168	-1.141117
C	-1.048263	-2.805841	-1.426686
H	-4.143849	-4.315323	-1.058367
C	-5.357019	5.282153	-0.842197
H	1.436372	3.214480	-1.314327
H	-1.346164	2.842875	-1.128935
H	2.920707	4.188612	-1.153427
H	5.785672	-0.229093	-1.038296
H	8.140899	-0.252456	-0.707009
H	-8.767387	1.341485	-0.551380
H	-7.617415	3.795845	-0.514434
N	3.263401	-1.117212	-0.981777
C	-5.498992	-2.053728	-0.709560
C	8.222178	-1.301426	-0.401367
C	5.706186	-1.244098	-0.652115
H	-0.311333	-2.309761	-0.789013
C	-2.337688	-3.122252	-0.667352
C	2.009672	3.859862	-0.639839
C	4.442796	-1.842926	-0.549402
C	-6.723695	3.245180	-0.212827

C	-5.474675	3.868338	-0.327378
C	-6.789083	-2.316913	-0.237488
C	6.860432	-1.939460	-0.277676
H	1.406225	4.751788	-0.419248
H	-5.044517	5.968380	-0.042741
N	-3.069614	-1.824035	-0.350332
Mo	-2.419261	0.030668	-0.423387
H	5.044517	-5.968380	0.042741
C	4.411296	1.997930	-0.172791
C	4.335092	-3.151279	-0.061086
C	-8.222178	1.301426	0.401367
C	6.723695	-3.245180	0.212827
H	3.351455	-3.614125	0.014212
C	-6.860432	1.939460	0.277676
H	-3.351455	3.614125	-0.014212
C	6.789083	2.316913	0.237488
C	-4.335092	3.151279	0.061086
H	8.767387	-1.341485	0.551380
N	-0.613688	0.005668	-0.106464
H	7.617415	-3.795845	0.514434
C	5.474675	-3.868338	0.327378
C	-4.411296	-1.997930	0.172791
H	-8.140899	0.252456	0.707009
N	0.613688	-0.005668	0.106464
H	8.607722	3.257704	0.938184
H	-1.406225	-4.751788	0.419248
N	3.069614	1.824035	0.350332
H	-8.839218	1.825393	1.144200
C	-5.706186	1.244098	0.652115
C	-4.442796	1.842926	0.549402
C	5.357019	-5.282153	0.842197
Mo	2.419261	-0.030668	0.423387
C	5.498992	2.053728	0.709560
C	-2.009672	-3.859862	0.639839
H	8.577811	1.503621	1.141493
C	2.337688	3.122252	0.667352
H	6.313365	-5.643982	1.235761
C	7.957464	2.410263	1.188897
C	-6.972977	-2.495168	1.141117
H	-5.785672	0.229093	1.038296
H	4.143849	4.315323	1.058367
H	0.311333	2.309761	0.789013
H	-7.975063	-2.706234	1.520672
N	-3.263401	1.117212	0.981777
H	-2.920707	-4.188612	1.153427
H	-1.436372	-3.214480	1.314327
H	4.610299	-5.358865	1.644051
H	1.346164	-2.842875	1.128935
C	-4.622535	-2.180099	1.544825
C	3.214617	4.020960	1.558695
C	1.048263	2.805841	1.426686
H	5.328001	1.918153	1.776608
H	2.648602	4.935382	1.785612
H	7.619238	2.527633	2.224567
H	0.608893	3.743135	1.790061
C	-5.907683	-2.424220	2.047401
H	-1.606255	3.067030	1.973988

H	0.153491	-1.729512	1.847564
H	5.292037	-1.673233	2.192247
H	-3.773076	-2.137645	2.225604
C	0.929038	-2.467722	2.073639
N	2.761860	-0.800333	2.205378
H	1.244166	2.171214	2.301224
H	3.463646	3.524609	2.505187
H	7.595884	-1.764105	2.778465
H	-0.786012	0.659304	2.265288
H	-3.260352	3.487827	2.494019
C	-2.859481	1.335343	2.433076
H	3.468615	-3.444136	2.488786
H	0.457935	-3.314886	2.587477
C	-2.425487	2.794424	2.649655
H	-1.959116	-0.651261	2.550493
C	5.148787	-0.799878	2.827164
H	8.366225	-0.230450	3.250548
C	3.880210	-0.213906	2.915278
C	-1.708739	0.391712	2.787740
C	2.014385	-1.880239	2.972541
H	-4.899183	1.685997	3.176419
C	7.579631	-0.950860	3.512333
H	-4.386453	-0.020011	3.224087
C	-6.128744	-2.619999	3.527378
H	-7.178903	-2.840140	3.748246
C	6.224136	-0.289639	3.564836
C	-4.050723	1.016043	3.355230
C	2.983023	-3.009802	3.371070
H	-5.521211	-3.449406	3.913680
H	-2.075038	2.919608	3.684153
C	3.689043	0.903808	3.739099
H	2.408000	-3.799140	3.875440
H	-5.848468	-1.721787	4.095752
H	2.697105	1.347324	3.813894
H	-1.518424	0.449423	3.866745
H	7.847048	-1.374090	4.490490
H	3.757960	-2.662167	4.063333
C	6.007756	0.833385	4.372395
H	0.698531	-0.459094	3.990256
H	-3.728076	1.146734	4.397715
C	4.749751	1.445295	4.472066
C	1.375563	-1.285934	4.239128
H	6.840829	1.239951	4.950699
H	4.895478	3.572741	4.841261
H	0.794059	-2.065688	4.751319
H	2.137273	-0.922544	4.939367
C	4.549006	2.659106	5.346569
H	3.492220	2.801338	5.600842
H	5.117071	2.573540	6.280621

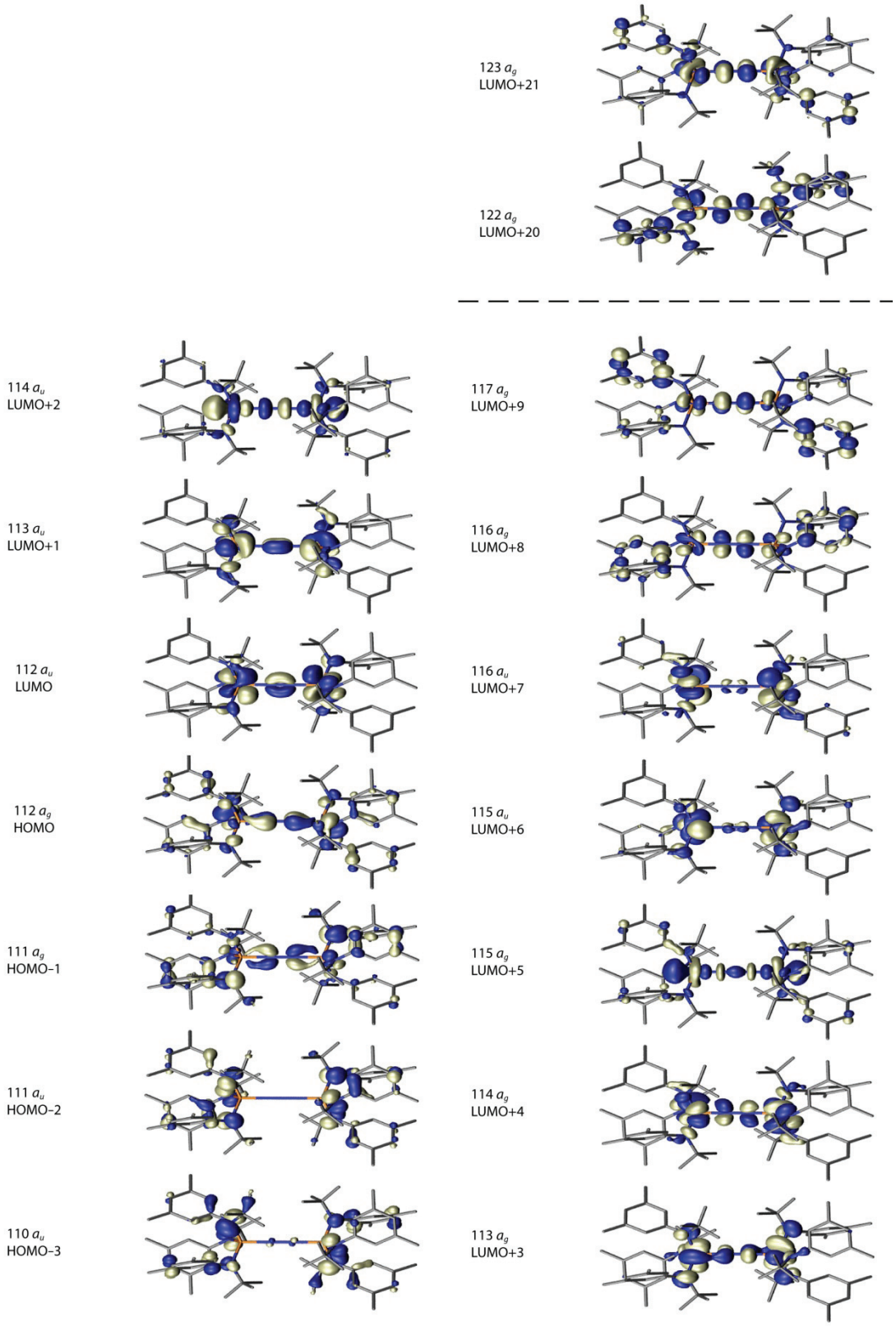

Figure S20. Selected molecular orbitals drawings for $\mathbf{2}^{2+}$

Table S5. Selected molecular orbitals energies for $\mathbf{2}^{2+}$

These molecular orbitals of $\mathbf{2}^{2+}$ were obtained from the DFT optimized geometry given above. Orbitals energies are uncorrected.

E(eV)	Occ	MO	%	SFO (first member)	E(eV)	Occ	Fragment
-9.766	2.00	110 A.u	17.28%	1 P:y	-5.422	0.67	133 C
			12.86%	1 P:y	-5.422	0.67	125 C
			10.23%	1 P:y	-5.422	0.67	129 C
			8.23%	1 P:y	-5.422	0.67	141 C
			4.32%	1 P:z	-5.422	0.67	116 C
			4.29%	1 P:z	-5.422	0.67	121 C
			3.29%	1 P:z	-5.422	0.67	115 C
			2.93%	1 P:y	-5.422	0.67	121 C
			2.69%	1 P:z	-5.422	0.67	110 C
			2.33%	1 P:y	-5.422	0.67	116 C
			2.04%	1 P:y	-5.422	0.67	115 C
			1.69%	1 P:y	-5.422	0.67	110 C
			1.36%	1 S	-6.630	1.00	9 H
			1.35%	1 P:z	-5.422	0.67	135 C
			1.35%	1 P:y	-5.422	0.67	143 C
			1.30%	1 P:z	-5.422	0.67	140 C
			1.27%	1 S	-6.630	1.00	11 H
			1.19%	1 S	-6.630	1.00	40 H
-9.671	2.00	110 A.g	20.18%	1 P:y	-7.225	1.00	182 N
			6.31%	1 P:y	-5.422	0.67	130 C
			5.85%	1 P:y	-5.422	0.67	129 C
			5.39%	1 P:x	-7.225	1.00	182 N
			5.34%	1 P:y	-7.225	1.00	181 N
			5.24%	1 P:y	-5.422	0.67	143 C
			4.60%	1 P:z	-7.225	1.00	183 N
			4.51%	1 P:y	-5.422	0.67	141 C
			4.40%	1 P:x	-7.225	1.00	181 N
			2.21%	1 P:z	-5.422	0.67	139 C
			1.97%	1 P:z	-5.422	0.67	144 C
			1.87%	1 P:y	-5.422	0.67	123 C
			1.79%	1 P:z	-7.225	1.00	184 N
			1.62%	1 P:z	-5.422	0.67	138 C
			1.44%	1 P:z	-7.225	1.00	181 N
			1.39%	1 P:y	-7.225	1.00	183 N
			1.16%	1 P:y	-5.422	0.67	116 C
-9.664	2.00	111 A.u	12.98%	1 P:z	-7.225	1.00	183 N
			9.71%	1 P:y	-7.225	1.00	182 N
			5.09%	1 P:z	-7.225	1.00	181 N
			4.52%	1 P:y	-7.225	1.00	181 N
			4.05%	1 P:x	-7.225	1.00	181 N
			3.79%	1 P:z	-5.422	0.67	144 C
			3.75%	1 P:z	-5.422	0.67	111 C
			3.50%	1 P:z	-5.422	0.67	120 C
			3.06%	1 P:y	-5.422	0.67	130 C
			2.83%	1 P:x	-7.225	1.00	182 N
			2.74%	1 P:y	-5.422	0.67	116 C
			2.52%	1 P:y	-5.422	0.67	143 C
			2.39%	1 P:y	-5.422	0.67	129 C
			2.18%	1 P:z	-5.422	0.67	139 C
			2.11%	1 P:y	-5.422	0.67	111 C
			2.09%	1 P:z	-5.422	0.67	142 C
			2.01%	1 P:y	-5.422	0.67	141 C
			1.64%	1 P:z	-5.422	0.67	115 C
			1.41%	1 P:z	-5.422	0.67	138 C
			1.20%	1 P:x	-7.225	1.00	183 N
			1.11%	1 P:z	-5.422	0.67	112 C
			1.10%	1 P:z	-5.422	0.67	116 C
			1.10%	1 P:y	-5.422	0.67	120 C
-9.638	2.00	111 A.g	18.71%	1 P:z	-7.225	1.00	183 N
			7.80%	1 P:y	-7.225	1.00	184 N

