

Supporting Information for the Paper Entitled:

Reductive Disproportionation of Nitric Oxide Mediated by Low-Valent Uranium

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Supporting Information Table of Contents

General Considerations	2
Synthetic and Spectroscopic Details.....	2
GC/MS Measurements:	7
SQUID Magnetization Data:	15
EPR spectroscopy	16
UV/Vis/NIR	18
X-Ray Crystal Structure Determinations.....	20
DFT	25
References.....	74

General Considerations

All air- and moisture-sensitive experiments were performed under a dry dinitrogen atmosphere, using standard Schlenk techniques or in an MBraun inert-gas glovebox containing an atmosphere of purified dinitrogen. The glovebox is equipped with a -35°C freezer. Solvents were purified using a two-column, solid-state purification system (Glass Contour System, Irvine, CA), transferred to the glovebox without exposure to air, and stored over molecular sieves and sodium (where appropriate). NMR solvents were obtained packaged under argon and stored over activated molecular sieves and sodium (where appropriate) prior to use or were vacuum transferred from purple ketyl solutions over sodium. Nitrous oxide (99.998 %), was purchased from Sigma-Aldrich and used without further purification. Nitric oxide (99.9 %) was purchased from Praxair and cleaned from trace amounts of higher nitrogen oxides by passing it through a concentrated KOH solution, an Ascarite II column (NaOH on silica gel, Sigma-Aldrich), and a phosphorus pentoxide column.^{1, 2} The precursor complex $\text{UI}_3(\text{dioxane})_{1.5}$ was prepared as described by Kiplinger and coworkers.³ ^1H NMR spectra were recorded on a JEOL ECX 400 MHz instrument operating at frequencies of 400.178 and 100.624 MHz for ^1H and ^{13}C NMR spectra, respectively, and a probe temperature of 23°C ; if not stated otherwise. Chemical shifts, δ , are reported relative to residual ^1H resonances of the solvent in ppm.⁴ Electronic absorption spectra were recorded from 250 to 2200 nm (Shimadzu, UV-3600) in the indicated solvent at room temperature. IR vibrational spectra were recorded from 3500 to 400 cm^{-1} (Shimadzu, IRAffinity-1) as KBr pellets at room temperature. Magnetization data of micro-crystalline and powdered samples (15–30 mg) were recorded with a SQUID magnetometer (Quantum Design) as a function of temperature (2–300 K). Values of the magnetic susceptibility were corrected for the underlying diamagnetic increment ($\chi_{\text{dia}} = -864.97 \times 10^{-6}\text{ cm}^3\text{mol}^{-1}$ (**1**), $-849.57 \times 10^{-6}\text{ cm}^3\text{mol}^{-1}$ (**2**)), by using tabulated Pascal constants, and the effect of the blank sample holders (gelatin capsule/straw).⁵ Data reproducibility was carefully checked on three independently synthesized and measured samples. EPR spectra were recorded on a JEOL CW spectrometer JESFA200 equipped with an X-band Gunn diode oscillator bridge, a cylindrical mode cavity, and a helium cryostat. The spectra were simulated with the program W95EPR.⁶ Elemental analyses were obtained using Euro EA 3000 (Euro Vector) and EA 1108 (Carlo-Erba) elemental analyzers in the Chair of Inorganic and General Chemistry at FAU. GC/MS measurements were carried out using a Bruker Scion 456-G-TQ equipped with a ShinCarbon ST column (Restek, 80/100, $2\text{ m} \times 0.53\text{ mm}$) utilizing He as carrier gas.

Synthetic and Spectroscopic Details

Synthesis of $\text{Ad,Ad,MeArOK} \cdot 1.5\text{ DME}$. To a suspension of Ad,Ad,MeArOH (3.00 g, 7.97 mmol, 1.0 eq.) in 25 mL DME a solution of potassium bis(trimethylsilyl)amide (1.75 g, 8.77 mmol, 1.1 eq.) in 5 mL DME was added dropwise. The color of the suspension turns immediately to yellow upon addition. After stirring overnight, the volatiles were removed *in vacuo* and the remaining white solid was washed two times with 5 mL DME and three times with 5 mL *n*-pentane each to obtain a white powder. The amount of coordinated DME depends on the drying conditions. If dried for 3 days at 70°C under high vacuum, one molecule remains. If dried for 5 h under 1 mbar, 1.5 molecules remain. Yield: 3.66 g, 7.45 mmol, 94%. **^1H NMR** (400 MHz, $\text{THF-}d_8$): $\delta = 1.69\text{--}1.79$ (m, 12 H, H3 or H5), $1.93\text{--}1.99$ (m, 6 H, H4), 2.05 (s, 3 H, H1), 2.28 (m, 12 H, H3 or H5), 6.43 (s, 2 H, H2) ppm. **^{13}C NMR** (100 MHz, $\text{THF-}d_8$): $\delta = 21.80$ (1 C, C1), 30.87 (6 C, C7), 37.74 (2 C, C5), 38.86 and 41.52 (12 C, C6 and C8), 124.03 (2 C, C3), 135.91 (2 C, C4) ppm. The carbon atoms C2 and C9 could not be detected even after increased number of scans and scan delays. **IR** (KBr pellet): $\nu [\text{cm}^{-1}]$: 2903 (vs), 2847 (s),

1441 (s), 1364 (w), 1342 (w), 1304 (w), 1277 (w), 1240 (m), 1188 (w), 1159 (w), 1110 (m), 1076 (m), 1028 (w), 980 (w), 852 (w), 820 (w), 794 (w), 758 (w). Elemental analysis calculated for $\text{Ad}_{\text{Ad,Me}}\text{ArOK} \cdot 1.5 \text{ DME C}_{33}\text{H}_{51}\text{KO}_4$: C, 71.95, H, 9.33. Found: C, 71.92, H, 9.10.

Synthesis of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (1). To a suspension of $\text{Ad}_{\text{Ad,Me}}\text{ArOK}$ (0.20 g, 4.1 mmol, 3.1 eq.) in 40 mL benzene solid $\text{UI}_3(\text{dioxane})_{1.5}$ (0.10 g, 0.13 mmol, 1.0 eq.) was slowly added as well as a few drops of THF to increase the solubility. The solution turned red-brown after 3 h and precipitation of KI was observed. After stirring for 5 h, the reaction mixture was filtered over celite and the solvent was removed *in vacuo*. The red powder was washed with *n*-pentane and Et_2O until the filtrate is colorless. Yield: 0.15 g, 0.65 mmol, 84%. **^1H NMR** (400 MHz, benzene- d_6): $\delta = -11.58$ (d, $|^2J_{\text{H,H}}| = 7.8$ Hz, 18 H, H5), -8.60 (s, 18 H, H4), -6.01 (d, $|^2J_{\text{H,H}}| = 7.8$ Hz, 18 H, H5), -3.60 (s, 18 H, H3), 7.56 (s, 9 H, H1), 9.25 (s, 18 H, H3), 16.41 (s, 6 H, H2) ppm. **^{13}C NMR** (100 MHz, benzene- d_6): $\delta = -37.52$ (18 C, C6), 15.15 (18 C, C8), 20.69 (18 C, C7), 26.35 (3 C, C1), 52.87 (6 C, C5), 138.13 (6 C, C3), 142.20 (CAr), 189.27 (CAr), 208.23 (CAr) ppm. **IR** (KBr pellet): ν [cm^{-1}]: 2904 (vs), 2849 (s), 1479 (w), 1448 (s), 1418 (m), 1362 (w), 1342 (m), 1311 (m), 1232 (m), 1212 (m), 1184 (m), 1161 (m), 1101 (m), 1082 (w), 1040 (w), 978 (w), 903 (w), 856 (w), 815 (m), 536 (w). Elemental analysis calculated for $\text{C}_{81}\text{H}_{105}\text{O}_3\text{U}$: C, 71.29, H, 7.75. Found: C, 71.71, H, 7.80.

Synthesis of $[(\text{Ad}_{\text{Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$ (2). **a.)** A red solution of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (22 mg, 0.016 mmol) in 5 mL benzene was reacted with 1 atm. of N_2O . The solution turned black instantly. After 10 minutes of stirring, the volatiles were removed *in vacuo*. The brown-black solid was triturated three times with 3 mL *n*-pentane and subsequently washed with *n*-pentane and dried *in vacuo* to obtain a grey-brown powder. Yield: 17 mg, 0.012 mmol, 75%. **b.)** A red solution of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (130 mg, 0.095 mmol) in 5 mL benzene was treated with 1 atm. of NO. The solution turned black instantly. After 10 minutes of stirring, the volatiles were removed *in vacuo*. The brown-black solid was triturated thrice with 3 mL *n*-pentane and subsequently washed with *n*-pentane until the filtrate is colorless and dried *in vacuo* to obtain a brown powder. Yield: 94 mg, 0.069 mmol, 73%. **c.)** Finely ground $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ was treated with 1 atm. of NO. The solid turns brown-black instantly to give the product in quantitative yield. **^1H NMR** (400 MHz, benzene- d_6): $\delta = -2.83$ (br s, 9 H, AdCH), 0.85 (br s, 9 H, AdCH), 1.34 (br s, 9 H, AdCH), 1.79 (br s, 9 H, AdCH), 2.59 (br s, 27 H, AdCH), 3.06 (br s, 9 H, AdCH), 3.80 (s, 9 H, CH₃), 4.34 (br s, 9 H, AdCH), 4.47 (br s, 9 H, AdCH), 6.91 (br s, 3 H, ArCH), 8.23 (br s, 3 H, ArCH) ppm. **IR** (KBr pellet): ν [cm^{-1}]: 2905 (vs), 2849 (s), 1445 (m), 1416 (m), 1346 (w), 1314 (w), 1263 (w), 1211 (m), 1184 (m), 1163 (m), 1101 (m), 1026 (w), 978 (w), 941 (w), 901 (w), 833 (m), 810 (m), 758 (w), 540 (m). Elemental analysis calculated for $\text{C}_{81}\text{H}_{105}\text{O}_4\text{U}$: C, 70.46, H, 7.67. Found: C, 70.01, H, 7.93.