				4.88%	1	D:xy	-3.873	1.00	189	Mo
				4.08%	1	P:y	-7.225	1.00	181	N
				3.82%	1	P:z	-5.422	0.67	111	C
				3.73%	1	P:z	-5.422	0.67	116	C
				2.94%	1	P:z	-5.422	0.67	139	C
				2.87%	1	P:z	-5.422	0.67	138	C
				2.68%	1	P:z	-5.422	0.67	120	C
				2.53%	1	P:x	-7.225	1.00	181	N
				2.34%	1	P:y	-5.422	0.67	111	C
				2.31%	1	P:z	-7.225	1.00	184	N
				2.23%	1	P:z	-5.422	0.67	115	C
				2.18%	1	P:y	-5.422	0.67	133	C
				2.11%	1	P:y	-5.422	0.67	120	C
				-1.86%	1	P:z	-0.498	0.00	189	Mo
				1.72%	1	P:y	-5.422	0.67	116	C
				1.60%	1	P:z	-7.225	1.00	182	N
				1.60%	1	P:y	-5.422	0.67	115	C
				1.57%	1	P:y	-7.225	1.00	183	N
				1.35%	1	P:z	-5.422	0.67	135	C
				1.35%	1	P:x	-7.225	1.00	183	N
				1.25%	1	P:y	-5.422	0.67	125	C
				1.21%	1	P:z	-5.422	0.67	140	C
				1.11%	1	P:y	-7.225	1.00	182	N
HOMO	-9.595	2.00	112 A.g	11.40%	1	P:z	-7.225	1.00	181	N
				7.71%	1	P:z	-7.225	1.00	184	N
				4.25%	1	P:y	-7.225	1.00	181	N
				3.82%	1	P:x	-7.225	1.00	181	N
				3.64%	1	P:y	-7.225	1.00	184	N
				3.36%	1	D:xz	-3.873	1.00	189	Mo
				3.24%	1	P:z	-5.422	0.67	144	C
				3.22%	1	P:z	-7.225	1.00	183	N
				3.08%	1	P:y	-7.225	1.00	182	N
				2.87%	1	P:y	-5.422	0.67	130	C
				2.83%	1	P:x	-7.225	1.00	182	N
				2.82%	1	P:z	-5.422	0.67	142	C
				2.58%	1	P:z	-5.422	0.67	139	C
				2.42%	1	P:z	-5.422	0.67	111	C
				2.20%	1	P:y	-5.422	0.67	143	C
				-2.02%	1	P:y	-0.498	0.00	189	Mo
				2.01%	1	D:z2	-3.873	1.00	189	Mo
				1.95%	1	P:z	-5.422	0.67	138	C
				1.93%	1	P:z	-5.422	0.67	121	C
				1.91%	1	P:y	-7.225	1.00	183	N
				1.85%	1	P:x	-7.225	1.00	183	N
				1.59%	1	P:z	-5.422	0.67	112	C
				1.58%	1	P:z	-5.422	0.67	120	C
				1.36%	1	P:y	-5.422	0.67	111	C
				1.17%	1	P:z	-7.225	1.00	182	N
				1.13%	1	P:y	-5.422	0.67	120	C
				1.04%	1	P:y	-5.422	0.67	144	C
				1.01%	1	P:y	-5.422	0.67	110	C
LUMO	-8.072	0.00	112 A.u	42.13%	1	D:xy	-3.873	1.00	189	Mo
				11.54%	1	D:z2	-3.873	1.00	189	Mo
				6.47%	1	P:y	-7.225	1.00	181	N
				5.73%	1	P:z	-7.225	1.00	183	N
				5.24%	1	D:xz	-3.873	1.00	189	Mo
				4.29%	1	P:x	-7.225	1.00	181	N
				3.88%	1	P:y	-7.225	1.00	184	N
				1.84%	1	D:x2-y2	-3.873	1.00	189	Mo
				1.25%	1	P:z	-5.422	0.67	124	C
				1.07%	1	P:z	-7.225	1.00	182	N
				1.02%	2	D:xy	3.474	0.00	189	Mo
	-8.021	0.00	113 A.u	37.00%	1	D:xz	-3.873	1.00	189	Mo
				11.04%	1	D:xy	-3.873	1.00	189	Mo
				7.08%	1	D:yz	-3.873	1.00	189	Mo
				5.84%	1	P:y	-7.225	1.00	182	N
				4.47%	1	P:z	-7.225	1.00	183	N
				4.31%	1	D:z2	-3.873	1.00	189	Mo
				4.19%	1	P:x	-7.225	1.00	182	N
				3.64%	1	P:z	-7.225	1.00	184	N
				1.84%	1	P:z	-7.225	1.00	181	N

			1.58%	1	P:x	-7.225	1.00	183	N
			1.39%	1	P:z	-7.225	1.00	182	N
			1.33%	1	D:x2-y2	-3.873	1.00	189	Mo
			1.27%	2	D:xz	3.474	0.00	189	Mo
-7.099	0.00	114 A.u	34.87%	1	D:x2-y2	-3.873	1.00	189	Mo
			10.85%	1	D:z2	-3.873	1.00	189	Mo
			6.49%	1	S	-18.740	2.00	184	N
			4.28%	2	P:x	7.798	0.00	184	N
			3.87%	1	D:xz	-3.873	1.00	189	Mo
			2.37%	1	P:y	-7.225	1.00	181	N
			2.01%	1	P:z	-7.225	1.00	183	N
			1.96%	1	P:z	-5.422	0.67	144	C
			1.95%	1	P:y	-5.422	0.67	129	C
			1.89%	1	P:y	-5.422	0.67	130	C
			1.88%	1	P:x	-7.225	1.00	182	N
			1.87%	1	P:z	-5.422	0.67	139	C
			1.66%	1	P:x	-7.225	1.00	181	N
			1.32%	1	P:z	-7.225	1.00	182	N
			1.27%	1	P:z	-5.422	0.67	111	C
			1.24%	1	P:y	-7.225	1.00	183	N
			1.21%	1	P:x	-7.225	1.00	183	N
			1.17%	1	P:z	-5.422	0.67	116	C
			1.07%	1	P:y	-5.422	0.67	133	C
-6.835	0.00	113 A.g	35.44%	1	D:yz	-3.873	1.00	189	Mo
			9.46%	1	P:z	-7.225	1.00	183	N
			8.48%	1	P:z	-7.225	1.00	184	N
			6.15%	1	P:x	-7.225	1.00	182	N
			4.24%	1	D:xz	-3.873	1.00	189	Mo
			3.62%	1	P:y	-7.225	1.00	184	N
			3.36%	1	P:z	-7.225	1.00	181	N
			2.62%	1	P:z	-7.225	1.00	182	N
			2.27%	1	D:xy	-3.873	1.00	189	Mo
			1.71%	1	D:z2	-3.873	1.00	189	Mo
			1.50%	1	P:x	-7.225	1.00	183	N
			1.39%	1	P:y	-7.225	1.00	182	N
			1.24%	1	D:x2-y2	-3.873	1.00	189	Mo
			1.09%	1	P:z	-5.422	0.67	111	C
			1.04%	1	P:z	-5.422	0.67	121	C
-6.805	0.00	114 A.g	27.17%	1	D:z2	-3.873	1.00	189	Mo
			10.64%	1	D:x2-y2	-3.873	1.00	189	Mo
			9.51%	1	P:y	-7.225	1.00	184	N
			5.99%	1	P:y	-7.225	1.00	181	N
			5.70%	1	P:x	-7.225	1.00	181	N
			5.66%	1	P:y	-7.225	1.00	182	N
			4.87%	1	D:yz	-3.873	1.00	189	Mo
			3.64%	1	P:z	-7.225	1.00	184	N
			3.03%	1	P:y	-7.225	1.00	183	N
			2.09%	1	P:x	-7.225	1.00	183	N
			1.71%	1	D:xy	-3.873	1.00	189	Mo
			1.25%	1	P:z	-7.225	1.00	183	N
			1.10%	1	P:y	-5.422	0.67	130	C
			1.08%	1	P:z	-5.422	0.67	139	C
			1.07%	1	P:z	-5.422	0.67	144	C
			1.03%	2	P:x	4.700	0.00	143	C
-6.414	0.00	115 A.g	22.59%	1	D:x2-y2	-3.873	1.00	189	Mo
			7.58%	1	D:z2	-3.873	1.00	189	Mo
			6.16%	1	P:x	-0.498	0.00	189	Mo
			5.26%	1	P:x	-7.225	1.00	184	N
			3.57%	1	P:z	-5.422	0.67	144	C
			3.45%	1	P:z	-5.422	0.67	139	C
			3.22%	1	P:y	-5.422	0.67	129	C
			3.19%	1	P:y	-5.422	0.67	130	C
			3.13%	1	S	-18.740	2.00	184	N
			2.29%	1	D:xz	-3.873	1.00	189	Mo
			2.15%	1	S	-4.293	1.00	189	Mo
			2.01%	1	P:y	-7.225	1.00	181	N
			1.93%	2	S	0.905	0.00	189	Mo
			1.87%	1	P:z	-5.422	0.67	111	C
			1.84%	1	P:z	-5.422	0.67	116	C
			1.64%	1	P:z	-5.422	0.67	138	C
			-1.47%	2	P:x	7.798	0.00	184	N

			1.46%	1	P:z	-7.225	1.00	182	N
			1.28%	1	P:z	-5.422	0.67	142	C
			1.26%	1	P:y	-5.422	0.67	111	C
			1.25%	1	P:y	-5.422	0.67	143	C
			1.25%	1	P:x	-7.225	1.00	182	N
			1.24%	2	S	16.016	0.00	184	N
			1.08%	1	P:y	-5.422	0.67	141	C
			1.03%	1	P:y	-5.422	0.67	133	C
			1.03%	1	P:y	-5.422	0.67	116	C
-6.261	0.00	115 A.u	30.95%	1	D:yz	-3.873	1.00	189	Mo
			11.45%	1	D:z2	-3.873	1.00	189	Mo
			7.50%	1	P:z	-7.225	1.00	181	N
			6.25%	1	P:z	-7.225	1.00	183	N
			4.32%	1	P:x	-7.225	1.00	182	N
			3.07%	1	D:xz	-3.873	1.00	189	Mo
			2.59%	1	D:xy	-3.873	1.00	189	Mo
			2.29%	1	S	-18.740	2.00	181	N
			2.07%	1	D:x2-y2	-3.873	1.00	189	Mo
			1.86%	1	P:y	-7.225	1.00	183	N
			1.68%	1	P:z	-5.422	0.67	111	C
			1.54%	1	P:z	-7.225	1.00	182	N
			1.52%	1	P:z	-5.422	0.67	121	C
			1.36%	1	P:y	-5.422	0.67	116	C
			1.23%	1	P:z	-5.422	0.67	120	C
			1.04%	1	P:y	-5.422	0.67	130	C
-6.245	0.00	116 A.u	14.53%	1	D:z2	-3.873	1.00	189	Mo
			10.33%	1	D:xz	-3.873	1.00	189	Mo
			8.79%	1	D:x2-y2	-3.873	1.00	189	Mo
			8.52%	1	P:y	-7.225	1.00	182	N
			8.35%	1	D:xy	-3.873	1.00	189	Mo
			8.25%	1	D:yz	-3.873	1.00	189	Mo
			3.94%	1	P:y	-7.225	1.00	183	N
			3.33%	1	P:x	-7.225	1.00	181	N
			3.06%	1	P:y	-7.225	1.00	181	N
			2.41%	1	P:x	-7.225	1.00	183	N
			2.08%	1	P:z	-5.422	0.67	139	C
			1.82%	1	S	-18.740	2.00	182	N
			1.69%	1	P:z	-5.422	0.67	144	C
			1.69%	1	P:y	-5.422	0.67	130	C
			1.66%	1	S	-18.740	2.00	183	N
			1.52%	1	P:y	-5.422	0.67	129	C
			1.26%	1	P:y	-5.422	0.67	143	C
			1.19%	1	P:z	-5.422	0.67	135	C
			-1.17%	2	P:y	7.798	0.00	182	N
-5.235	0.00	116 A.g	18.74%	1	P:y	-7.225	1.00	184	N
			11.92%	1	D:xy	-3.873	1.00	189	Mo
			8.61%	1	P:z	-5.422	0.67	120	C
			7.59%	1	P:y	-5.422	0.67	143	C
			6.64%	1	P:z	-5.422	0.67	111	C
			5.96%	1	P:y	-5.422	0.67	130	C
			5.69%	1	P:y	-5.422	0.67	129	C
			4.55%	1	P:y	-5.422	0.67	141	C
			4.06%	1	P:y	-5.422	0.67	120	C
			3.94%	1	P:y	-5.422	0.67	111	C
			2.50%	1	P:z	-5.422	0.67	121	C
			2.30%	1	P:z	-5.422	0.67	116	C
			-2.23%	2	P:y	7.798	0.00	184	N
			-1.72%	2	P:z	4.700	0.00	120	C
			1.63%	1	P:y	-5.422	0.67	121	C
			-1.49%	2	P:y	4.700	0.00	143	C
			1.49%	1	P:z	-5.422	0.67	115	C
			1.45%	1	P:z	-5.422	0.67	110	C
			1.23%	1	D:z2	-3.873	1.00	189	Mo
-5.200	0.00	117 A.g	18.82%	1	P:z	-7.225	1.00	184	N
			11.63%	1	P:z	-5.422	0.67	138	C
			9.93%	1	P:z	-5.422	0.67	139	C
			9.26%	1	D:xz	-3.873	1.00	189	Mo
			5.16%	1	P:z	-5.422	0.67	144	C
			4.38%	1	P:y	-5.422	0.67	143	C
			3.99%	1	P:z	-5.422	0.67	142	C
			3.57%	1	P:y	-5.422	0.67	130	C

			3.23%	1	D:z2	-3.873	1.00	189	Mo
			2.97%	1	P:y	-5.422	0.67	129	C
			2.34%	1	P:y	-5.422	0.67	138	C
			2.34%	1	P:y	-5.422	0.67	141	C
			2.32%	1	P:z	-5.422	0.67	135	C
			-2.28%	2	P:z	4.700	0.00	138	C
			-2.22%	2	P:z	7.798	0.00	184	N
			1.78%	1	P:z	-5.422	0.67	120	C
			1.60%	1	P:y	-5.422	0.67	139	C
			1.30%	1	P:z	-5.422	0.67	111	C
			1.28%	1	D:yz	-3.873	1.00	189	Mo
			1.19%	1	P:z	-5.422	0.67	140	C
-5.126	0.00	117 A.u	15.09%	1	P:y	-5.422	0.67	141	C
			12.42%	1	P:y	-5.422	0.67	129	C
			9.50%	1	P:y	-5.422	0.67	125	C
			8.11%	1	P:z	-5.422	0.67	142	C
			7.78%	1	P:y	-5.422	0.67	133	C
			6.40%	1	P:z	-5.422	0.67	144	C
			5.48%	1	P:z	-5.422	0.67	140	C
			4.58%	1	P:z	-5.422	0.67	135	C
			2.85%	1	P:z	-5.422	0.67	110	C
			-2.43%	2	P:y	4.700	0.00	141	C
			2.11%	1	P:z	-5.422	0.67	121	C
			2.01%	1	S	-6.630	1.00	40	H
			1.61%	1	P:y	-5.422	0.67	110	C
			1.51%	1	P:y	-5.422	0.67	121	C
			1.40%	1	P:z	-5.422	0.67	115	C
			-1.37%	2	P:y	4.700	0.00	125	C
			-1.29%	2	P:z	4.700	0.00	142	C
			1.21%	2	D:x2-y2	3.474	0.00	189	Mo
			1.17%	1	S	-6.630	1.00	11	H
			1.15%	1	P:y	-5.422	0.67	142	C
			1.12%	1	D:x2-y2	-3.873	1.00	189	Mo
			-1.10%	2	P:y	4.700	0.00	129	C
			1.09%	1	S	-6.630	1.00	9	H
-5.094	0.00	118 A.g	14.95%	1	P:y	-5.422	0.67	125	C
			13.64%	1	P:y	-5.422	0.67	133	C
			8.91%	1	P:z	-5.422	0.67	140	C
			7.79%	1	P:z	-5.422	0.67	135	C
			6.81%	1	P:z	-5.422	0.67	142	C
			6.75%	1	P:y	-5.422	0.67	141	C
			5.10%	1	P:z	-5.422	0.67	144	C
			4.36%	1	P:y	-5.422	0.67	129	C
			2.57%	1	P:z	-5.422	0.67	110	C
			-2.26%	2	P:y	4.700	0.00	125	C
			2.03%	1	P:y	-5.422	0.67	130	C
			1.97%	1	P:z	-5.422	0.67	115	C
			1.96%	1	P:y	-5.422	0.67	143	C
			1.60%	1	P:z	-5.422	0.67	121	C
			1.43%	1	P:y	-5.422	0.67	110	C
			1.41%	1	P:z	-5.422	0.67	116	C
			1.40%	1	S	-6.630	1.00	9	H
			1.29%	1	P:y	-5.422	0.67	140	C
			-1.29%	2	P:z	4.700	0.00	140	C
			1.27%	1	S	-6.630	1.00	11	H
			1.26%	1	P:y	-5.422	0.67	115	C
			-1.24%	2	P:y	4.700	0.00	141	C
			-1.23%	2	P:z	4.700	0.00	142	C
			1.20%	1	P:y	-7.225	1.00	184	N
			1.14%	1	S	-6.630	1.00	53	H
			1.14%	1	P:y	-5.422	0.67	121	C
			1.04%	1	P:y	-5.422	0.67	135	C
-5.083	0.00	118 A.u	9.45%	1	P:z	-5.422	0.67	142	C
			8.92%	1	P:z	-5.422	0.67	120	C
			8.41%	1	P:z	-5.422	0.67	144	C
			7.71%	1	P:z	-5.422	0.67	111	C
			5.02%	1	P:y	-5.422	0.67	111	C
			4.64%	1	P:y	-5.422	0.67	120	C
			3.78%	1	P:z	-5.422	0.67	138	C
			3.59%	1	P:y	-5.422	0.67	129	C
			3.25%	1	P:y	-5.422	0.67	141	C

			2.84%	1	P:z	-5.422	0.67	110	C
			2.55%	1	P:z	-5.422	0.67	121	C
			2.15%	1	P:y	-5.422	0.67	121	C
			2.12%	1	P:z	-5.422	0.67	139	C
			2.11%	1	P:z	-5.422	0.67	140	C
			2.04%	1	D:z2	-3.873	1.00	189	Mo
			2.00%	1	P:y	-5.422	0.67	143	C
			1.87%	1	P:y	-5.422	0.67	144	C
			1.86%	1	P:y	-5.422	0.67	110	C
			1.84%	1	P:z	-5.422	0.67	135	C
			-1.37%	2	P:z	4.700	0.00	142	C
			1.36%	1	P:y	-5.422	0.67	142	C
			1.35%	1	P:z	-5.422	0.67	116	C
			1.33%	1	P:y	-5.422	0.67	130	C
			1.27%	1	P:z	-5.422	0.67	115	C
			-1.17%	2	P:z	4.700	0.00	120	C
			-1.10%	2	P:z	4.700	0.00	138	C
			1.09%	1	S	-6.630	1.00	41	H
-5.021	0.00	119 A.u	10.14%	1	P:z	-5.422	0.67	138	C
			8.22%	1	P:z	-5.422	0.67	139	C
			7.83%	1	P:z	-5.422	0.67	115	C
			7.74%	1	P:z	-5.422	0.67	116	C
			5.00%	1	P:z	-5.422	0.67	120	C
			4.66%	1	P:y	-5.422	0.67	115	C
			3.80%	1	P:y	-5.422	0.67	130	C
			3.68%	1	P:z	-5.422	0.67	144	C
			3.52%	1	P:z	-5.422	0.67	142	C
			3.44%	1	P:z	-5.422	0.67	111	C
			3.33%	1	P:y	-5.422	0.67	143	C
			3.31%	1	P:y	-5.422	0.67	116	C
			2.69%	1	P:y	-5.422	0.67	120	C
			2.43%	1	D:yz	-3.873	1.00	189	Mo
			2.36%	1	P:y	-5.422	0.67	125	C
			2.33%	1	P:y	-5.422	0.67	133	C
			-2.05%	2	P:z	4.700	0.00	138	C
			2.00%	1	P:y	-5.422	0.67	111	C
			1.61%	1	P:z	-5.422	0.67	135	C
			1.49%	1	P:y	-5.422	0.67	138	C
			1.40%	1	S	-6.630	1.00	6	H
			1.33%	1	P:y	-5.422	0.67	139	C
			1.22%	1	P:z	-5.422	0.67	140	C
			-1.11%	2	P:z	4.700	0.00	115	C
-5.002	0.00	119 A.g	13.96%	1	P:z	-5.422	0.67	140	C
			12.25%	1	P:z	-5.422	0.67	135	C
			10.44%	1	P:z	-5.422	0.67	142	C
			8.86%	1	P:z	-5.422	0.67	144	C
			8.45%	1	P:y	-5.422	0.67	125	C
			8.12%	1	P:y	-5.422	0.67	133	C
			7.87%	1	P:y	-5.422	0.67	141	C
			7.22%	1	P:y	-5.422	0.67	129	C
			2.62%	1	P:y	-7.225	1.00	184	N
			-2.16%	2	P:z	4.700	0.00	140	C
			2.01%	1	P:y	-5.422	0.67	135	C
			1.97%	1	P:y	-5.422	0.67	140	C
			1.90%	1	S	-6.630	1.00	53	H
			-1.64%	2	P:z	4.700	0.00	142	C
			1.59%	1	P:y	-5.422	0.67	144	C
			1.52%	1	P:y	-5.422	0.67	142	C
			1.47%	1	D:xy	-3.873	1.00	189	Mo
			-1.38%	2	P:z	4.700	0.00	135	C
			1.33%	1	S	-6.630	1.00	34	H
			-1.18%	2	P:y	4.700	0.00	141	C
			-1.16%	2	P:y	4.700	0.00	125	C
			1.11%	1	S	-6.630	1.00	11	H
			-1.05%	2	P:y	4.700	0.00	133	C
-4.995	0.00	120 A.u	13.91%	1	P:y	-5.422	0.67	143	C
			10.81%	1	P:z	-5.422	0.67	140	C
			9.92%	1	P:y	-5.422	0.67	130	C
			8.71%	1	P:z	-5.422	0.67	135	C
			6.86%	1	P:z	-5.422	0.67	139	C
			6.75%	1	P:y	-5.422	0.67	129	C

			6.21%	1	P:y	-5.422	0.67	141	C
			6.13%	1	P:z	-5.422	0.67	138	C
			3.84%	1	D:x2-y2	-3.873	1.00	189	Mo
			-2.83%	2	P:y	4.700	0.00	143	C
			-1.94%	2	P:z	4.700	0.00	140	C
			1.73%	1	P:z	-5.422	0.67	110	C
			1.68%	1	P:z	-5.422	0.67	120	C
			1.46%	1	P:y	-5.422	0.67	140	C
			1.18%	1	P:z	-5.422	0.67	111	C
			-1.15%	2	P:z	4.700	0.00	138	C
			1.13%	1	P:z	-5.422	0.67	121	C
			1.13%	1	P:y	-5.422	0.67	110	C
			1.08%	1	P:y	-5.422	0.67	138	C
			1.05%	1	S	-6.630	1.00	53	H
			1.00%	1	P:y	-5.422	0.67	121	C
-4.949	0.00	120 A.g	14.12%	1	P:z	-5.422	0.67	110	C
			11.78%	1	P:z	-5.422	0.67	121	C
			8.61%	1	P:y	-5.422	0.67	110	C
			8.59%	1	P:z	-5.422	0.67	115	C
			7.93%	1	P:z	-5.422	0.67	116	C
			7.45%	1	P:y	-5.422	0.67	121	C
			5.09%	1	P:y	-5.422	0.67	115	C
			4.72%	1	P:y	-5.422	0.67	116	C
			4.09%	1	P:y	-5.422	0.67	125	C
			3.41%	1	P:y	-5.422	0.67	133	C
			2.92%	1	P:y	-5.422	0.67	141	C
			2.67%	1	P:y	-5.422	0.67	129	C
			-2.39%	2	P:z	4.700	0.00	110	C
			2.24%	1	P:z	-7.225	1.00	184	N
			2.05%	1	S	-6.630	1.00	4	H
			1.44%	1	D:xz	-3.873	1.00	189	Mo
			-1.30%	2	P:y	4.700	0.00	110	C
			-1.27%	2	P:z	4.700	0.00	121	C
			1.18%	1	P:x	-5.422	0.67	110	C
			-1.14%	2	P:z	4.700	0.00	115	C
			1.12%	1	P:z	-5.422	0.67	144	C
			1.09%	1	P:z	-5.422	0.67	142	C
			-1.03%	2	P:y	4.700	0.00	115	C
			1.02%	1	P:z	-5.422	0.67	138	C
-4.942	0.00	121 A.u	19.19%	1	P:y	-5.422	0.67	125	C
			17.54%	1	P:y	-5.422	0.67	133	C
			7.70%	1	P:y	-5.422	0.67	130	C
			6.90%	1	P:y	-5.422	0.67	143	C
			5.02%	1	P:z	-5.422	0.67	142	C
			4.47%	1	P:z	-5.422	0.67	144	C
			-3.10%	2	P:y	4.700	0.00	125	C
			2.78%	1	P:y	-5.422	0.67	141	C
			2.59%	1	D:yz	-3.873	1.00	189	Mo
			2.48%	1	P:z	-5.422	0.67	111	C
			2.21%	1	P:z	-5.422	0.67	140	C
			2.20%	1	P:y	-5.422	0.67	129	C
			2.13%	1	P:z	-5.422	0.67	120	C
			-1.95%	2	P:y	4.700	0.00	133	C
			1.82%	1	P:z	-5.422	0.67	135	C
			1.78%	1	P:z	-5.422	0.67	121	C
			1.71%	1	P:z	-5.422	0.67	110	C
			1.60%	1	P:y	-5.422	0.67	121	C
			1.56%	1	S	-6.630	1.00	11	H
			1.54%	1	S	-6.630	1.00	9	H
			1.33%	1	P:y	-5.422	0.67	111	C
			1.24%	1	P:y	-5.422	0.67	120	C
			1.20%	1	P:y	-5.422	0.67	110	C
			-1.05%	2	P:y	4.700	0.00	143	C
-4.895	0.00	122 A.u	9.85%	1	P:z	-5.422	0.67	110	C
			8.34%	1	P:z	-5.422	0.67	121	C
			7.86%	1	P:z	-5.422	0.67	115	C
			7.40%	1	P:z	-5.422	0.67	140	C
			7.13%	1	P:z	-5.422	0.67	135	C
			6.90%	1	P:z	-5.422	0.67	116	C
			5.80%	1	P:y	-5.422	0.67	110	C
			4.97%	1	P:y	-5.422	0.67	121	C