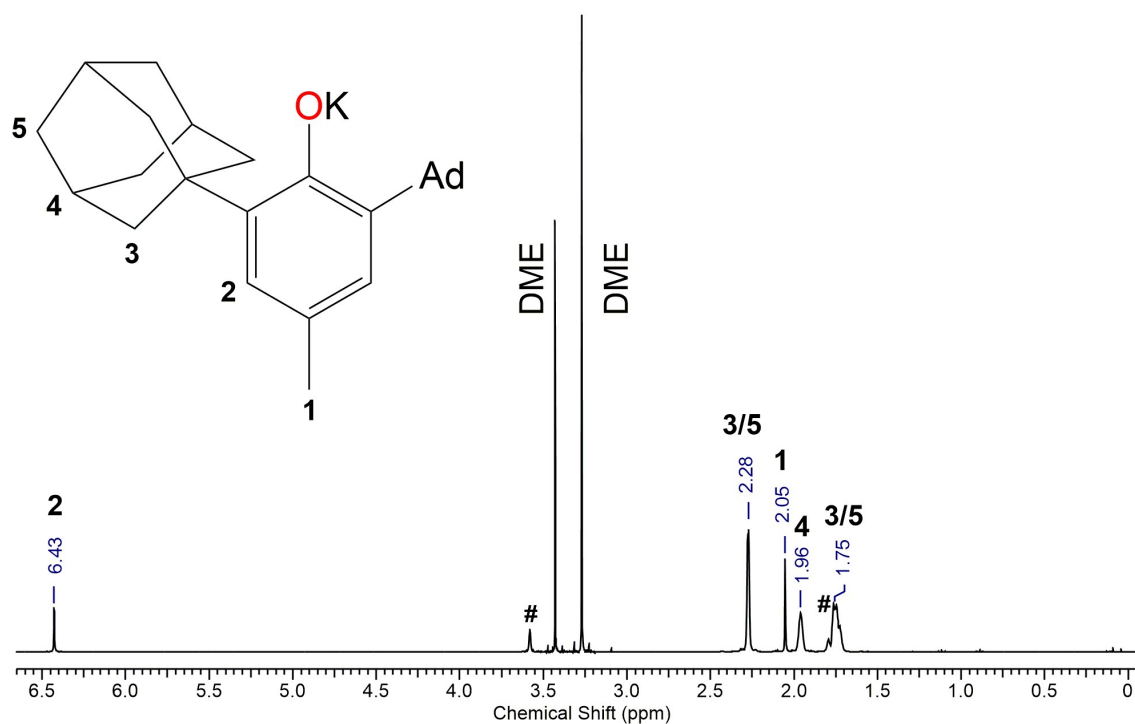


Figure S1: ^1H NMR spectrum of Ad,Ad,MeArOK in THF- d_8 (#). Signals from DME are labelled.

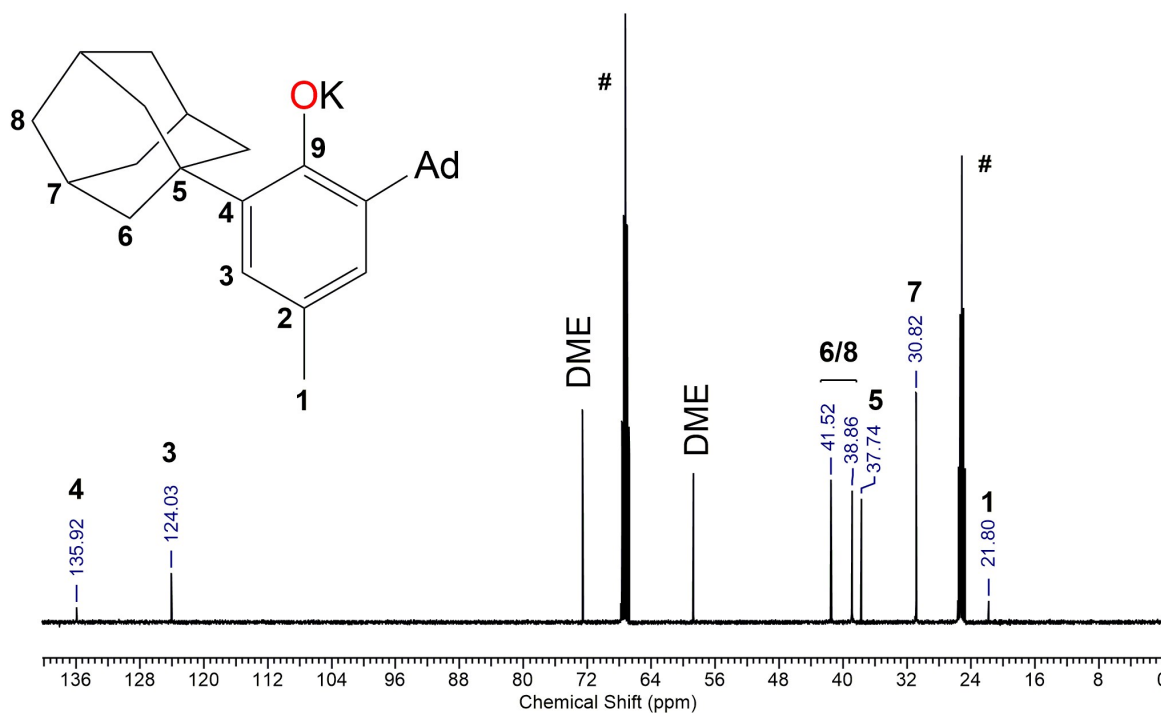


Figure S2: ^{13}C NMR spectrum of Ad,Ad,MeArOK in THF- d_8 (#). Signals from DME are labelled.

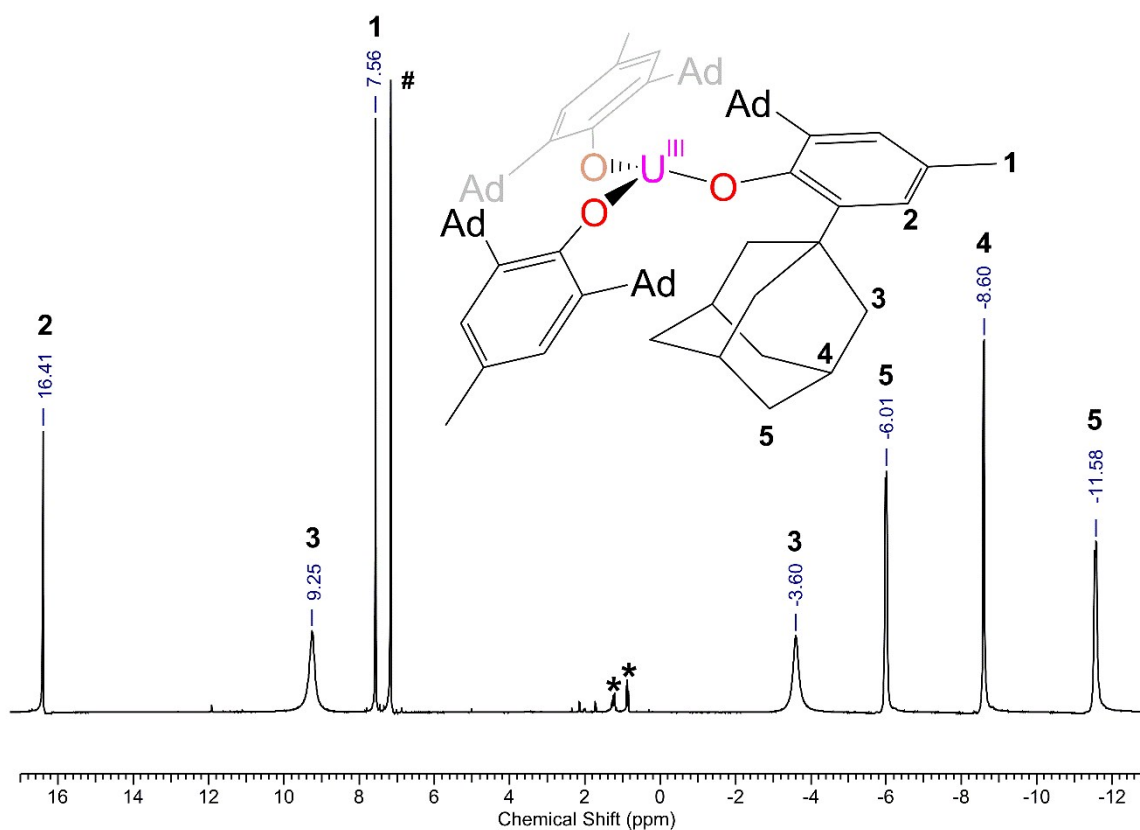


Figure S3: ¹H NMR spectrum of [U^{III}(OAr^{Ad,Ad,Me})₃] (1) in benzene-*d*₆ (#). Residual pentane is marked with an asterisk (*).

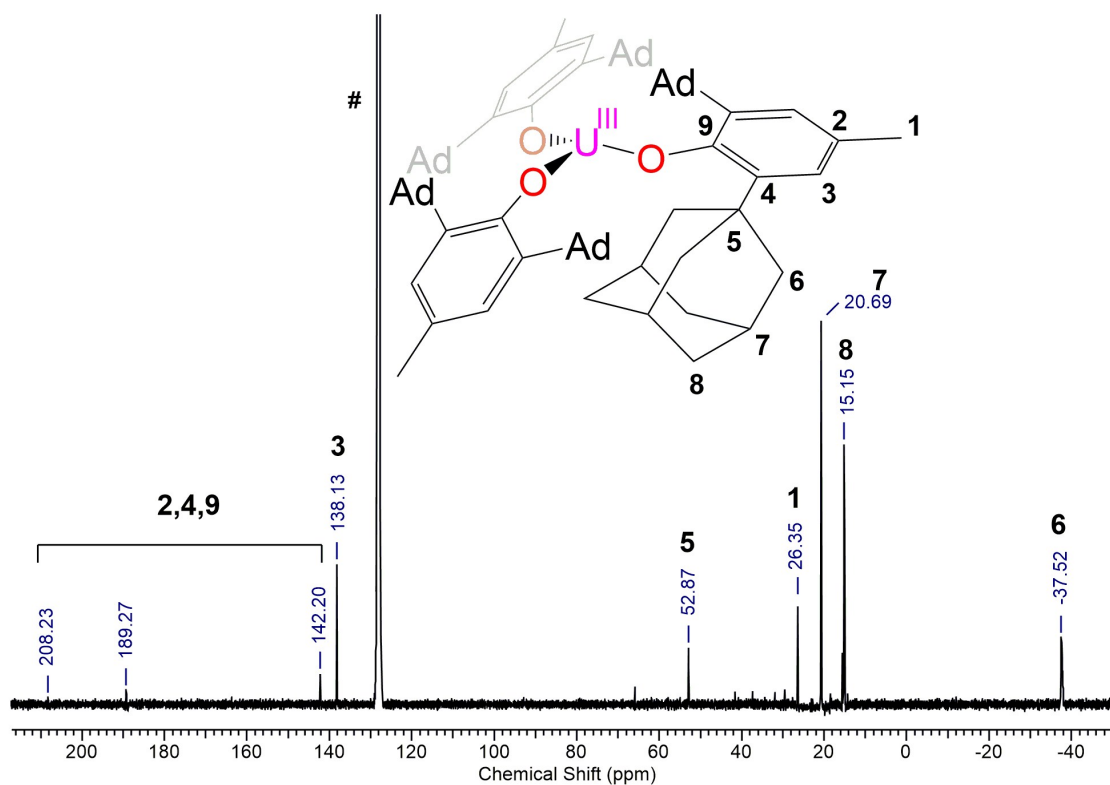


Figure S4: ¹³C NMR spectrum of [U^{III}(OAr^{Ad,Ad,Me})₃] (1) in benzene-*d*₆ (#).