			4.92%	1	P:y	-5.422	0.67	116	C
			4.80%	1	P:y	-5.422	0.67	115	C
			4.70%	1	P:z	-5.422	0.67	139	C
			4.14%	1	P:z	-5.422	0.67	138	C
			2.13%	1	P:y	-5.422	0.67	143	C
			1.83%	1	P:y	-5.422	0.67	141	C
			1.77%	1	P:y	-5.422	0.67	130	C
			1.76%	1	P:y	-5.422	0.67	129	C
			1.66%	1	D:z2	-3.873	1.00	189	Mo
			-1.65%	2	P:z	4.700	0.00	110	C
			1.59%	1	S	-6.630	1.00	4	H
			-1.11%	2	P:z	4.700	0.00	115	C
			-1.11%	2	P:z	4.700	0.00	140	C
			-1.04%	2	P:z	4.700	0.00	135	C
-4.794	0.00	121 A.g	6.92%	1	P:z	-5.422	0.67	120	C
			6.41%	1	D:z2	-3.873	1.00	189	Mo
			4.94%	1	P:z	-5.422	0.67	111	C
			4.93%	1	D:x2-y2	-3.873	1.00	189	Mo
			4.79%	1	P:z	-5.422	0.67	115	C
			4.51%	1	P:z	-5.422	0.67	138	C
			4.41%	1	P:z	-5.422	0.67	139	C
			4.29%	1	P:y	-7.225	1.00	184	N
			3.64%	1	P:z	-5.422	0.67	116	C
			3.55%	1	P:y	-5.422	0.67	143	C
			3.30%	1	P:y	-5.422	0.67	111	C
			3.24%	1	P:y	-5.422	0.67	120	C
			2.95%	1	P:y	-5.422	0.67	115	C
			2.56%	1	P:z	-5.422	0.67	140	C
			2.39%	1	P:x	-0.498	0.00	189	Mo
			2.35%	1	P:y	-5.422	0.67	130	C
			2.31%	1	D:xy	-3.873	1.00	189	Mo
			1.90%	1	P:y	-5.422	0.67	141	C
			1.81%	1	P:y	-5.422	0.67	116	C
			1.79%	1	S	-4.293	1.00	189	Mo
			1.52%	1	P:z	-5.422	0.67	135	C
			1.51%	1	P:y	-5.422	0.67	129	C
			1.42%	1	S	-18.740	2.00	181	N
			1.41%	1	S	-6.630	1.00	16	H
			1.37%	1	P:x	-7.225	1.00	184	N
			1.36%	1	P:z	-7.225	1.00	181	N
			-1.15%	2	P:z	4.700	0.00	138	C
			1.12%	1	D:xz	-3.873	1.00	189	Mo
			1.03%	1	P:y	-5.422	0.67	138	C
-4.769	0.00	122 A.g	11.87%	1	P:y	-7.225	1.00	184	N
			11.84%	1	P:y	-5.422	0.67	143	C
			10.89%	1	P:y	-5.422	0.67	130	C
			8.50%	1	D:xy	-3.873	1.00	189	Mo
			7.93%	1	D:x2-y2	-3.873	1.00	189	Mo
			7.55%	1	P:z	-7.225	1.00	184	N
			4.64%	1	D:xz	-3.873	1.00	189	Mo
			4.33%	1	P:y	-5.422	0.67	125	C
			2.90%	1	S	-18.740	2.00	183	N
			2.79%	1	P:y	-5.422	0.67	133	C
			2.38%	1	P:y	-7.225	1.00	183	N
			2.35%	1	P:y	-5.422	0.67	141	C
			-1.83%	2	P:y	4.700	0.00	143	C
			-1.78%	2	P:y	7.798	0.00	184	N
			1.76%	1	P:y	-7.225	1.00	182	N
			1.70%	1	P:y	-5.422	0.67	129	C
			1.61%	1	P:y	-5.422	0.67	136	C
			1.09%	1	D:z2	-3.873	1.00	189	Mo
			1.05%	1	P:x	-7.225	1.00	183	N
-4.741	0.00	123 A.g	15.70%	1	P:z	-7.225	1.00	184	N
			10.70%	1	D:yz	-3.873	1.00	189	Mo
			10.70%	1	D:xz	-3.873	1.00	189	Mo
			7.51%	1	P:y	-7.225	1.00	184	N
			6.81%	1	P:z	-5.422	0.67	138	C
			6.55%	1	P:z	-5.422	0.67	139	C
			3.04%	1	D:xy	-3.873	1.00	189	Mo
			2.66%	1	P:z	-7.225	1.00	181	N
			2.33%	1	P:z	-5.422	0.67	142	C

			-2.27%	2	P:z	7.798	0.00	184	N
			2.03%	1	P:z	-5.422	0.67	140	C
			1.64%	1	S	-18.740	2.00	182	N
			1.62%	1	S	-18.740	2.00	181	N
			1.56%	2	D:xy	3.474	0.00	189	Mo
			1.39%	1	P:z	-5.422	0.67	144	C
			1.30%	1	P:z	-5.422	0.67	110	C
			1.28%	1	P:z	-5.422	0.67	135	C
			1.28%	1	P:x	-7.225	1.00	182	N
			-1.28%	2	P:z	4.700	0.00	138	C
			1.23%	1	P:z	-5.422	0.67	124	C
			1.20%	1	P:z	-5.422	0.67	111	C
			1.15%	1	P:y	-5.422	0.67	119	C
			1.02%	1	P:x	-7.225	1.00	184	N
			1.01%	1	P:y	-5.422	0.67	121	C
			1.01%	1	P:y	-5.422	0.67	139	C
-4.137	0.00	124 A.g	9.52%	2	S	0.905	0.00	189	Mo
			5.86%	2	S	2.533	0.00	45	H
			5.84%	2	S	2.533	0.00	31	H
			5.68%	2	S	2.533	0.00	27	H
			5.63%	1	S	-4.293	1.00	189	Mo
			4.93%	2	S	2.533	0.00	17	H
			4.57%	2	S	2.533	0.00	38	H
			-4.39%	2	S	2.533	0.00	29	H
			4.35%	1	S	-6.630	1.00	31	H
			4.28%	1	S	-6.630	1.00	45	H
			4.16%	1	S	-6.630	1.00	27	H
			4.11%	2	S	2.533	0.00	55	H
			-4.08%	2	S	2.533	0.00	37	H
			4.01%	2	S	2.533	0.00	52	H
			-3.91%	2	S	2.533	0.00	51	H
			3.87%	2	S	2.533	0.00	25	H
			3.71%	2	S	2.533	0.00	15	H
			3.61%	2	S	2.533	0.00	18	H
			3.45%	2	S	2.533	0.00	30	H
			3.14%	2	S	2.533	0.00	7	H
			2.11%	1	S	-6.630	1.00	55	H
			2.04%	1	S	-6.630	1.00	15	H
			1.99%	1	S	-6.630	1.00	52	H
			1.94%	1	S	-6.630	1.00	17	H
			-1.88%	1	S	-6.630	1.00	29	H
			1.83%	1	S	-6.630	1.00	30	H
			1.74%	1	S	-6.630	1.00	18	H
			1.74%	1	S	-6.630	1.00	38	H
			-1.68%	1	S	-6.630	1.00	51	H
			-1.63%	1	S	-6.630	1.00	37	H
			1.61%	2	S	2.533	0.00	35	H
			1.61%	2	S	2.533	0.00	13	H
			1.57%	2	S	2.533	0.00	8	H
			1.51%	2	S	2.533	0.00	14	H
			1.49%	2	S	2.533	0.00	2	H
			1.49%	1	S	-6.630	1.00	7	H
			-1.47%	2	S	2.533	0.00	22	H
			1.46%	2	S	2.533	0.00	32	H
			1.45%	1	S	-6.630	1.00	25	H
			-1.32%	2	S	11.657	0.00	131	C
			-1.30%	2	S	11.657	0.00	122	C
			-1.26%	2	S	2.533	0.00	19	H
			-1.15%	2	S	11.657	0.00	126	C
			-1.15%	2	S	2.533	0.00	47	H
			-1.12%	2	S	2.533	0.00	26	H
			-1.09%	2	S	2.533	0.00	36	H

Table S6. TDDFT spin-allowed electronic transitions

The first 30 spin-allowed electronic transitions are given (energies are uncorrected).

no.	E/a.u.	E/eV	f	Symmetry
1:	0.05743	1.56269	0.7835E-03	A.u
2:	0.05895	1.60411	0.9388E-03	A.u
3:	0.06014	1.63647	0.4574E-03	A.u
4:	0.06168	1.67831	0.3466E-02	A.u
5:	0.06265	1.70467	0.4555E-02	A.u
6:	0.06334	1.72357	0.1890E-02	A.u
7:	0.06400	1.74143	0.2872E-02	A.u
8:	0.06483	1.76404	0.5044E-02	A.u
9:	0.06515	1.77269	0.7042E-03	A.u
10:	0.06786	1.84647	0.7003E-01	A.u
11:	0.07432	2.02234	0.2935E-02	A.u
12:	0.07617	2.07265	0.3201E-02	A.u
13:	0.07772	2.11488	0.1091E-01	A.u
14:	0.08003	2.17776	0.1337E-02	A.u
15:	0.08083	2.19941	0.8289E-02	A.u
16:	0.08438	2.29623	0.8081E-02	A.u
17:	0.08625	2.34688	0.8472E-02	A.u
18:	0.09346	2.54321	0.1625	A.u
19:	0.09447	2.57056	0.1342	A.u
20:	0.09544	2.59705	0.1483E-01	A.u
21:	0.09837	2.67688	0.2506	A.u
22:	0.09978	2.71522	0.2781E-02	A.u
23:	0.09992	2.71897	0.3970E-02	A.u
24:	0.10672	2.90413	0.6856E-02	A.u
25:	0.10739	2.92216	0.4881E-02	A.u
26:	0.10818	2.94367	0.8112E-04	A.u
27:	0.10851	2.95281	0.1128E-01	A.u
28:	0.10930	2.97412	0.3574E-02	A.u
29:	0.10955	2.98103	0.2702E-02	A.u
30:	0.11069	3.01216	0.1086E-03	A.u

Table S7. TDDFT orbital contributions to electronic transitions

Excitation Nr.	Occupied to virtual orbitals	Contribution weight (sum=1)	contribibutions to transition dipole moment x	y	z
1: 112a.g	-> 112a.u	0.8693	-0.1287	0.5076	-0.7206
1: 110a.g	-> 112a.u	0.0592	0.1683	-0.1113	0.2091
1: 111a.g	-> 113a.u	0.0549	0.0079	-0.1504	0.0661
1: 112a.g	-> 113a.u	0.0058	0.2496	-0.0257	0.0359
1: 108a.g	-> 112a.u	0.0024	0.0088	-0.0040	0.0121
1: 106a.g	-> 112a.u	0.0024	-0.0951	-0.0125	-0.0030
1: 111a.g	-> 112a.u	0.0009	0.0908	0.0167	0.0220
1: 106a.g	-> 113a.u	0.0008	-0.0763	0.0034	-0.0089
1: 104a.g	-> 112a.u	0.0004	-0.0059	-0.0147	0.0227
1: 110a.g	-> 113a.u	0.0004	-0.0215	0.0175	0.0159
1: 103a.g	-> 112a.u	0.0003	-0.0229	-0.0021	0.0170
1: 112a.g	-> 116a.u	0.0003	-0.0032	-0.0113	0.0149
1: 102a.g	-> 113a.u	0.0003	-0.0128	0.0027	-0.0220
1: 111a.u	-> 114a.g	0.0002	-0.0014	0.0037	0.0235
1: 107a.u	-> 114a.g	0.0002	-0.0216	0.0018	0.0125
1: 110a.g	-> 114a.u	0.0002	-0.0085	-0.0053	0.0016
2: 111a.g	-> 112a.u	0.4940	-2.1016	-0.3873	-0.5083
2: 112a.g	-> 113a.u	0.4301	2.1305	-0.2193	0.3065
2: 111a.g	-> 113a.u	0.0341	-0.0061	0.1169	-0.0514
2: 110a.g	-> 113a.u	0.0235	-0.1613	0.1309	0.1189
2: 110a.g	-> 112a.u	0.0091	0.0652	-0.0431	0.0810
2: 109a.g	-> 112a.u	0.0024	0.0442	0.0079	0.0118

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2: 105a.g     -> 112a.u        0.0017  0.1070  0.0126  0.0221
2: 106a.g     -> 112a.u        0.0013  0.0705  0.0093  0.0022
2: 106a.g     -> 113a.u        0.0009 -0.0781  0.0035 -0.0091
2: 105a.g     -> 113a.u        0.0005 -0.0381  0.0053 -0.0112
2: 108a.g     -> 113a.u        0.0004 -0.0164  0.0031 -0.0025

3: 110a.g     -> 112a.u        0.4838  0.4703 -0.3111  0.5841
3: 111a.g     -> 113a.u        0.3752 -0.0201  0.3840 -0.1687
3: 112a.g     -> 113a.u        0.0725 -0.8658  0.0891 -0.1246
3: 110a.g     -> 113a.u        0.0593  0.2536 -0.2059 -0.1870
3: 111a.g     -> 112a.u        0.0026 -0.1512 -0.0279 -0.0366
3: 105a.g     -> 113a.u        0.0018  0.0699 -0.0098  0.0205
3: 108a.g     -> 113a.u        0.0010  0.0251 -0.0047  0.0038
3: 105a.g     -> 112a.u        0.0010  0.0803  0.0094  0.0166
3: 107a.g     -> 112a.u        0.0006 -0.0126  0.0095 -0.0169
3: 109a.g     -> 112a.u        0.0003 -0.0159 -0.0028 -0.0042

4: 111a.g     -> 113a.u        0.4561  0.0219 -0.4180  0.1837
4: 110a.g     -> 112a.u        0.3634  0.4025 -0.2662  0.4999
4: 112a.g     -> 112a.u        0.0927  0.0405 -0.1599  0.2271
4: 108a.g     -> 112a.u        0.0389 -0.0337  0.0154 -0.0466
4: 109a.g     -> 113a.u        0.0127  0.0125  0.0139 -0.0188
4: 111a.g     -> 112a.u        0.0070 -0.2443 -0.0450 -0.0591
4: 107a.g     -> 112a.u        0.0062 -0.0399  0.0301 -0.0535
4: 104a.g     -> 112a.u        0.0038  0.0166  0.0412 -0.0638
4: 105a.g     -> 113a.u        0.0026 -0.0812  0.0113 -0.0238
4: 108a.g     -> 113a.u        0.0017 -0.0331  0.0062 -0.0051
4: 111a.g     -> 114a.u        0.0014 -0.0009  0.0010 -0.0416
4: 111a.u     -> 114a.g        0.0014  0.0033 -0.0090 -0.0571
4: 111a.u     -> 113a.g        0.0014 -0.0078  0.0568 -0.0162
4: 110a.g     -> 113a.u        0.0014 -0.0382  0.0310  0.0281
4: 106a.g     -> 112a.u        0.0014  0.0695  0.0091  0.0022
4: 112a.g     -> 116a.u        0.0007  0.0049  0.0176 -0.0232
4: 111a.g     -> 115a.u        0.0007  0.0026  0.0285 -0.0112
4: 112a.g     -> 115a.u        0.0005 -0.0372 -0.0006 -0.0318
4: 105a.u     -> 114a.g        0.0005  0.0074  0.0229 -0.0326
4: 104a.g     -> 113a.u        0.0004 -0.0034  0.0241  0.0130

5: 109a.g     -> 112a.u        0.6047 -0.6850 -0.1224 -0.1825
5: 110a.g     -> 113a.u        0.1062 -0.3326  0.2700  0.2452
5: 111a.g     -> 112a.u        0.0956  0.8968  0.1653  0.2169
5: 108a.g     -> 112a.u        0.0710 -0.0452  0.0207 -0.0625
5: 112a.g     -> 113a.u        0.0703  0.8355 -0.0860  0.1202
5: 111a.g     -> 113a.u        0.0245 -0.0050  0.0962 -0.0423
5: 110a.g     -> 112a.u        0.0074  0.0568 -0.0376  0.0706
5: 108a.g     -> 113a.u        0.0057 -0.0598  0.0112 -0.0091
5: 106a.g     -> 112a.u        0.0027 -0.0975 -0.0128 -0.0031
5: 105a.g     -> 112a.u        0.0027 -0.1321 -0.0155 -0.0273
5: 106a.g     -> 113a.u        0.0019 -0.1113  0.0049 -0.0129
5: 109a.g     -> 113a.u        0.0018 -0.0047 -0.0052  0.0071
5: 107a.g     -> 113a.u        0.0010  0.0109 -0.0199 -0.0148
5: 105a.g     -> 113a.u        0.0007 -0.0428  0.0060 -0.0126
5: 104a.g     -> 113a.u        0.0007  0.0042 -0.0294 -0.0159
5: 111a.u     -> 113a.g        0.0004  0.0040 -0.0290  0.0083
5: 107a.g     -> 112a.u        0.0003 -0.0091  0.0068 -0.0122
5: 112a.g     -> 114a.u        0.0003  0.0057 -0.0159 -0.0009
5: 112a.g     -> 112a.u        0.0002  0.0019 -0.0076  0.0108

6: 108a.g     -> 112a.u        0.8068 -0.1515  0.0694 -0.2096
6: 109a.g     -> 112a.u        0.1491  0.3383  0.0604  0.0901
6: 111a.g     -> 113a.u        0.0147 -0.0039  0.0740 -0.0325
6: 112a.g     -> 112a.u        0.0074 -0.0113  0.0445 -0.0632
6: 109a.g     -> 113a.u        0.0057 -0.0083 -0.0092  0.0125
6: 111a.g     -> 112a.u        0.0050  0.2043  0.0376  0.0494
6: 110a.g     -> 112a.u        0.0047 -0.0454  0.0300 -0.0564
6: 112a.g     -> 113a.u        0.0020  0.1388 -0.0143  0.0200
6: 106a.g     -> 112a.u        0.0013 -0.0663 -0.0087 -0.0021
6: 110a.g     -> 113a.u        0.0007 -0.0259  0.0211  0.0191
6: 106a.g     -> 113a.u        0.0005 -0.0571  0.0025 -0.0066
6: 104a.g     -> 112a.u        0.0004 -0.0052 -0.0130  0.0200
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 7: 110a.g     -> 113a.u        0.6987 -0.8441  0.6852  0.6223
 7: 109a.g     -> 112a.u        0.1221  0.3046  0.0544  0.0811
 7: 108a.g     -> 112a.u        0.0313  0.0297 -0.0136  0.0411
 7: 108a.g     -> 113a.u        0.0309  0.1373 -0.0258  0.0210
 7: 111a.g     -> 112a.u        0.0237  0.4416  0.0814  0.1068
 7: 110a.g     -> 112a.u        0.0236  0.1006 -0.0665  0.1249
 7: 111a.g     -> 113a.u        0.0156 -0.0040  0.0759 -0.0333
 7: 112a.g     -> 113a.u        0.0106 -0.3210  0.0330 -0.0462
 7: 107a.g     -> 113a.u        0.0100  0.0347 -0.0635 -0.0472
 7: 109a.g     -> 113a.u        0.0085  0.0101  0.0112 -0.0151
 7: 104a.g     -> 113a.u        0.0044  0.0106 -0.0742 -0.0401
 7: 111a.u     -> 113a.g        0.0018  0.0088 -0.0635  0.0182
 7: 107a.g     -> 112a.u        0.0018 -0.0208  0.0157 -0.0279
 7: 105a.g     -> 112a.u        0.0016 -0.1006 -0.0118 -0.0208
 7: 112a.g     -> 114a.u        0.0016  0.0127 -0.0357 -0.0019
 7: 111a.u     -> 114a.g        0.0015  0.0034 -0.0091 -0.0582
 7: 105a.g     -> 113a.u        0.0012  0.0551 -0.0077  0.0162
 7: 106a.g     -> 113a.u        0.0011  0.0840 -0.0037  0.0097
 7: 110a.g     -> 116a.u        0.0010  0.0178 -0.0267 -0.0406
 7: 112a.g     -> 112a.u        0.0008  0.0037 -0.0144  0.0205

 8: 108a.g     -> 113a.u        0.6555  0.6283 -0.1179  0.0960
 8: 109a.g     -> 113a.u        0.1499  0.0419  0.0466 -0.0630
 8: 109a.g     -> 112a.u        0.0578 -0.2081 -0.0372 -0.0554
 8: 111a.g     -> 112a.u        0.0513 -0.6457 -0.1190 -0.1562
 8: 112a.g     -> 113a.u        0.0294 -0.5308  0.0546 -0.0764
 8: 108a.g     -> 112a.u        0.0246 -0.0262  0.0120 -0.0362
 8: 110a.g     -> 112a.u        0.0107 -0.0675  0.0447 -0.0838
 8: 105a.g     -> 112a.u        0.0058  0.1911  0.0224  0.0395
 8: 106a.g     -> 112a.u        0.0036  0.1101  0.0145  0.0035
 8: 112a.g     -> 112a.u        0.0026 -0.0066  0.0260 -0.0369
 8: 105a.g     -> 113a.u        0.0019  0.0677 -0.0094  0.0199
 8: 107a.g     -> 112a.u        0.0018  0.0208 -0.0157  0.0279
 8: 106a.g     -> 113a.u        0.0017  0.1039 -0.0046  0.0121
 8: 111a.g     -> 113a.u        0.0009  0.0009 -0.0179  0.0079
 8: 110a.g     -> 113a.u        0.0006  0.0245 -0.0199 -0.0181

 9: 109a.g     -> 113a.u        0.7988  0.0966  0.1073 -0.1450
 9: 108a.g     -> 113a.u        0.1794 -0.3279  0.0616 -0.0501
 9: 111a.g     -> 113a.u        0.0097 -0.0031  0.0593 -0.0260
 9: 110a.g     -> 112a.u        0.0027 -0.0338  0.0224 -0.0420
 9: 112a.g     -> 112a.u        0.0025 -0.0065  0.0257 -0.0366
 9: 108a.g     -> 112a.u        0.0013 -0.0061  0.0028 -0.0084
 9: 111a.g     -> 112a.u        0.0011  0.0923  0.0170  0.0223
 9: 109a.g     -> 112a.u        0.0007  0.0227  0.0041  0.0061
 9: 106a.g     -> 112a.u        0.0006 -0.0457 -0.0060 -0.0015
 9: 105a.g     -> 113a.u        0.0005  0.0356 -0.0050  0.0105
 9: 107a.g     -> 112a.u        0.0005  0.0109 -0.0083  0.0147
 9: 110a.g     -> 113a.u        0.0004  0.0209 -0.0169 -0.0154

10: 112a.g     -> 113a.u        0.2488 -1.5103  0.1555 -0.2173
10: 111a.g     -> 112a.u        0.1906 -1.2167 -0.2242 -0.2943
10: 108a.g     -> 113a.u        0.1177 -0.2603  0.0489 -0.0398
10: 105a.g     -> 112a.u        0.0721  0.6573  0.0772  0.1360
10: 106a.g     -> 113a.u        0.0674  0.6306 -0.0279  0.0732
10: 110a.g     -> 113a.u        0.0650 -0.2499  0.2029  0.1843
10: 106a.g     -> 112a.u        0.0596  0.4393  0.0578  0.0140
10: 109a.g     -> 112a.u        0.0518 -0.1926 -0.0344 -0.0513
10: 105a.g     -> 113a.u        0.0416  0.3127 -0.0436  0.0918
10: 109a.g     -> 113a.u        0.0203 -0.0151 -0.0168  0.0227
10: 108a.g     -> 112a.u        0.0203 -0.0232  0.0106 -0.0321
10: 110a.g     -> 112a.u        0.0119 -0.0695  0.0460 -0.0863
10: 107a.g     -> 112a.u        0.0115  0.0517 -0.0390  0.0693
10: 112a.g     -> 112a.u        0.0079 -0.0113  0.0445 -0.0632
10: 110a.g     -> 114a.u        0.0026 -0.0294 -0.0185  0.0055
10: 107a.g     -> 113a.u        0.0022  0.0158 -0.0289 -0.0214
10: 111a.g     -> 113a.u        0.0017  0.0013 -0.0246  0.0108
10: 104a.g     -> 114a.u        0.0010  0.0900  0.0030  0.0163
10: 112a.g     -> 116a.u        0.0005 -0.0038 -0.0136  0.0179
10: 103a.g     -> 113a.u        0.0005  0.0257  0.0232  0.0062
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11: 107a.g     -> 112a.u        0.9539 -0.4497  0.3394 -0.6027
11: 105a.g     -> 112a.u        0.0131  0.2674  0.0314  0.0553
11: 104a.g     -> 112a.u        0.0078 -0.0216 -0.0539  0.0834
11: 106a.g     -> 112a.u        0.0072  0.1462  0.0192  0.0047
11: 110a.g     -> 112a.u        0.0050 -0.0432  0.0285 -0.0536
11: 105a.g     -> 113a.u        0.0027  0.0763 -0.0106  0.0224
11: 112a.g     -> 112a.u        0.0017 -0.0050  0.0198 -0.0282
11: 106a.g     -> 113a.u        0.0010  0.0719 -0.0032  0.0083
11: 107a.g     -> 113a.u        0.0008 -0.0092  0.0169  0.0125
11: 111a.g     -> 114a.u        0.0008  0.0006 -0.0007  0.0289
11: 111a.u     -> 114a.g        0.0008 -0.0023  0.0061  0.0391
11: 111a.g     -> 112a.u        0.0007 -0.0680 -0.0125 -0.0164
11: 111a.g     -> 113a.u        0.0005 -0.0007  0.0128 -0.0056
11: 112a.g     -> 113a.u        0.0003 -0.0520  0.0054 -0.0075
11: 108a.g     -> 112a.u        0.0003 -0.0025  0.0012 -0.0035
11: 109a.g     -> 112a.u        0.0003 -0.0128 -0.0023 -0.0034
11: 112a.g     -> 116a.u        0.0002 -0.0026 -0.0092  0.0121
11: 111a.u     -> 113a.g        0.0002  0.0029 -0.0211  0.0060
11: 112a.g     -> 115a.u        0.0002  0.0215  0.0004  0.0183
11: 110a.g     -> 113a.u        0.0002  0.0125 -0.0101 -0.0092

12: 107a.g     -> 113a.u        0.9565  0.3101 -0.5677 -0.4217
12: 106a.g     -> 113a.u        0.0098 -0.2270  0.0100 -0.0263
12: 105a.g     -> 112a.u        0.0085  0.2125  0.0250  0.0440
12: 104a.g     -> 113a.u        0.0081 -0.0132  0.0922  0.0498
12: 110a.g     -> 113a.u        0.0070  0.0776 -0.0630 -0.0572
12: 106a.g     -> 112a.u        0.0022 -0.0798 -0.0105 -0.0025
12: 112a.g     -> 114a.u        0.0011 -0.0096  0.0271  0.0015
12: 111a.u     -> 113a.g        0.0009 -0.0056  0.0406 -0.0116
12: 105a.g     -> 113a.u        0.0008 -0.0401  0.0056 -0.0118
12: 107a.g     -> 112a.u        0.0005 -0.0106  0.0080 -0.0143
12: 111a.u     -> 114a.g        0.0004 -0.0016  0.0043  0.0276
12: 104a.g     -> 112a.u        0.0004 -0.0048 -0.0119  0.0184
12: 110a.g     -> 116a.u        0.0003 -0.0094  0.0141  0.0214
12: 111a.g     -> 113a.u        0.0003  0.0005 -0.0098  0.0043
12: 112a.g     -> 113a.u        0.0002  0.0419 -0.0043  0.0060
12: 111a.g     -> 112a.u        0.0002 -0.0357 -0.0066 -0.0086
12: 107a.u     -> 113a.g        0.0002 -0.0003  0.0119 -0.0018
12: 102a.g     -> 113a.u        0.0002  0.0082 -0.0017  0.0142
12: 106a.u     -> 113a.g        0.0002 -0.0017  0.0110  0.0049
12: 105a.u     -> 113a.g        0.0002 -0.0015  0.0175  0.0119