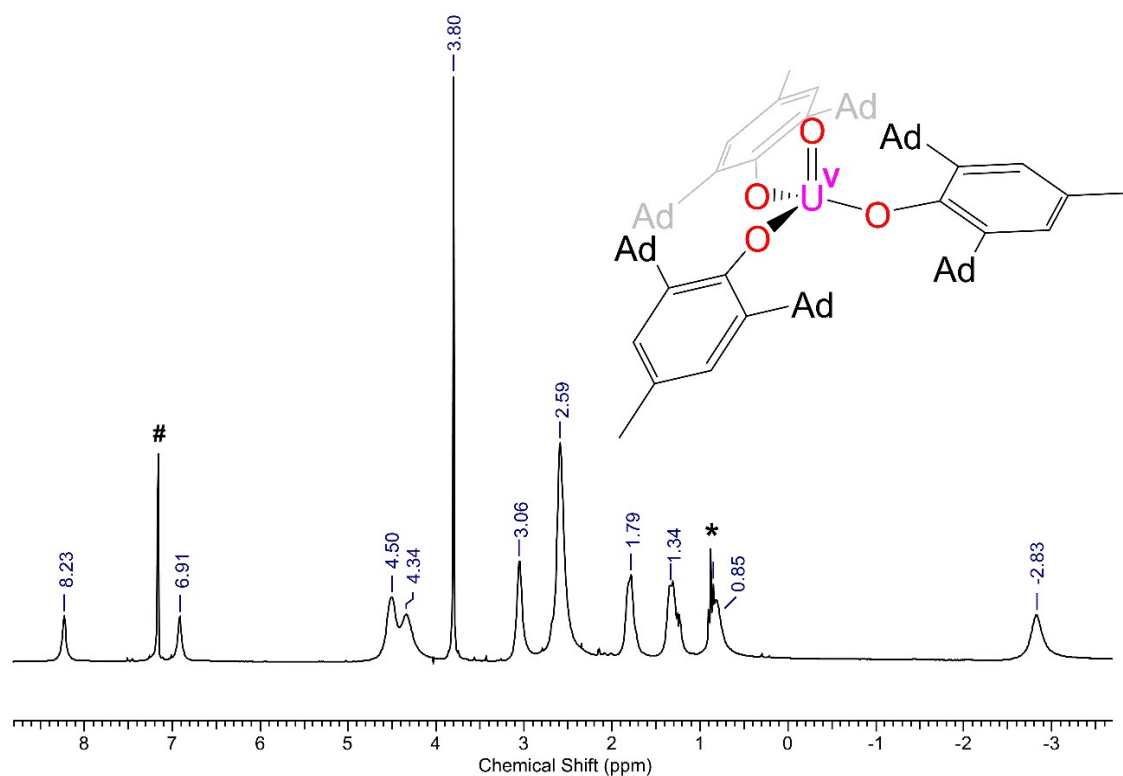


Figure S5: ^1H NMR spectrum of $[(\text{Ad,Ad,MeArO})_3\text{U}^{\text{V}}(\text{O})]$ (**2**) in benzene- d_6 (#). Residual pentane is marked with an asterisk (*).

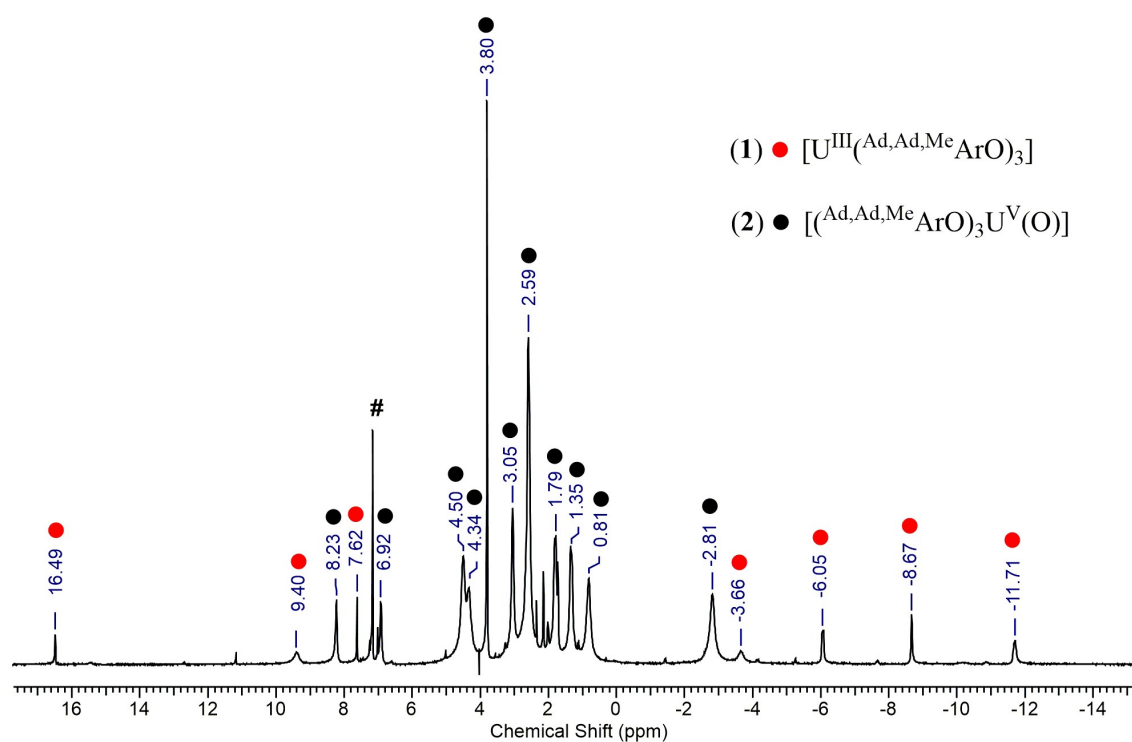


Figure S6: ^1H NMR spectrum in benzene- d_6 (#) of the reaction mixture of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (**1**) and $[(\text{Ad,Ad,MeArO})_3\text{U}^{\text{V}}(\text{O})]$ (**2**) obtained when solid **1** is reacted with N_2O (approximately 90% conversion).

GC/MS Measurements:

Gas Chromatography: Reaction of **1** with NO:

The gaseous products from the reaction of solid **1** with an excess of NO were examined. The samples were prepared in the glovebox in a 20 mL vial, sealed with a rubber septum, and subsequently flushed with argon for 10 minutes. NO was then added all at once directly *via* a syringe. Control experiments with pure NO and argon confirm that the N₂O was produced during the reaction. The formation of N₂ is not observed.

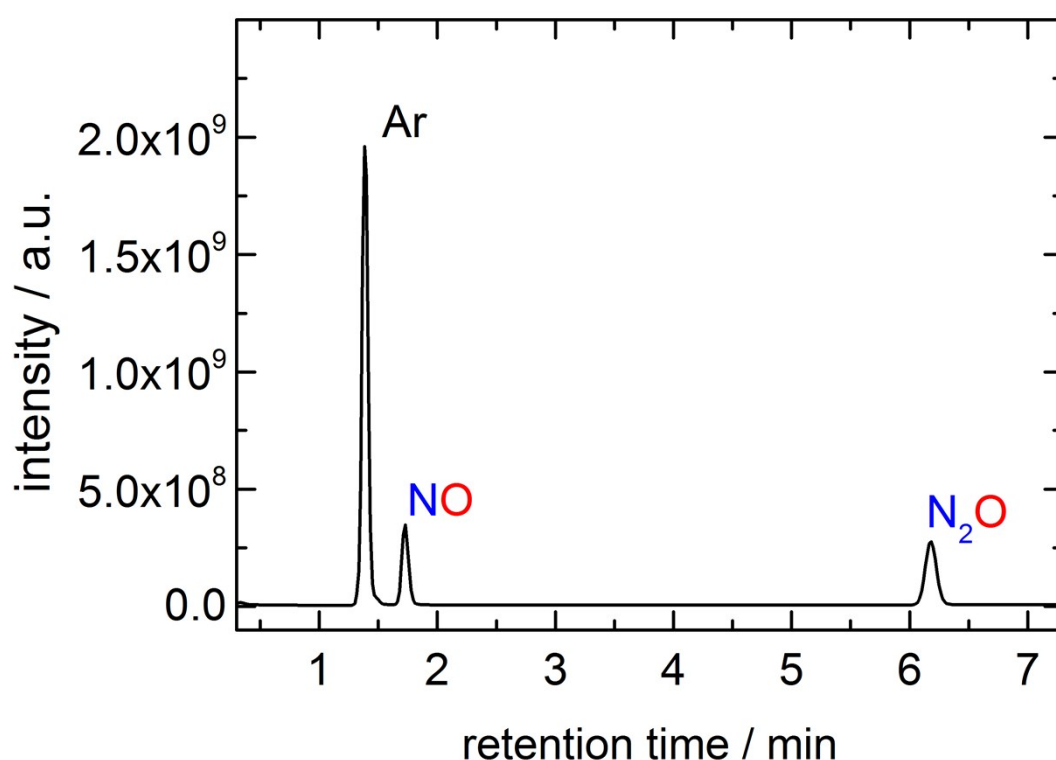


Figure S7: Chromatogram of the head space (injection volume 50 μ L) from the reaction of **1** in the solid state with excess NO to form **2** with liberation of N₂O (retention time = 6.18 min) at 50 °C on a 100 mg scale.

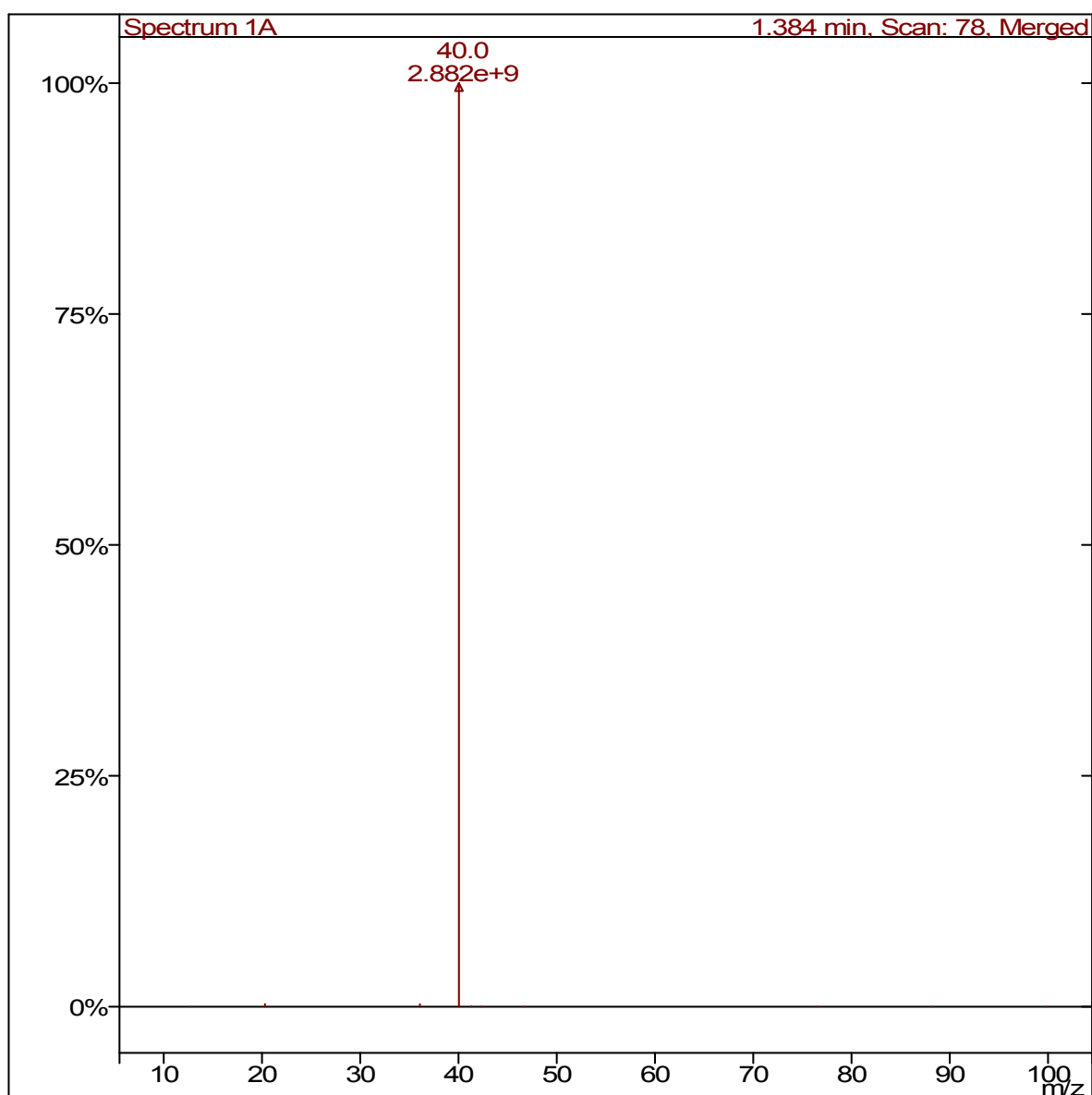


Figure S8: Mass spectrum of the signal corresponding to argon at a retention time of 1.38 min.

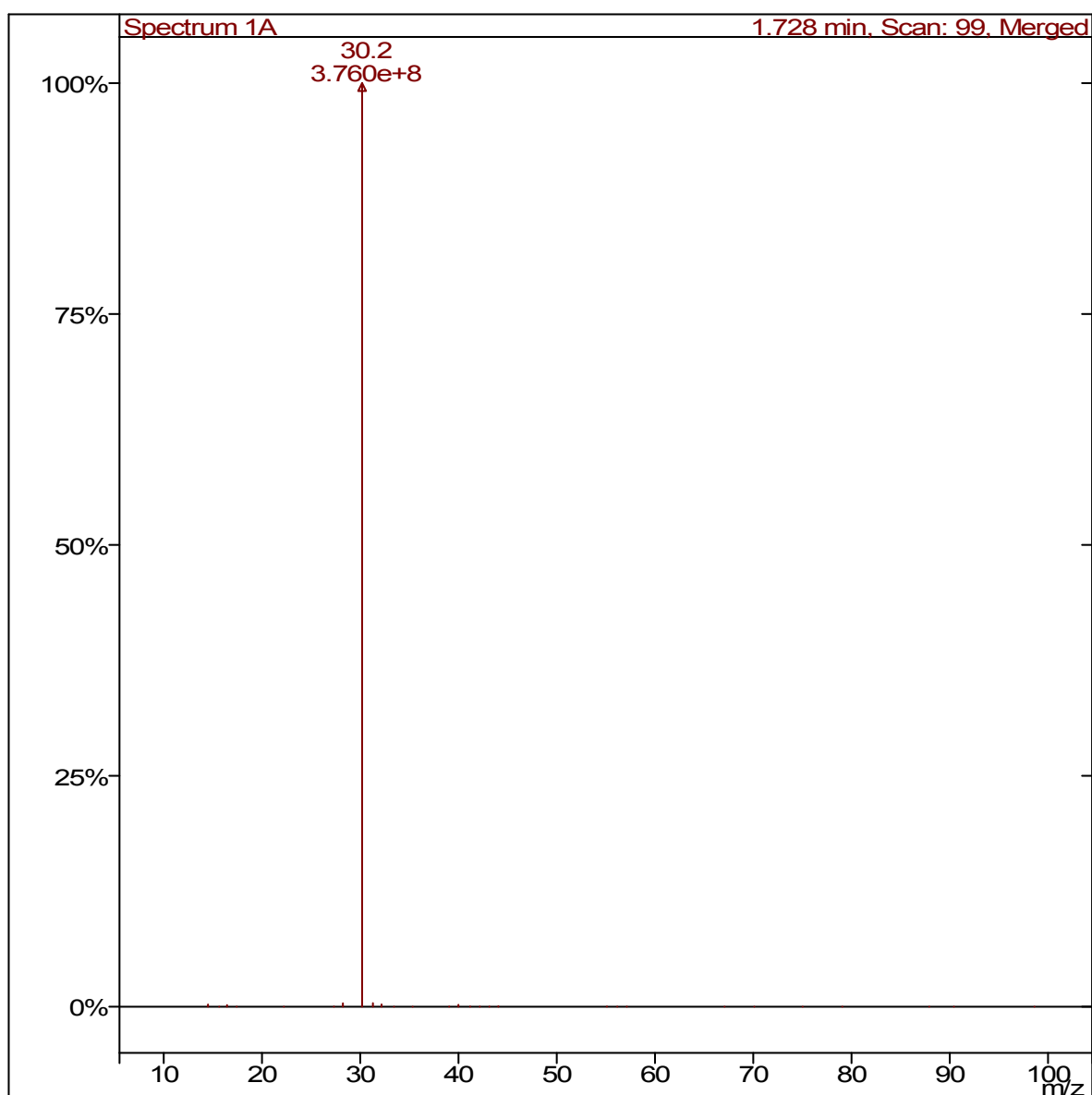


Figure S9: Mass spectrum of the signal corresponding to nitric oxide at a retention time of 1.73 min.

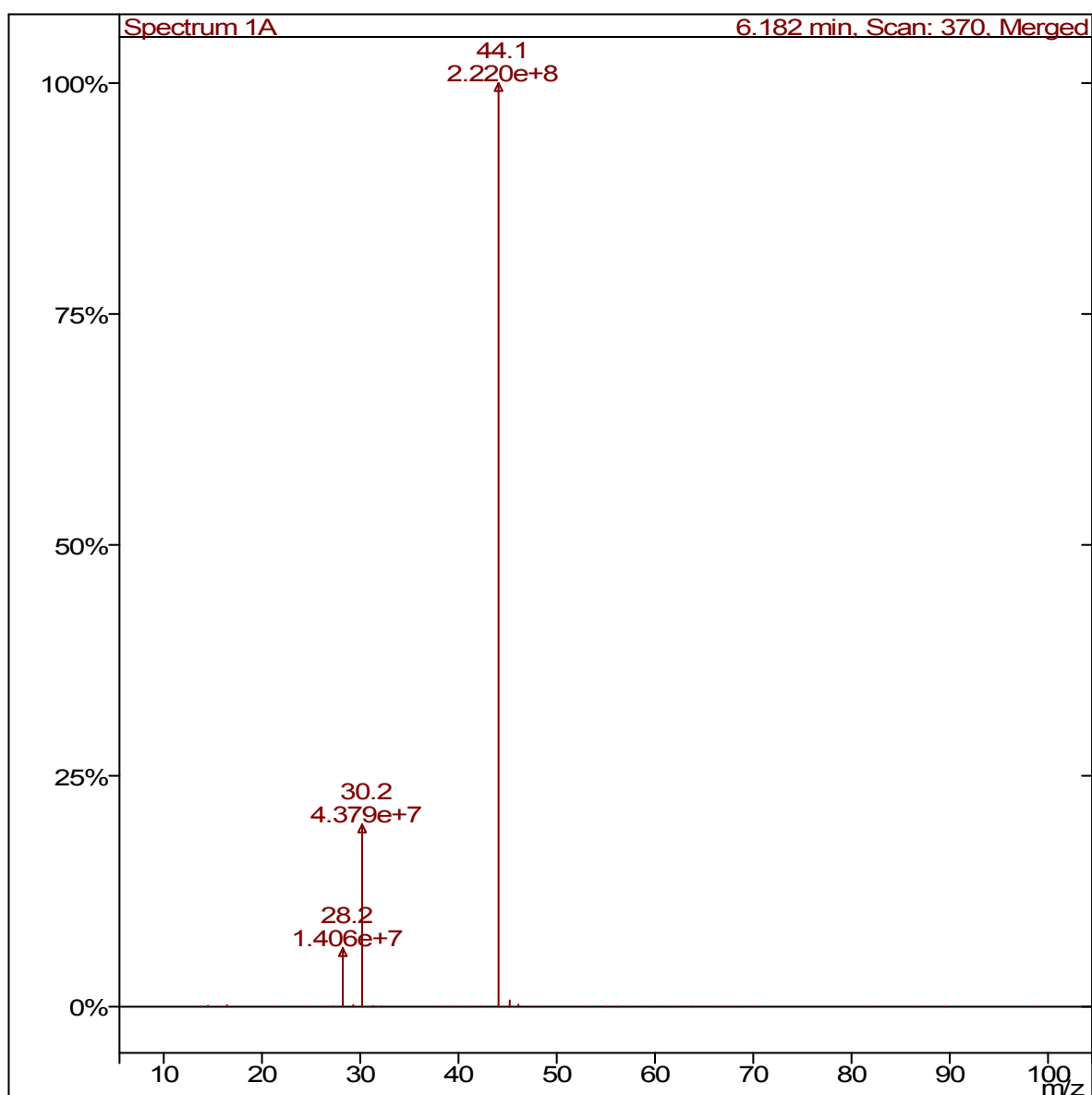


Figure S10: Mass spectrum of the signals corresponding to nitrous oxide at a retention time of 6.18 min.

Gas Chromatography: Reaction of **1** with N₂O:

The gaseous products from the reaction of solid **1** with an excess of N₂O were examined. The samples were prepared in the glovebox in a 20 mL vial, sealed with a rubber septum, and subsequently flushed with argon for 10 minutes. N₂O was then added all at once directly *via* a syringe. Control experiments with pure N₂O and argon confirm that N₂ was produced during the reaction.