13: 106a.g     -> 112a.u        0.5089  1.1994  0.1577  0.0382
13: 105a.g     -> 112a.u        0.2938 -1.2400 -0.1456 -0.2566
13: 106a.g     -> 113a.u        0.1292 -0.8161  0.0361 -0.0947
13: 105a.g     -> 113a.u        0.0588  0.3472 -0.0485  0.1020
13: 107a.g     -> 113a.u        0.0028  0.0165 -0.0303 -0.0225
13: 104a.g     -> 112a.u        0.0011 -0.0079 -0.0198  0.0306
13: 112a.g     -> 112a.u        0.0009 -0.0036  0.0141 -0.0199
13: 102a.g     -> 112a.u        0.0007 -0.0308  0.0257 -0.0033
13: 103a.g     -> 112a.u        0.0006 -0.0263 -0.0024  0.0195
13: 104a.g     -> 114a.u        0.0005  0.0600  0.0020  0.0109
13: 102a.g     -> 113a.u        0.0004 -0.0138  0.0029 -0.0237
13: 112a.g     -> 113a.u        0.0002 -0.0429  0.0044 -0.0062
13: 110a.g     -> 113a.u        0.0002  0.0135 -0.0110 -0.0100

14: 106a.g     -> 113a.u        0.4928 -1.5705  0.0695 -0.1822
14: 105a.g     -> 112a.u        0.4136  1.4498  0.1703  0.3000
14: 106a.g     -> 112a.u        0.0357  0.3131  0.0412  0.0100
14: 105a.g     -> 113a.u        0.0136 -0.1645  0.0230 -0.0483
14: 107a.g     -> 113a.u        0.0114 -0.0330  0.0604  0.0449
14: 104a.g     -> 113a.u        0.0097  0.0141 -0.0986 -0.0533
14: 111a.g     -> 112a.u        0.0046  0.1734  0.0320  0.0419
14: 104a.g     -> 112a.u        0.0034  0.0138  0.0345 -0.0533
14: 107a.g     -> 112a.u        0.0034  0.0258 -0.0195  0.0345
14: 103a.g     -> 112a.u        0.0024 -0.0514 -0.0046  0.0380
14: 110a.g     -> 113a.u        0.0017 -0.0374  0.0303  0.0275
14: 102a.g     -> 113a.u        0.0011  0.0215 -0.0045  0.0370
14: 112a.g     -> 112a.u        0.0005  0.0027 -0.0107  0.0152
14: 103a.g     -> 113a.u        0.0005 -0.0248 -0.0223 -0.0060
14: 111a.u     -> 113a.g        0.0005  0.0040 -0.0292  0.0084
```

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14: 109a.g     -> 112a.u        0.0004  0.0164  0.0029  0.0044
14: 112a.g     -> 113a.u        0.0004 -0.0572  0.0059 -0.0082
14: 112a.g     -> 114a.u        0.0003  0.0052 -0.0147 -0.0008
14: 111a.u     -> 114a.g        0.0002  0.0012 -0.0033 -0.0209
14: 111a.g     -> 114a.u        0.0002  0.0003 -0.0004  0.0147

15: 105a.g     -> 113a.u        0.6647 -1.1448  0.1598 -0.3361
15: 106a.g     -> 112a.u        0.2002  0.7378  0.0970  0.0235
15: 106a.g     -> 113a.u        0.0884  0.6618 -0.0293  0.0768
15: 104a.g     -> 112a.u        0.0204 -0.0335 -0.0835  0.1293
15: 104a.g     -> 113a.u        0.0070  0.0119 -0.0834 -0.0451
15: 111a.g     -> 113a.u        0.0033 -0.0016  0.0311 -0.0137
15: 111a.g     -> 112a.u        0.0033  0.1459  0.0269  0.0353
15: 102a.g     -> 112a.u        0.0024 -0.0563  0.0470 -0.0060
15: 105a.g     -> 112a.u        0.0019  0.0991  0.0116  0.0205
15: 112a.g     -> 112a.u        0.0017 -0.0047  0.0187 -0.0265
15: 107a.g     -> 113a.u        0.0009  0.0095 -0.0173 -0.0129
15: 111a.u     -> 113a.g        0.0008  0.0054 -0.0387  0.0111
15: 107a.g     -> 112a.u        0.0006  0.0111 -0.0084  0.0149
15: 111a.g     -> 114a.u        0.0005  0.0005 -0.0005  0.0216
15: 103a.g     -> 113a.u        0.0005  0.0238  0.0215  0.0058
15: 109a.g     -> 113a.u        0.0004  0.0019  0.0021 -0.0029
15: 109a.g     -> 112a.u        0.0003  0.0135  0.0024  0.0036
15: 102a.g     -> 113a.u        0.0003  0.0107 -0.0022  0.0185
15: 110a.g     -> 112a.u        0.0002  0.0083 -0.0055  0.0103
15: 108a.u     -> 113a.g        0.0002  0.0137  0.0032  0.0156

16: 104a.g     -> 112a.u        0.9465 -0.2233 -0.5564  0.8610
16: 105a.g     -> 113a.u        0.0097  0.1353 -0.0189  0.0397
16: 107a.g     -> 112a.u        0.0057  0.0326 -0.0246  0.0436
16: 106a.g     -> 112a.u        0.0048 -0.1116 -0.0147 -0.0036
16: 111a.u     -> 114a.g        0.0042  0.0049 -0.0133 -0.0851
16: 106a.g     -> 113a.u        0.0042 -0.1411  0.0062 -0.0164
16: 111a.g     -> 114a.u        0.0036 -0.0013  0.0014 -0.0570
16: 110a.g     -> 112a.u        0.0023  0.0276 -0.0183  0.0343
16: 112a.g     -> 112a.u        0.0022  0.0053 -0.0210  0.0298
16: 105a.g     -> 112a.u        0.0021  0.0996  0.0117  0.0206
16: 112a.g     -> 114a.u        0.0014  0.0103 -0.0291 -0.0016
16: 111a.g     -> 113a.u        0.0011  0.0009 -0.0174  0.0076
16: 111a.u     -> 113a.g        0.0010 -0.0058  0.0420 -0.0120
16: 105a.u     -> 114a.g        0.0009  0.0087  0.0271 -0.0385
16: 104a.g     -> 113a.u        0.0007 -0.0038  0.0263  0.0142
16: 107a.g     -> 113a.u        0.0007 -0.0081  0.0149  0.0110
16: 110a.g     -> 113a.u        0.0006 -0.0223  0.0181  0.0164
16: 112a.g     -> 116a.u        0.0006  0.0038  0.0136 -0.0179
16: 107a.u     -> 114a.g        0.0005  0.0292 -0.0025 -0.0169
16: 110a.g     -> 116a.u        0.0004  0.0104 -0.0156 -0.0238

17: 104a.g     -> 113a.u        0.9523 -0.1343  0.9404  0.5080
17: 107a.g     -> 113a.u        0.0064 -0.0239  0.0437  0.0324
17: 105a.g     -> 113a.u        0.0062 -0.1067  0.0149 -0.0313
17: 111a.u     -> 113a.g        0.0058  0.0137 -0.0987  0.0282
17: 112a.g     -> 114a.u        0.0050  0.0195 -0.0548 -0.0030
17: 110a.g     -> 113a.u        0.0039 -0.0546  0.0443  0.0402
17: 106a.g     -> 112a.u        0.0030  0.0872  0.0115  0.0028
17: 105a.g     -> 112a.u        0.0028  0.1149  0.0135  0.0238
17: 111a.g     -> 112a.u        0.0010  0.0799  0.0147  0.0193
17: 111a.g     -> 114a.u        0.0010  0.0007 -0.0007  0.0299
17: 105a.u     -> 113a.g        0.0009  0.0035 -0.0408 -0.0277
17: 106a.g     -> 113a.u        0.0009 -0.0638  0.0028 -0.0074
17: 111a.u     -> 114a.g        0.0007  0.0020 -0.0054 -0.0342
17: 111a.g     -> 113a.u        0.0007 -0.0007  0.0136 -0.0060
17: 110a.g     -> 115a.u        0.0006 -0.0113 -0.0265  0.0030
17: 105a.g     -> 114a.u        0.0005  0.0024 -0.0374  0.0085
17: 110a.g     -> 116a.u        0.0005  0.0110 -0.0165 -0.0252
17: 104a.g     -> 112a.u        0.0005  0.0051  0.0126 -0.0195
17: 106a.u     -> 113a.g        0.0004  0.0026 -0.0174 -0.0077
17: 108a.u     -> 114a.g        0.0004 -0.0009 -0.0194  0.0026

18: 112a.g     -> 114a.u        0.5772  0.2009 -0.5653 -0.0307
18: 110a.g     -> 114a.u        0.1546  0.1933  0.1215 -0.0365
```

```
18: 106a.g     -> 113a.u        0.0470  0.4487 -0.0199  0.0521
18: 105a.g     -> 113a.u        0.0388  0.2573 -0.0359  0.0756
18: 105a.g     -> 112a.u        0.0347  0.3885  0.0456  0.0804
18: 106a.g     -> 112a.u        0.0331  0.2790  0.0367  0.0089
18: 112a.g     -> 113a.u        0.0171  0.3375 -0.0347  0.0485
18: 111a.g     -> 114a.u        0.0166  0.0026 -0.0029  0.1159
18: 111a.g     -> 112a.u        0.0132  0.2731  0.0503  0.0660
18: 103a.g     -> 112a.u        0.0123 -0.1073 -0.0096  0.0794
18: 102a.g     -> 113a.u        0.0081 -0.0535  0.0111 -0.0919
18: 102a.g     -> 112a.u        0.0072 -0.0905  0.0756 -0.0096
18: 111a.u     -> 113a.g        0.0054 -0.0127  0.0915 -0.0262
18: 110a.g     -> 113a.u        0.0040  0.0528 -0.0429 -0.0390
18: 103a.g     -> 113a.u        0.0037 -0.0603 -0.0543 -0.0146
18: 108a.u     -> 114a.g        0.0024  0.0021  0.0438 -0.0059
18: 111a.g     -> 116a.u        0.0022 -0.0683  0.0078  0.0087
18: 111a.u     -> 114a.g        0.0018 -0.0031  0.0083  0.0528
18: 107a.g     -> 112a.u        0.0013  0.0149 -0.0112  0.0200
18: 108a.g     -> 113a.u        0.0012  0.0228 -0.0043  0.0035

19: 112a.g     -> 114a.u        0.3743  0.1609 -0.4528 -0.0245
19: 110a.g     -> 114a.u        0.3285 -0.2802 -0.1761  0.0529
19: 111a.g     -> 114a.u        0.0573 -0.0047  0.0053 -0.2139
19: 105a.g     -> 113a.u        0.0388 -0.2558  0.0357 -0.0751
19: 105a.g     -> 112a.u        0.0368 -0.3983 -0.0468 -0.0824
19: 106a.g     -> 113a.u        0.0367 -0.3942  0.0175 -0.0457
19: 106a.g     -> 112a.u        0.0252 -0.2423 -0.0319 -0.0077
19: 111a.g     -> 112a.u        0.0167 -0.3056 -0.0563 -0.0739
19: 112a.g     -> 113a.u        0.0167 -0.3315  0.0341 -0.0477
19: 102a.g     -> 113a.u        0.0097  0.0584 -0.0121  0.1004
19: 103a.g     -> 112a.u        0.0086  0.0890  0.0080 -0.0659
19: 103a.g     -> 113a.u        0.0071  0.0835  0.0752  0.0202
19: 111a.u     -> 114a.g        0.0053 -0.0052  0.0141  0.0899
19: 102a.g     -> 112a.u        0.0045  0.0713 -0.0595  0.0076
19: 111a.u     -> 113a.g        0.0036 -0.0102  0.0736 -0.0210
19: 112a.g     -> 115a.u        0.0033  0.0766  0.0013  0.0655
19: 107a.u     -> 113a.g        0.0030 -0.0010  0.0437 -0.0065
19: 108a.g     -> 114a.u        0.0024 -0.0038  0.0024  0.0120
19: 107a.g     -> 112a.u        0.0022 -0.0193  0.0146 -0.0259
19: 110a.g     -> 112a.u        0.0019 -0.0234  0.0155 -0.0290

20: 111a.g     -> 114a.u        0.8776  0.0184 -0.0207  0.8331
20: 110a.g     -> 114a.u        0.0553 -0.1144 -0.0719  0.0216
20: 111a.u     -> 113a.g        0.0126 -0.0190  0.1376 -0.0393
20: 111a.u     -> 114a.g        0.0085  0.0066 -0.0178 -0.1136
20: 109a.g     -> 114a.u        0.0054  0.0027  0.0174 -0.0081
20: 105a.g     -> 112a.u        0.0043 -0.1347 -0.0158 -0.0279
20: 106a.g     -> 112a.u        0.0040 -0.0959 -0.0126 -0.0031
20: 106a.g     -> 113a.u        0.0031 -0.1148  0.0051 -0.0133
20: 108a.g     -> 114a.u        0.0025  0.0039 -0.0025 -0.0124
20: 112a.g     -> 113a.u        0.0021 -0.1173  0.0121 -0.0169
20: 103a.g     -> 112a.u        0.0020  0.0433  0.0039 -0.0320
20: 112a.g     -> 114a.u        0.0020  0.0116 -0.0326 -0.0018
20: 111a.g     -> 112a.u        0.0019 -0.1012 -0.0186 -0.0245
20: 108a.u     -> 113a.g        0.0017 -0.0384 -0.0090 -0.0436
20: 105a.g     -> 113a.u        0.0015 -0.0505  0.0071 -0.0148
20: 104a.g     -> 112a.u        0.0014 -0.0081 -0.0201  0.0311
20: 107a.u     -> 114a.g        0.0014  0.0459 -0.0039 -0.0265
20: 111a.g     -> 115a.u        0.0012  0.0029  0.0309 -0.0121
20: 105a.g     -> 114a.u        0.0011 -0.0033  0.0506 -0.0115
20: 103a.g     -> 113a.u        0.0010  0.0304  0.0274  0.0074

21: 110a.g     -> 114a.u        0.4325 -0.3151 -0.1980  0.0595
21: 106a.g     -> 113a.u        0.0769  0.5596 -0.0248  0.0649
21: 105a.g     -> 113a.u        0.0712  0.3397 -0.0474  0.0997
21: 105a.g     -> 112a.u        0.0665  0.5242  0.0616  0.1085
21: 106a.g     -> 112a.u        0.0595  0.3646  0.0479  0.0116
21: 112a.g     -> 113a.u        0.0510  0.5681 -0.0585  0.0817
21: 111a.g     -> 112a.u        0.0464  0.4986  0.0919  0.1206
21: 103a.g     -> 112a.u        0.0248 -0.1483 -0.0133  0.1097
21: 102a.g     -> 112a.u        0.0234 -0.1595  0.1332 -0.0170
21: 102a.g     -> 113a.u        0.0207 -0.0835  0.0173 -0.1434
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21: 103a.g     -> 113a.u        0.0190 -0.1336 -0.1203 -0.0324
21: 112a.g     -> 114a.u        0.0095 -0.0252  0.0708  0.0038
21: 107a.g     -> 114a.u        0.0076  0.0512  0.0175  0.0257
21: 111a.u     -> 115a.g        0.0066  0.0687  0.0062  0.0201
21: 110a.g     -> 113a.u        0.0064  0.0651 -0.0528 -0.0480
21: 109a.g     -> 114a.u        0.0054  0.0026  0.0171 -0.0080
21: 108a.g     -> 114a.u        0.0043  0.0051 -0.0032 -0.0160
21: 111a.g     -> 114a.u        0.0039 -0.0012  0.0014 -0.0548
21: 112a.g     -> 115a.u        0.0039 -0.0817 -0.0013 -0.0698
21: 109a.g     -> 112a.u        0.0039  0.0436  0.0078  0.0116

22: 109a.g     -> 114a.u        0.9387  0.0344  0.2239 -0.1050
22: 108a.g     -> 114a.u        0.0379 -0.0148  0.0094  0.0469
22: 111a.u     -> 113a.g        0.0071  0.0140 -0.1013  0.0290
22: 110a.g     -> 114a.u        0.0031  0.0265  0.0167 -0.0050
22: 111a.g     -> 114a.u        0.0016 -0.0008  0.0009 -0.0345
22: 111a.u     -> 114a.g        0.0013 -0.0025  0.0068  0.0433
22: 110a.u     -> 114a.g        0.0009 -0.0232 -0.0057 -0.0032
22: 109a.u     -> 115a.g        0.0006  0.0064  0.0108 -0.0134
22: 109a.u     -> 114a.g        0.0006  0.0071 -0.0008 -0.0054
22: 112a.g     -> 114a.u        0.0006 -0.0063  0.0177  0.0010
22: 110a.u     -> 115a.g        0.0006  0.0016 -0.0142 -0.0110
22: 110a.u     -> 113a.g        0.0006 -0.0054 -0.0003 -0.0049
22: 108a.u     -> 115a.g        0.0005 -0.0053 -0.0013  0.0263
22: 109a.u     -> 113a.g        0.0004  0.0162  0.0001  0.0044
22: 112a.g     -> 116a.u        0.0003 -0.0027 -0.0095  0.0125
22: 105a.g     -> 114a.u        0.0003  0.0018 -0.0275  0.0063
22: 106a.u     -> 114a.g        0.0003  0.0013  0.0053 -0.0128
22: 105a.g     -> 113a.u        0.0002 -0.0177  0.0025 -0.0052
22: 111a.g     -> 115a.u        0.0002 -0.0010 -0.0108  0.0043
22: 108a.u     -> 114a.g        0.0001 -0.0005 -0.0105  0.0014

23: 108a.g     -> 114a.u        0.9394 -0.0738  0.0470  0.2333
23: 109a.g     -> 114a.u        0.0345 -0.0066 -0.0429  0.0201
23: 111a.u     -> 114a.g        0.0050  0.0049 -0.0133 -0.0848
23: 111a.g     -> 114a.u        0.0032  0.0011 -0.0012  0.0491
23: 110a.g     -> 114a.u        0.0024 -0.0233 -0.0146  0.0044
23: 112a.g     -> 114a.u        0.0014 -0.0097  0.0273  0.0015
23: 110a.u     -> 114a.g        0.0013  0.0276  0.0067  0.0038
23: 110a.u     -> 113a.g        0.0012 -0.0077 -0.0005 -0.0069
23: 109a.u     -> 113a.g        0.0010 -0.0255 -0.0002 -0.0069
23: 109a.u     -> 115a.g        0.0008  0.0072  0.0122 -0.0151
23: 107a.u     -> 114a.g        0.0005  0.0283 -0.0024 -0.0163
23: 105a.g     -> 113a.u        0.0005  0.0295 -0.0041  0.0087
23: 107a.u     -> 115a.g        0.0005  0.0027 -0.0307 -0.0024
23: 111a.g     -> 112a.u        0.0005  0.0502  0.0092  0.0121
23: 109a.u     -> 114a.g        0.0005  0.0061 -0.0007 -0.0047
23: 106a.u     -> 113a.g        0.0004 -0.0025  0.0163  0.0072
23: 106a.g     -> 113a.u        0.0004  0.0420 -0.0019  0.0049
23: 105a.g     -> 112a.u        0.0004  0.0419  0.0049  0.0087
23: 110a.u     -> 115a.g        0.0004 -0.0013  0.0119  0.0092
23: 112a.g     -> 115a.u        0.0004 -0.0253 -0.0004 -0.0216

24: 111a.u     -> 113a.g        0.8095  0.1445 -1.0450  0.2988
24: 111a.u     -> 114a.g        0.0392  0.0134 -0.0361 -0.2305
24: 110a.u     -> 113a.g        0.0244  0.0335  0.0020  0.0302
24: 108a.u     -> 114a.g        0.0176  0.0054  0.1112 -0.0151
24: 107a.u     -> 113a.g        0.0149 -0.0022  0.0922 -0.0137
24: 109a.u     -> 113a.g        0.0141  0.0908  0.0006  0.0247
24: 109a.u     -> 114a.g        0.0108 -0.0287  0.0033  0.0218
24: 110a.g     -> 115a.u        0.0101  0.0418  0.0977 -0.0110
24: 111a.g     -> 115a.u        0.0073  0.0067  0.0721 -0.0283
24: 112a.g     -> 114a.u        0.0063  0.0196 -0.0550 -0.0030
24: 106a.u     -> 113a.g        0.0050 -0.0081  0.0532  0.0236
24: 108a.u     -> 113a.g        0.0035 -0.0522 -0.0123 -0.0592
24: 111a.g     -> 114a.u        0.0034  0.0011 -0.0012  0.0493
24: 105a.u     -> 113a.g        0.0030 -0.0055  0.0653  0.0445
24: 104a.g     -> 113a.u        0.0026  0.0063 -0.0442 -0.0239
24: 109a.g     -> 114a.u        0.0023 -0.0017 -0.0108  0.0051
24: 112a.g     -> 116a.u        0.0023  0.0066  0.0234 -0.0309
24: 105a.g     -> 114a.u        0.0019 -0.0041  0.0634 -0.0144
```