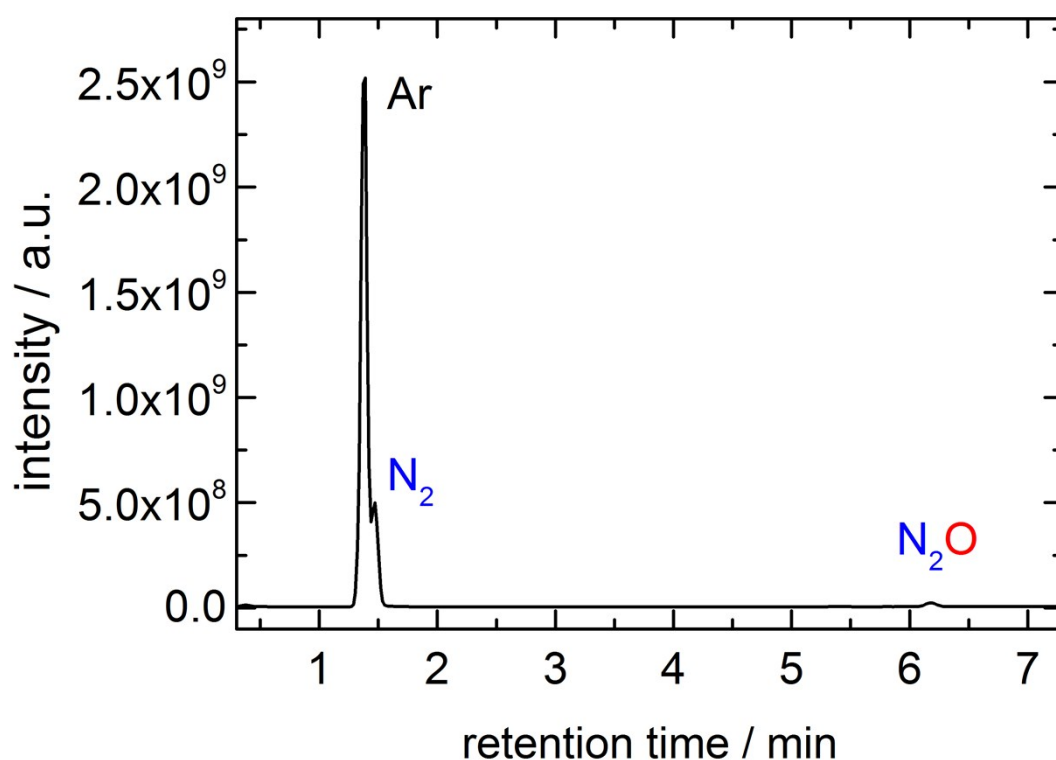


Figure S11: Chromatogram of the head space (injection volume 50 μ L) from the reaction of **1** in the solid state with excess N₂O to form **2** with liberation of N₂ (retention time = 1.47 min) at 50 °C on a 100 mg scale and an injection volume of 50 μ L.

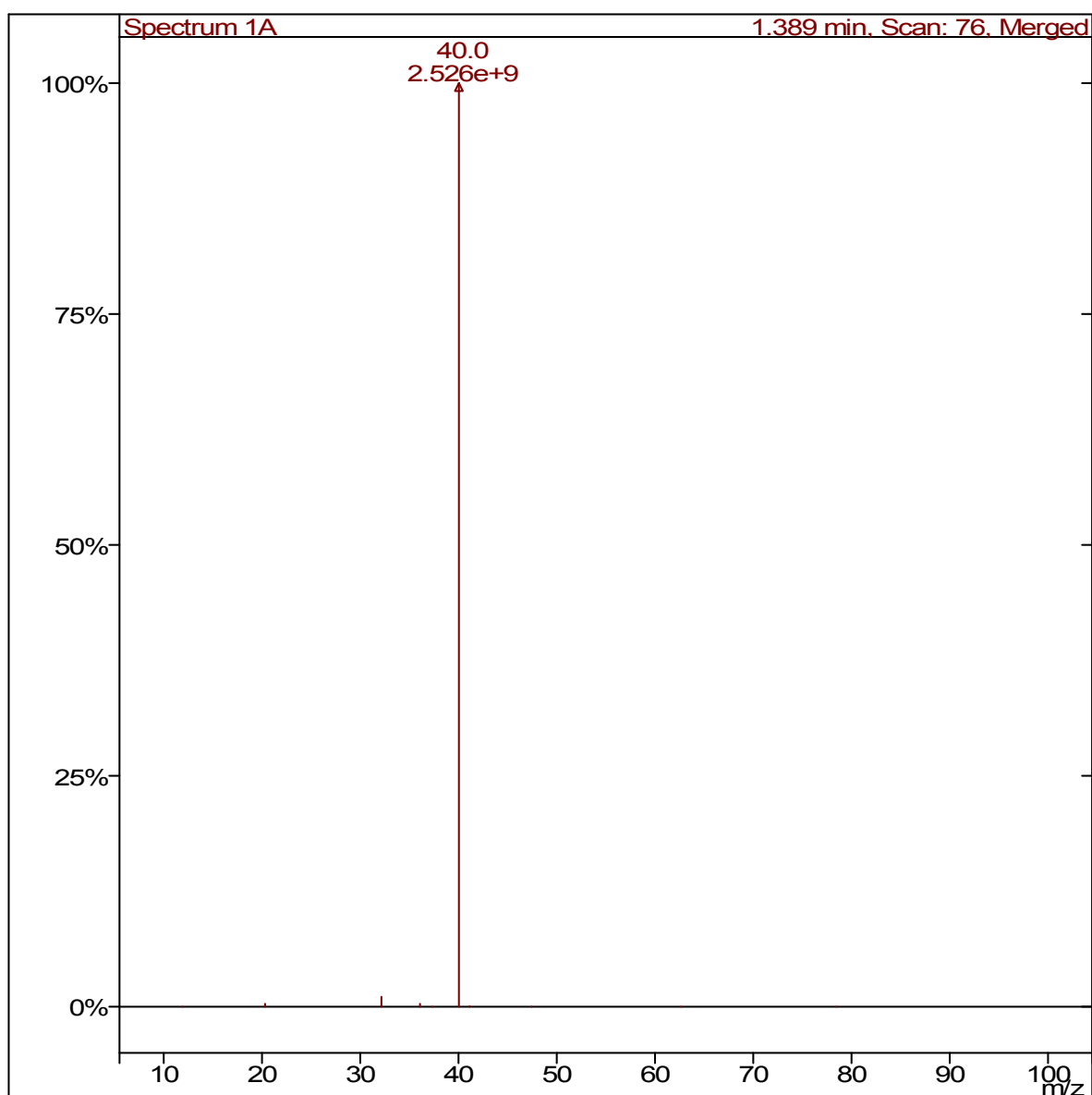


Figure S12: Mass spectrum of the signal corresponding to argon at a retention time of 1.39 min.

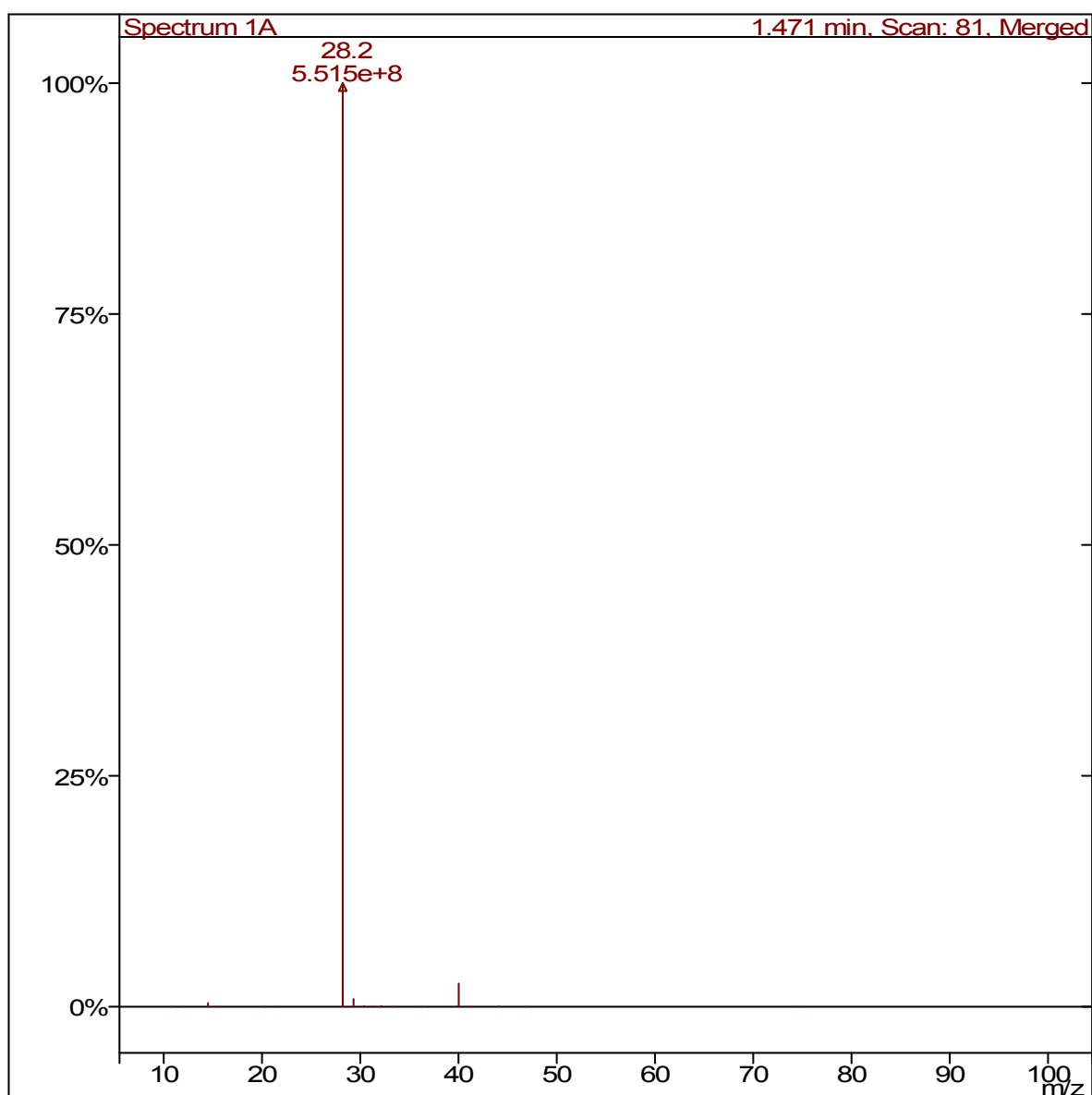


Figure S13: Mass spectrum of the signal corresponding to dinitrogen at a retention time of 1.47 min.

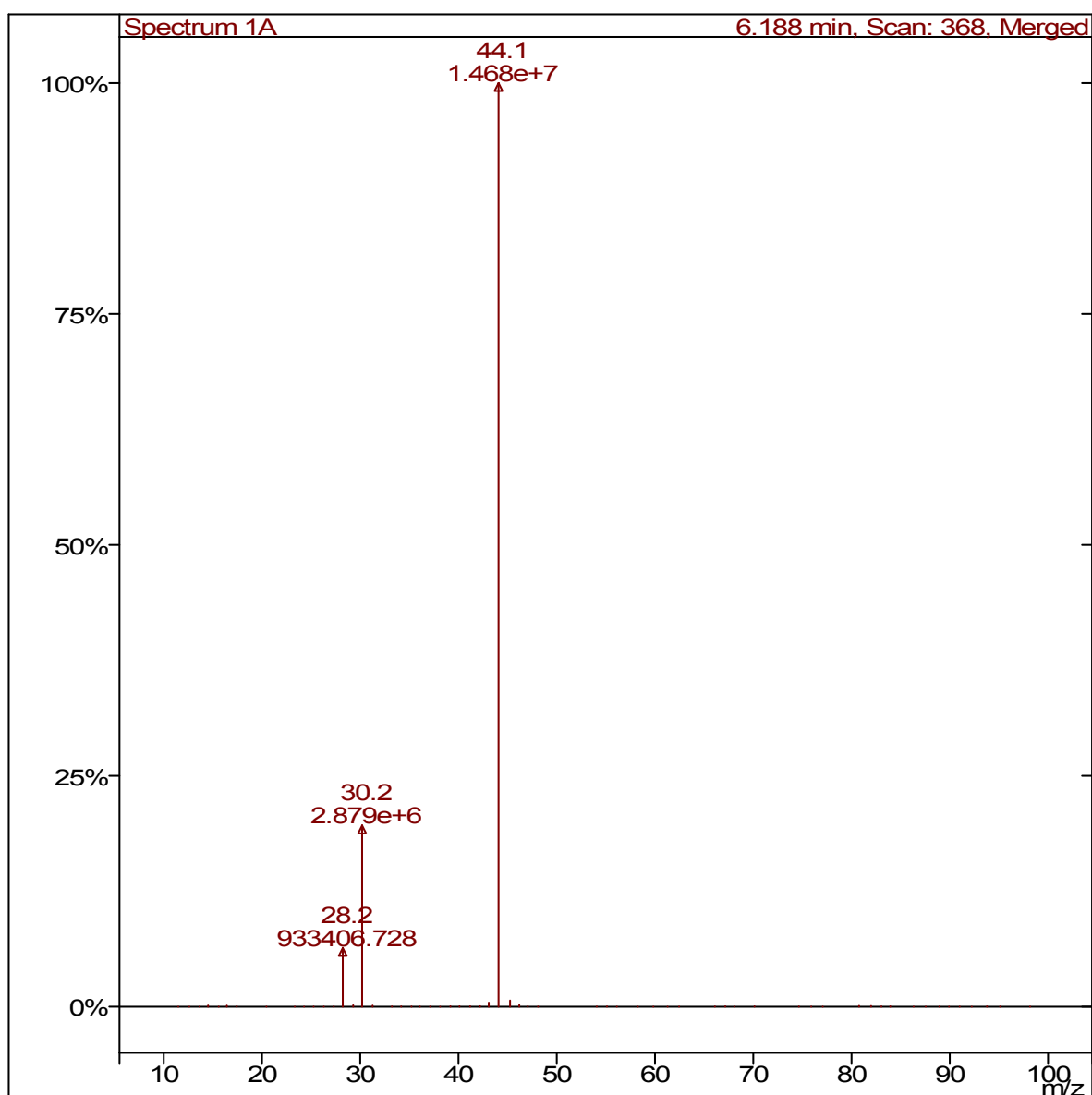


Figure S14: Mass spectrum of the signals corresponding to nitrous oxide at a retention time of 6.19 min.

SQUID Magnetization Data:

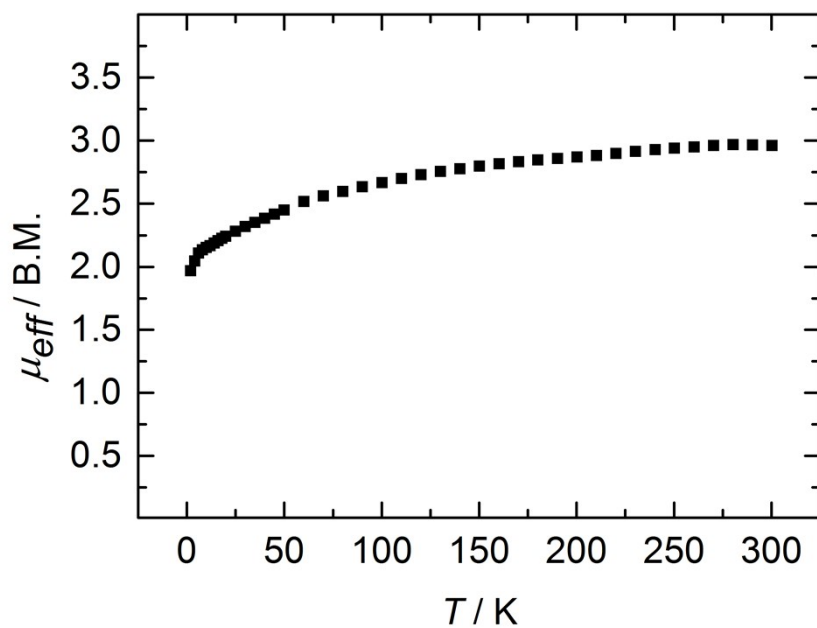


Figure S15: Temperature dependent SQUID magnetization measurements of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (1).

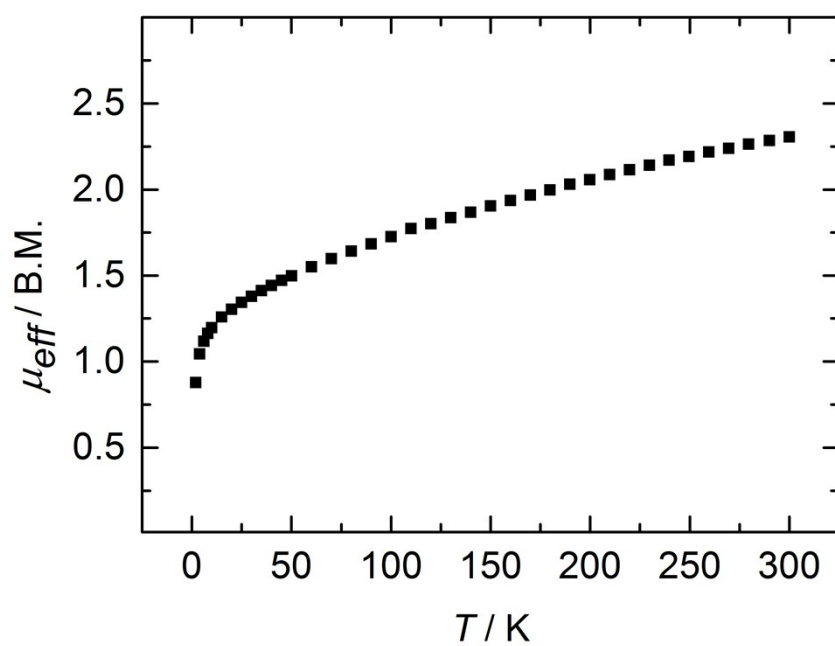


Figure S16: Temperature dependent SQUID magnetization measurements of $[(\text{Ar}^{\text{Ad,Ad,Me}}\text{O})_3\text{U}^{\text{V}}(\text{O})]$ (2).

EPR spectroscopy

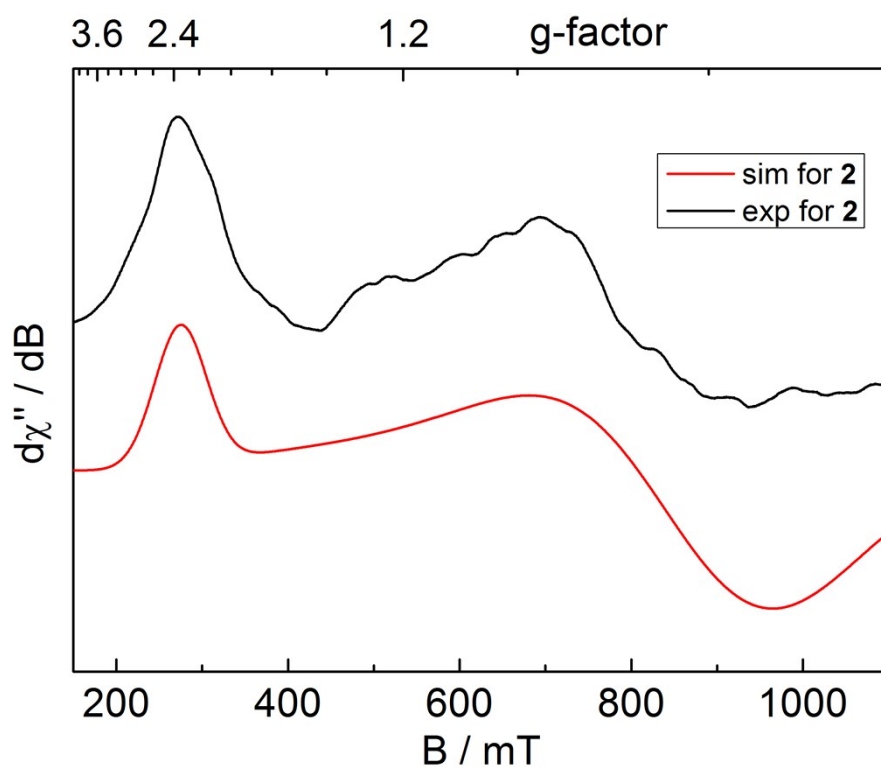


Figure S17: X-band EPR measurements of $[(^{\text{Ad,Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$ (**2**) recorded in 10.0 mM frozen toluene solution at 12 K (black trace) and its simulation (red trace). Experimental conditions: Microwave frequency $\nu = 8.968$ GHz, modulation width = 1.0 mT, modulation frequency = 100 kHz, microwave power = 0.50 mW, time constant = 3 s. Simulation parameters: $g_{\parallel} = 2.25$, $g_{\perp} = 0.71$, $W_{\perp} = 30$ mT, $W_{\parallel} = 50$ mT.

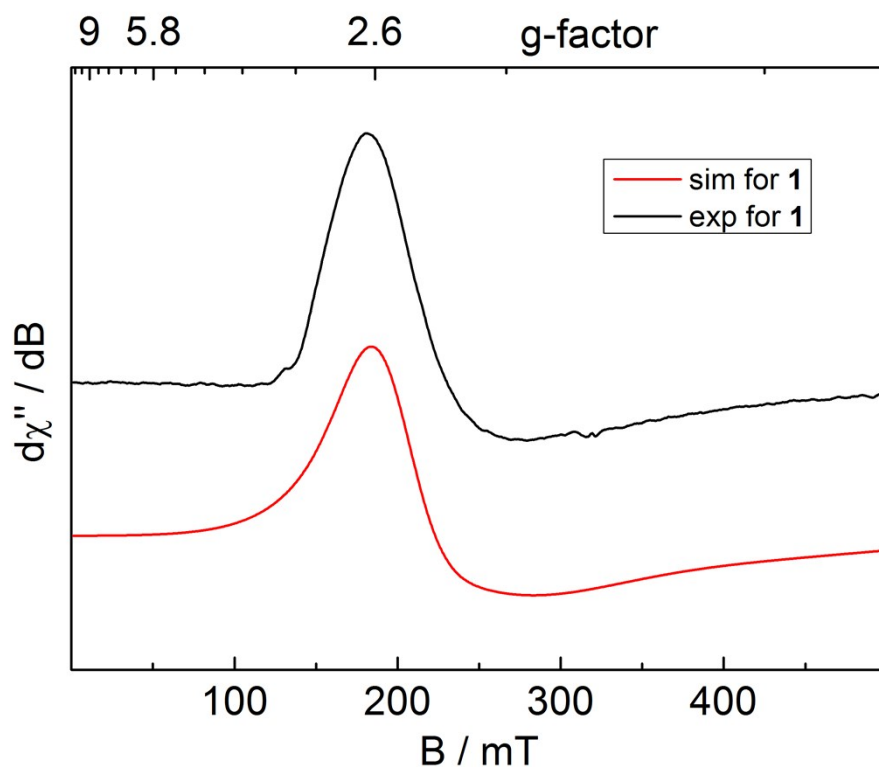


Figure S18: X-band EPR measurements of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3]$ (**1**) recorded in 10.0 mM frozen toluene solution at 8 K (black trace) and its simulation (red trace). Experimental conditions: Microwave frequency $\nu = 8.958$ GHz, modulation width = 1.0 mT, modulation frequency = 100 kHz, microwave power = 0.01 mW, time constant = 0.03 s. Simulation parameters: $g_1 = 3.20$, $g_2 = 2.73$, $g_3 = 1.42$, $W_x = 21$ mT, $W_y = 73$ mT, $W_z = 115$ mT.