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24: 110a.g     -> 116a.u        0.0018 -0.0188  0.0282  0.0429
24: 108a.u     -> 115a.g        0.0016  0.0095  0.0023 -0.0472

25: 111a.u     -> 114a.g        0.7887 -0.0597  0.1615  1.0302
25: 109a.u     -> 113a.g        0.0427 -0.1576 -0.0011 -0.0429
25: 111a.u     -> 113a.g        0.0375  0.0310 -0.2243  0.0641
25: 108a.u     -> 113a.g        0.0265 -0.1429 -0.0336 -0.1621
25: 107a.u     -> 114a.g        0.0154  0.1450 -0.0124 -0.0837
25: 110a.u     -> 113a.g        0.0154  0.0266  0.0016  0.0240
25: 110a.g     -> 116a.u        0.0093  0.0428 -0.0642 -0.0977
25: 110a.u     -> 114a.g        0.0091  0.0716  0.0175  0.0099
25: 111a.g     -> 114a.u        0.0073  0.0016 -0.0018  0.0718
25: 109a.u     -> 114a.g        0.0068  0.0226 -0.0026 -0.0172
25: 112a.g     -> 116a.u        0.0046  0.0093  0.0330 -0.0434
25: 112a.g     -> 115a.u        0.0044 -0.0833 -0.0014 -0.0711
25: 106a.u     -> 114a.g        0.0035  0.0043  0.0178 -0.0433
25: 105a.u     -> 114a.g        0.0025  0.0133  0.0412 -0.0586
25: 105a.g     -> 114a.u        0.0020 -0.0042  0.0644 -0.0147
25: 104a.g     -> 112a.u        0.0017 -0.0084 -0.0210  0.0325
25: 108a.u     -> 114a.g        0.0017 -0.0017 -0.0346  0.0047
25: 109a.g     -> 114a.u        0.0016 -0.0014 -0.0090  0.0042
25: 102a.g     -> 112a.u        0.0016 -0.0394  0.0329 -0.0042
25: 107a.u     -> 115a.g        0.0013  0.0042 -0.0476 -0.0037

26: 110a.u     -> 113a.g        0.7586 -0.1858 -0.0112 -0.1674
26: 109a.u     -> 113a.g        0.1758  0.3187  0.0022  0.0868
26: 111a.u     -> 114a.g        0.0235 -0.0103  0.0278  0.1773
26: 111a.u     -> 113a.g        0.0117  0.0172 -0.1246  0.0356
26: 108a.u     -> 113a.g        0.0103 -0.0887 -0.0208 -0.1007
26: 110a.u     -> 114a.g        0.0096  0.0735  0.0180  0.0102
26: 109a.g     -> 114a.u        0.0013 -0.0013 -0.0081  0.0038
26: 111a.g     -> 115a.u        0.0010  0.0025  0.0268 -0.0105
26: 103a.g     -> 113a.u        0.0006  0.0235  0.0212  0.0057
26: 111a.g     -> 114a.u        0.0006  0.0004 -0.0005  0.0202
26: 111a.u     -> 115a.g        0.0006 -0.0194 -0.0017 -0.0057
26: 109a.u     -> 114a.g        0.0005 -0.0059  0.0007  0.0045
26: 110a.g     -> 114a.u        0.0004  0.0090  0.0056 -0.0017
26: 103a.g     -> 112a.u        0.0004  0.0175  0.0016 -0.0129
26: 102a.g     -> 112a.u        0.0004 -0.0193  0.0161 -0.0021
26: 110a.g     -> 116a.u        0.0004  0.0083 -0.0124 -0.0189
26: 112a.g     -> 116a.u        0.0003  0.0024  0.0085 -0.0111
26: 108a.g     -> 114a.u        0.0003  0.0012 -0.0008 -0.0039
26: 109a.u     -> 115a.g        0.0003 -0.0040 -0.0067  0.0083
26: 105a.u     -> 114a.g        0.0002  0.0037  0.0116 -0.0165

27: 109a.u     -> 113a.g        0.6860 -0.6287 -0.0044 -0.1711
27: 110a.u     -> 113a.g        0.1759 -0.0893 -0.0054 -0.0805
27: 107a.g     -> 114a.u        0.0671  0.1446  0.0494  0.0727
27: 111a.u     -> 113a.g        0.0161  0.0202 -0.1462  0.0418
27: 110a.u     -> 114a.g        0.0161 -0.0949 -0.0232 -0.0132
27: 111a.u     -> 114a.g        0.0136  0.0078 -0.0211 -0.1347
27: 108a.u     -> 113a.g        0.0054  0.0642  0.0151  0.0728
27: 109a.u     -> 114a.g        0.0027 -0.0142  0.0016  0.0108
27: 107a.u     -> 113a.g        0.0022 -0.0008  0.0350 -0.0052
27: 108a.u     -> 114a.g        0.0017  0.0017  0.0347 -0.0047
27: 108a.g     -> 114a.u        0.0016  0.0029 -0.0019 -0.0092
27: 110a.g     -> 115a.u        0.0012  0.0145  0.0338 -0.0038
27: 111a.g     -> 115a.u        0.0011  0.0026  0.0277 -0.0109
27: 103a.g     -> 113a.u        0.0008  0.0261  0.0235  0.0063
27: 112a.g     -> 115a.u        0.0006  0.0309  0.0005  0.0264
27: 110a.g     -> 116a.u        0.0005 -0.0101  0.0152  0.0231
27: 104a.g     -> 114a.u        0.0005  0.0521  0.0017  0.0094
27: 105a.u     -> 113a.g        0.0005 -0.0022  0.0256  0.0174
27: 107a.u     -> 114a.g        0.0004  0.0236 -0.0020 -0.0137
27: 111a.g     -> 112a.u        0.0004 -0.0414 -0.0076 -0.0100