UV/Vis/NIR

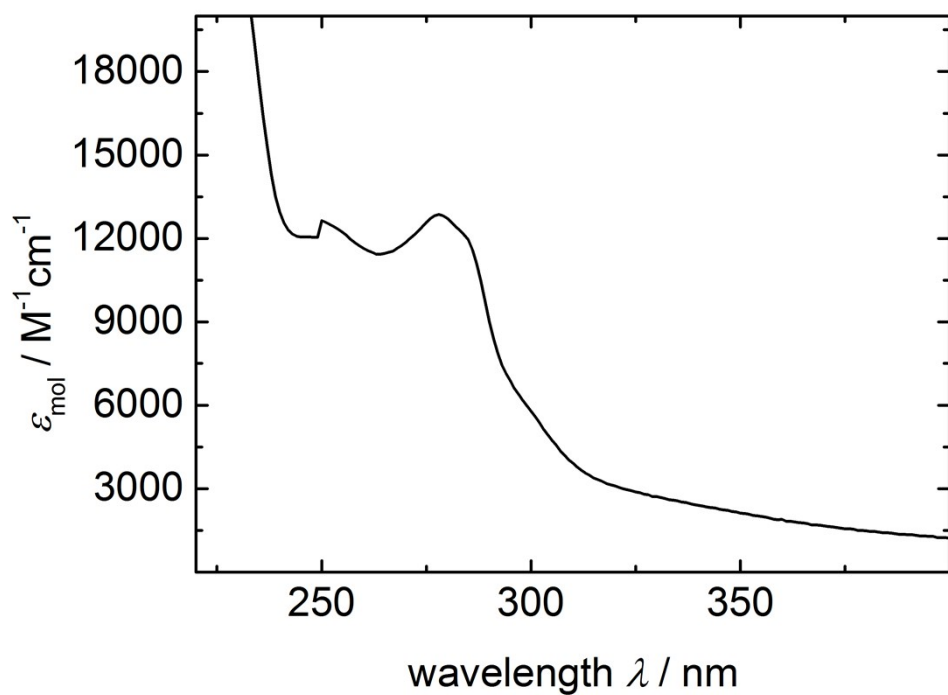


Figure S19: UV/vis/NIR spectrum of $[U^{III}(OAr^{Ad,Ad,Me})_3]$ (1) in THF, $c = 0.05$ mmol.

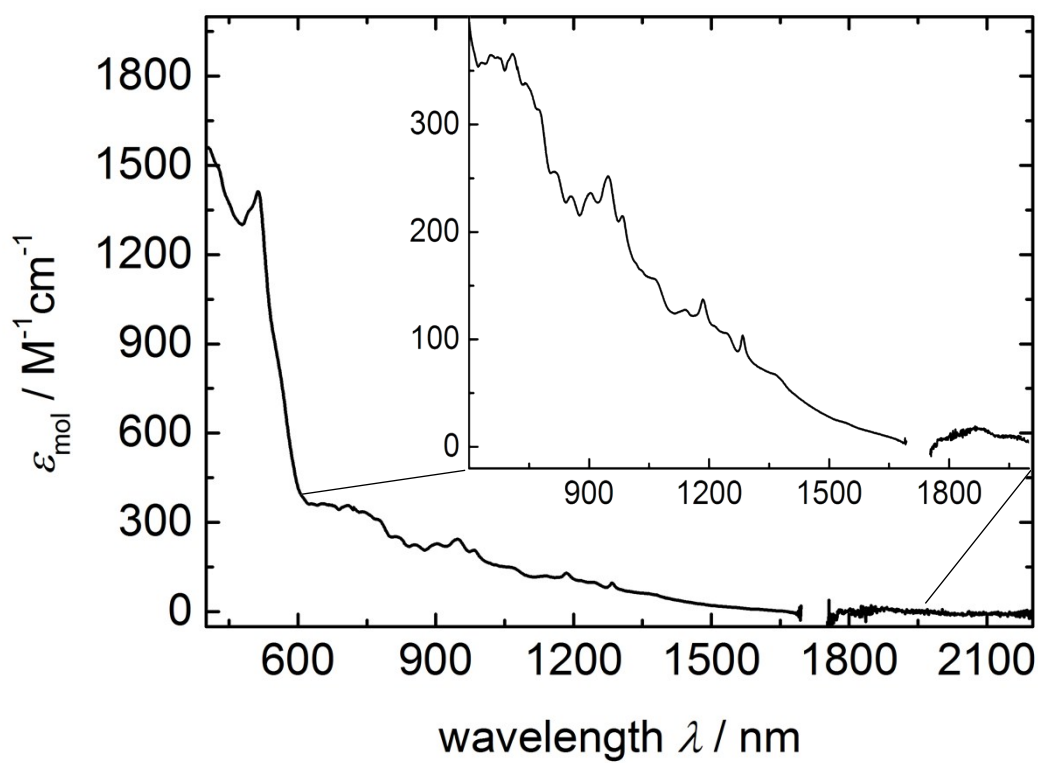


Figure S20: UV/vis/NIR spectrum of $[U^{III}(OAr^{Ad,Ad,Me})_3]$ (1) in THF, $c = 10$ mmol.

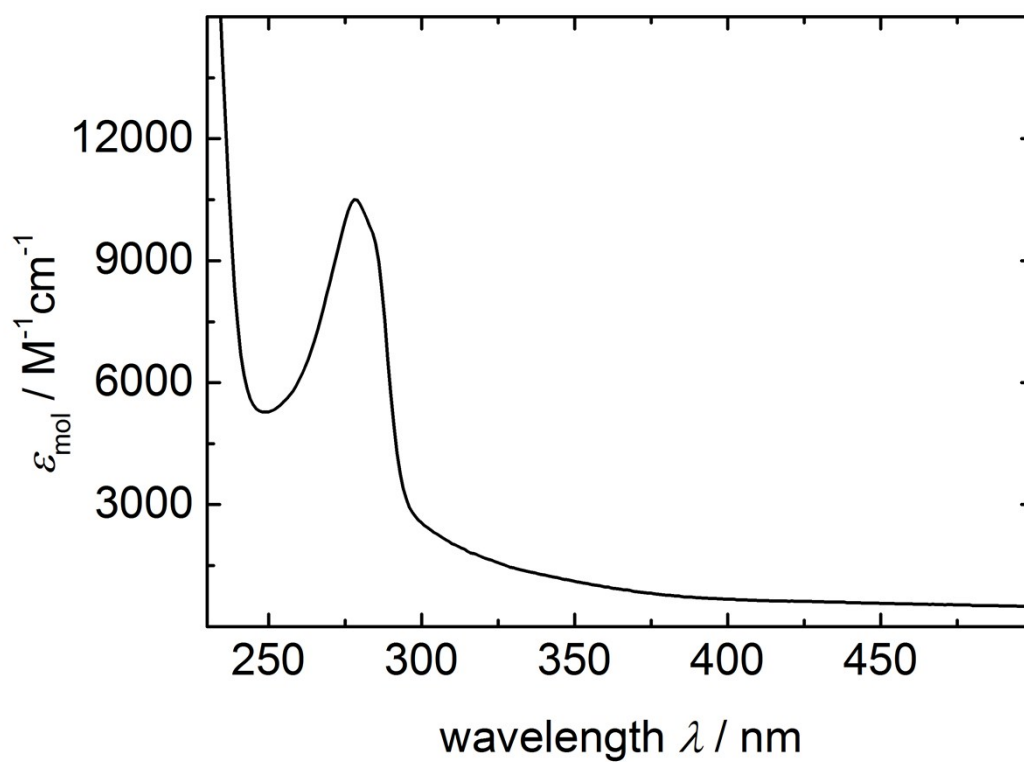


Figure S21: UV/vis/NIR spectrum of $[(^{\text{Ad,Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$ (**2**) in THF, $c = 0.1$ mmol.

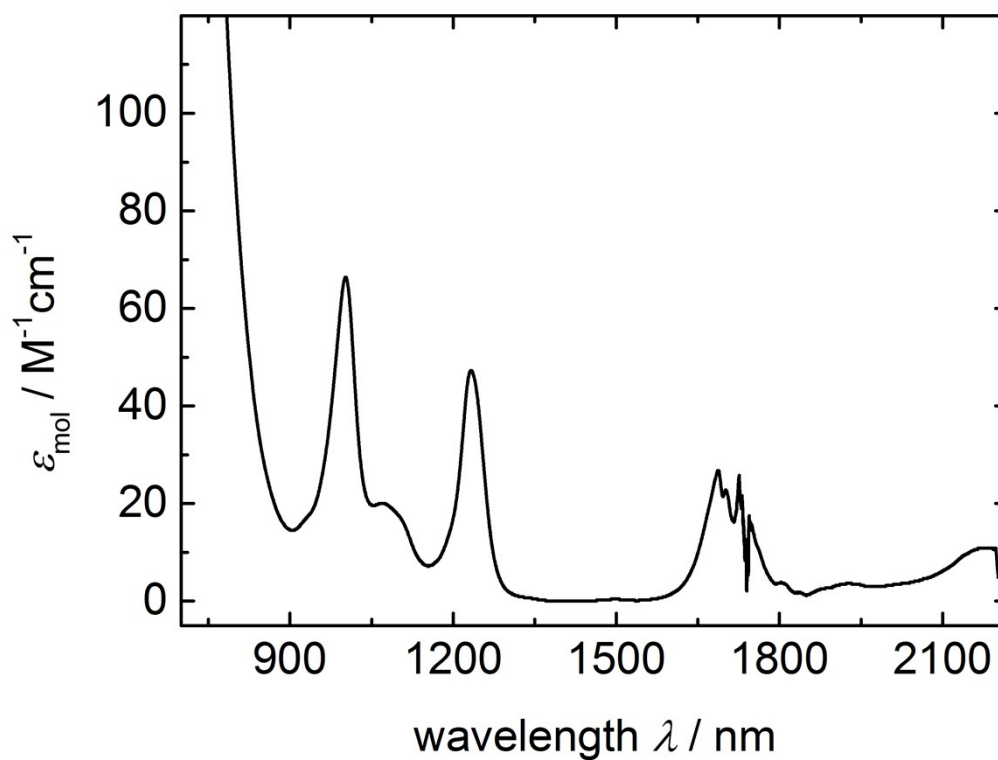


Figure S22: NIR spectrum of $[(^{\text{Ad,Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$ (**2**) in THF, $c = 4.3$ mmol.