28: 110a.u     -> 114a.g        0.8608  0.6917  0.1690  0.0960
28: 109a.u     -> 114a.g        0.0622 -0.0679  0.0078  0.0517
28: 107a.g     -> 114a.u        0.0291 -0.0948 -0.0324 -0.0476
28: 109a.u     -> 113a.g        0.0278 -0.1260 -0.0009 -0.0343
28: 111a.u     -> 114a.g        0.0085  0.0062 -0.0167 -0.1063
```

```
28: 107a.u     -> 114a.g        0.0028 -0.0614  0.0052  0.0355
28: 109a.g     -> 114a.u        0.0019  0.0015  0.0097 -0.0046
28: 103a.g     -> 112a.u        0.0007 -0.0240 -0.0021  0.0177
28: 108a.g     -> 114a.u        0.0006  0.0019 -0.0012 -0.0059
28: 110a.u     -> 115a.g        0.0004  0.0013 -0.0117 -0.0090
28: 112a.g     -> 116a.u        0.0004 -0.0027 -0.0095  0.0125
28: 102a.g     -> 113a.u        0.0003  0.0100 -0.0021  0.0171
28: 110a.g     -> 116a.u        0.0003 -0.0078  0.0117  0.0178
28: 112a.g     -> 115a.u        0.0003  0.0220  0.0004  0.0188
28: 111a.u     -> 115a.g        0.0003 -0.0138 -0.0012 -0.0040
28: 111a.g     -> 116a.u        0.0002 -0.0202  0.0023  0.0026
28: 107a.u     -> 115a.g        0.0002 -0.0017  0.0193  0.0015
28: 105a.u     -> 114a.g        0.0002 -0.0036 -0.0112  0.0159
28: 108a.u     -> 113a.g        0.0002  0.0115  0.0027  0.0131
28: 106a.u     -> 113a.g        0.0001  0.0013 -0.0088 -0.0039

29: 109a.u     -> 114a.g        0.8434  0.2497 -0.0286 -0.1901
29: 107a.g     -> 114a.u        0.0699 -0.1468 -0.0502 -0.0738
29: 110a.u     -> 114a.g        0.0282  0.1251  0.0306  0.0174
29: 108a.u     -> 113a.g        0.0103  0.0882  0.0207  0.1001
29: 111a.u     -> 114a.g        0.0102  0.0067 -0.0182 -0.1162
29: 109a.u     -> 113a.g        0.0073 -0.0645 -0.0005 -0.0176
29: 111a.u     -> 113a.g        0.0062  0.0124 -0.0900  0.0257
29: 110a.u     -> 113a.g        0.0044 -0.0141 -0.0008 -0.0127
29: 107a.u     -> 113a.g        0.0037 -0.0011  0.0457 -0.0068
29: 108a.u     -> 114a.g        0.0027  0.0021  0.0427 -0.0058
29: 110a.g     -> 116a.u        0.0021 -0.0201  0.0302  0.0459
29: 106a.g     -> 114a.u        0.0017 -0.0143  0.0126  0.0548
29: 108a.g     -> 114a.u        0.0014  0.0027 -0.0017 -0.0085
29: 102a.g     -> 112a.u        0.0013 -0.0361  0.0301 -0.0038
29: 110a.g     -> 115a.u        0.0007  0.0106  0.0248 -0.0028
29: 106a.u     -> 114a.g        0.0005 -0.0016 -0.0066  0.0160
29: 110a.g     -> 114a.u        0.0004 -0.0093 -0.0058  0.0018
29: 106a.g     -> 113a.u        0.0004  0.0364 -0.0016  0.0042
29: 103a.g     -> 112a.u        0.0003 -0.0164 -0.0015  0.0121
29: 111a.u     -> 115a.g        0.0003  0.0145  0.0013  0.0042

30: 107a.g     -> 114a.u        0.7699  0.4848  0.1657  0.2436
30: 110a.u     -> 114a.g        0.0603  0.1819  0.0444  0.0252
30: 109a.u     -> 114a.g        0.0600  0.0663 -0.0076 -0.0504
30: 108a.u     -> 113a.g        0.0310 -0.1520 -0.0357 -0.1725
30: 109a.u     -> 113a.g        0.0229  0.1138  0.0008  0.0310
30: 110a.u     -> 113a.g        0.0138  0.0248  0.0015  0.0223
30: 107a.u     -> 113a.g        0.0103 -0.0018  0.0753 -0.0112
30: 107a.u     -> 114a.g        0.0096 -0.1128  0.0096  0.0651
30: 108a.u     -> 114a.g        0.0028 -0.0021 -0.0439  0.0060
30: 106a.u     -> 115a.g        0.0026 -0.0704 -0.0023 -0.0086
30: 106a.g     -> 114a.u        0.0014  0.0126 -0.0111 -0.0482
30: 105a.g     -> 114a.u        0.0013  0.0033 -0.0513  0.0117
30: 102a.g     -> 112a.u        0.0013  0.0350 -0.0292  0.0037
30: 108a.g     -> 115a.u        0.0012 -0.0177  0.0193  0.0009
30: 109a.g     -> 116a.u        0.0011 -0.0128 -0.0216 -0.0086
30: 103a.g     -> 113a.u        0.0008  0.0256  0.0230  0.0062
30: 104a.g     -> 114a.u        0.0007  0.0608  0.0020  0.0110
30: 111a.u     -> 114a.g        0.0006  0.0016 -0.0043 -0.0276
30: 103a.g     -> 112a.u        0.0004 -0.0178 -0.0016  0.0131
30: 112a.g     -> 113a.u        0.0004 -0.0467  0.0048 -0.0067
```

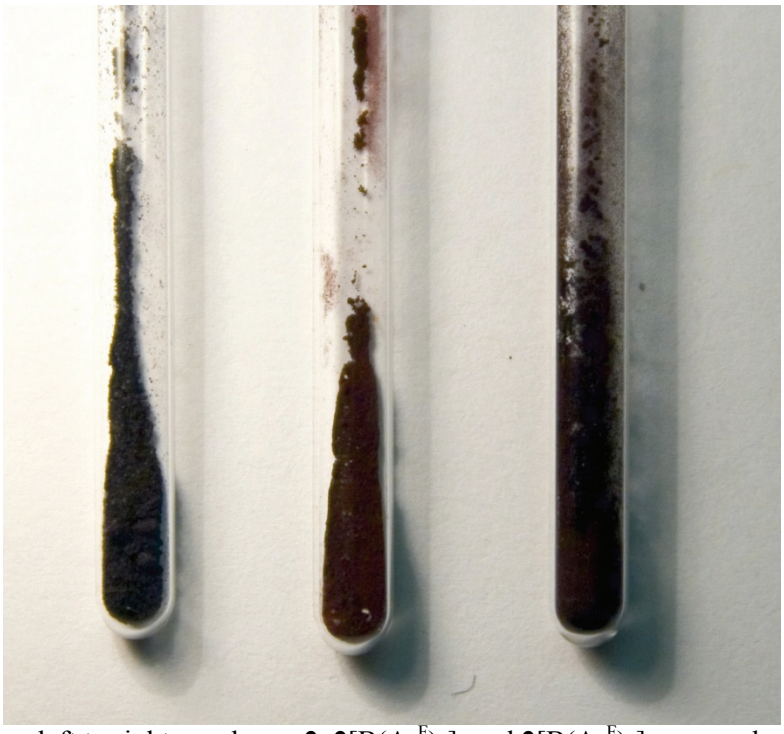

Figure S21. From left to right are shown **2**, **2**[$B(Ar^F)_4$], and **2**[$B(Ar^F)_4]_2$ as powders.

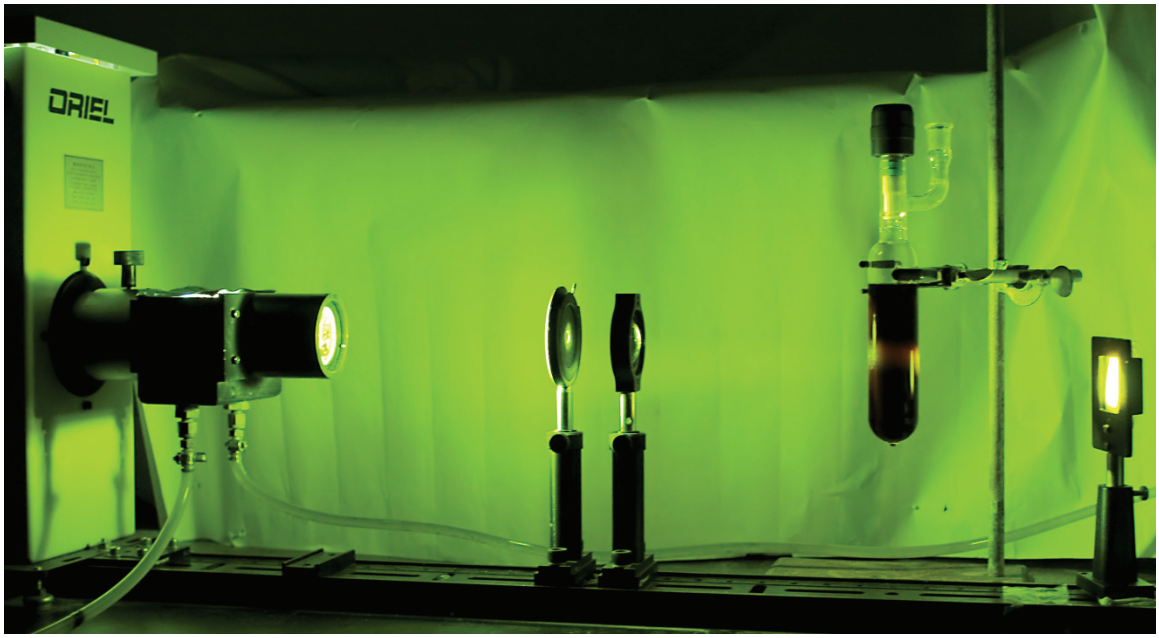

Figure S22. Table of Contents Graphic: This photograph shows the photochemical bleach of **2** when irradiated by an Oriel 1000 W Hg-Xe arc lamp equipped with a $\lambda \geq 480$ nm filter. The area above and below the bleach are still purple because these areas were not directly in the beam of light. The backstop is illuminated upon completion of the photochemical bleach when light at this wavelength is no longer absorbed by the solution.

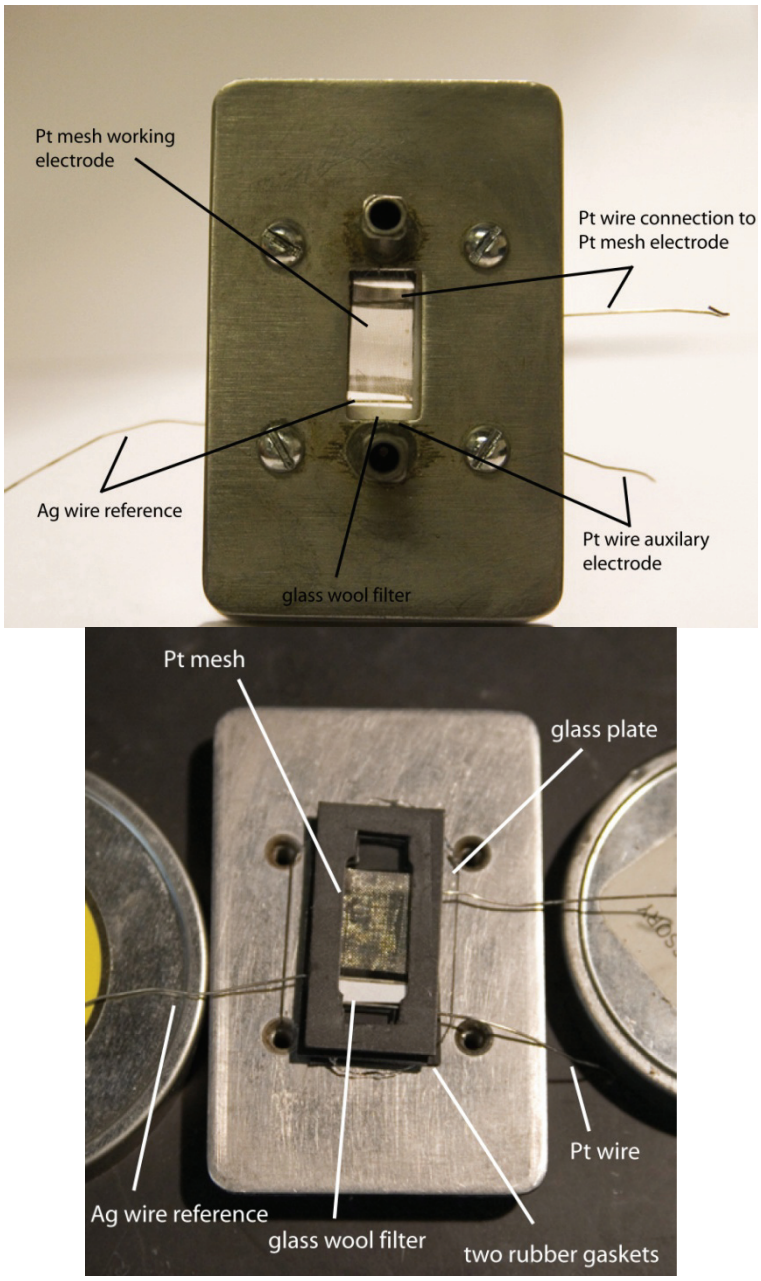

Figure S23. An optically transparent thin-layer electrode (OTTLE) constructed from a solution IR spectroscopy cell is suitable for the study of air-sensitive compounds. This electrochemical cell is adapted from literature designs.[32,33]

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