X-Ray Crystal Structure Determinations

CCDC-1477612 (for **1** · 1.445 C₆H₁₄ · 0.555 C₆H₆, [U^{III}(OAr^{Ad,Ad,Me})₃] · 1.44 C₆H₁₄ · 0.56 C₆H₆) and CCDC-1477613 (for **2**, [(^{Ad,Ad,Me}ArO)₃U^V(O)]) contain the supplementary crystallographic data for this paper. This data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/products/csd/request/> (or from Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK. fax: ++44-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Crystals of [U^{III}(OAr^{Ad,Ad,Me})₃] · 1.445 C₆H₁₄ · 0.555 C₆H₆ and [(^{Ad,Ad,Me}ArO)₃U^V(O)] were coated with perfluoropolyalkylether oil on a microscope slide. A suitable single crystal of each compound was selected, mounted on a MiTeGen micromount, and brought into the cold nitrogen gas stream of the diffractometer. Intensity data were collected at 100 K on a Bruker SMART APEX II diffractometer and at 150 K on a Bruker-Nonius KappaCCD diffractometer using MoK α radiation in both cases (λ = 0.71073 Å, graphite monochromator). Data were corrected for Lorentz and polarization effects, semi-empirical absorption corrections were performed on the basis of multiple scans using SADABS⁷. The structures were solved by direct methods and refined by full-matrix least-squares procedures on F^2 using SHELXTL NT 6.12.⁸ All non-hydrogen atoms were refined anisotropically. In [U^{III}(OAr^{Ad,Ad,Me})₃] · 1.44 C₆H₁₄ · 0.56 C₆H₆ the central uranium atom is disordered over two alternative positions above and beyond the plane formed by the three oxygen donor atoms with refined occupancies of 53(1) and 47(1) % for U1 and U1A. The compound crystallized with a total of 1.44 molecules of *n*-hexane and 0.56 molecules of benzene per formula unit. All solvent molecules were disordered. The *n*-hexane molecules were distributed over three crystallographic sites, one of which roughly shared its site with the benzene molecule. The refined site occupancies for the *n*-hexanes were 37.7(5)% for C101 – C106, 62.3(5)% for C111 – C116, and 44.5(5)% for C211 – C216, and 55.5(5)% for the benzene C201 – C206. DFIX and SIMU restraints were applied in the treatment of the disordered solvent molecules. Treatment of hydrogen atoms: All hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to those of their corresponding carrier atoms by a factor of 1.2 or 1.5.

Crystallographic Details for $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3] \cdot 1.445 \text{ C}_6\text{H}_{14} \cdot 0.555 \text{ C}_6\text{H}_6$

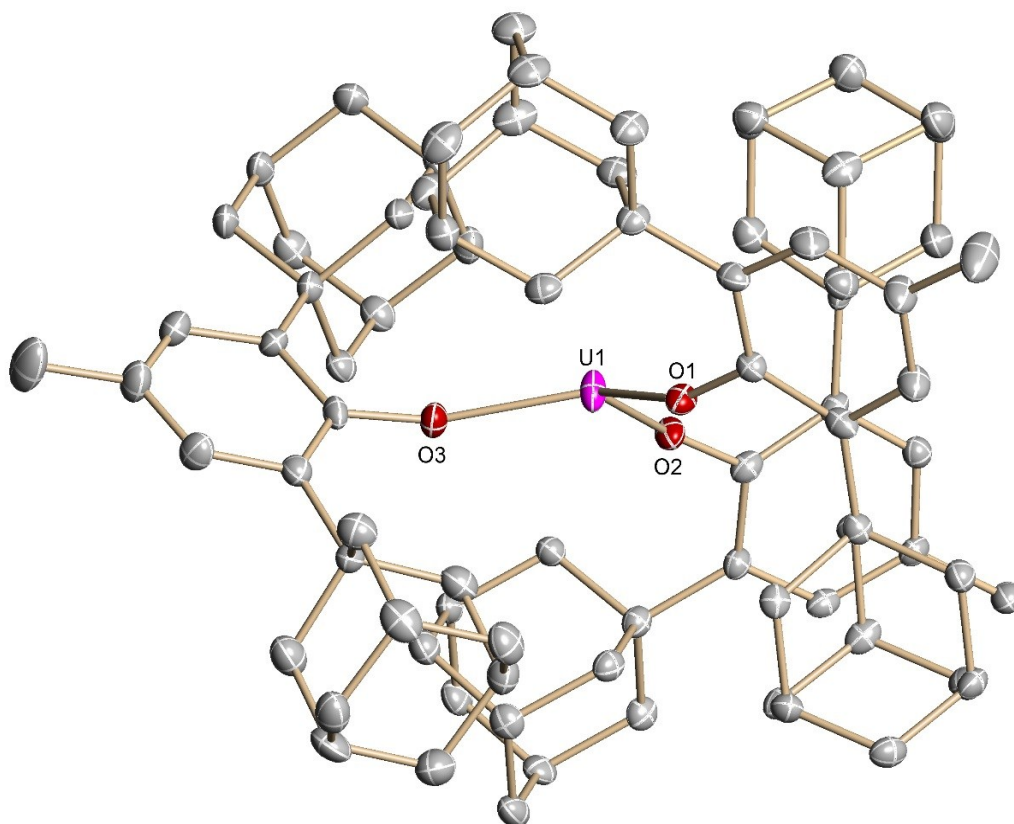
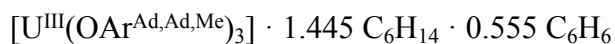


Figure S23: Solid-state molecular structure of **1** in crystals of $[\text{U}^{\text{III}}(\text{OAr}^{\text{Ad,Ad,Me}})_3] \cdot 1.44 \text{ C}_6\text{H}_{14} \cdot 0.56 \text{ C}_6\text{H}_6$. Hydrogen atoms, co-crystallized solvent molecules and disorder are omitted for clarity. Thermal ellipsoids are at the 50 % probability level.



Empirical formula	$\text{C}_{93}\text{H}_{128.56}\text{O}_3\text{U}$	
Formula weight	1532.56 g/mol	
Temperature	100 (2) K	
Wavelength	$\lambda = 0.71073 \text{ \AA}$	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	$a = 16.6756(14) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 37.752(3) \text{ \AA}$	$\beta = 93.136(5)^\circ$
	$c = 12.3496(11) \text{ \AA}$	$\gamma = 90^\circ$
Volume, Z	$7762.9(11) \text{ \AA}^3$, $Z = 4$	
Calculated density	1.311 mg/m ³	
Absorption coefficient	2.141 mm ⁻¹	
F (000)	3210	
Crystal size	0.26 x 0.26 x 0.25 mm	
Theta range for data collection	1.08 to 26.26 °	
Limiting indices	$-19 \leq h \leq 20$, $-46 \leq k \leq 46$, $-15 \leq l \leq 14$	
Reflections collected / unique	77570 / 14670 [$R(\text{int}) = 0.0496$]	
Completeness to theta	98.5 %	
Absorption correction	SADABS	
Max. and min. transmission	0.7460 and 0.662	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14670 / 162 / 991	
Goodness-of-fit on F^2	1.036	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0433$, $wR_2 = 0.0983$	
R indices (all data)	$R_1 = 0.0719$, $wR_2 = 0.1085$	
Largest diff. peak and hole	0.949 and -0.684 eÅ ⁻³	

Crystallographic Details for $[(^{\text{Ad,Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$

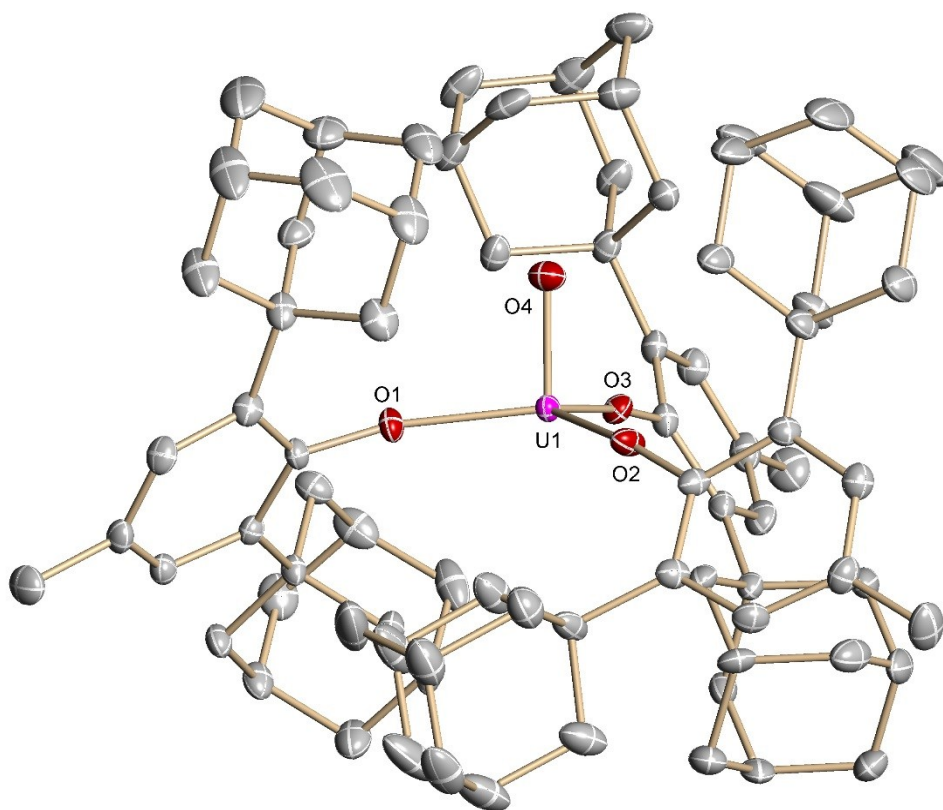


Figure S24: Solid-state molecular structure of **2** in crystals of $[(^{\text{Ad,Ad,Me}}\text{ArO})_3\text{U}^{\text{V}}(\text{O})]$. Hydrogen atoms are omitted for clarity. Thermal ellipsoids are at the 50 % probability level.



Empirical formula	$\text{C}_{81}\text{H}_{105}\text{O}_4\text{U}$	
Formula weight	1380.68 g/mol	
Temperature	150 (2) K	
Wavelength	$\lambda = 0.71073 \text{ \AA}$	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	$a = 21.4453(13) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 13.7404(11) \text{ \AA}$	$\beta = 119.622(6)^\circ$
	$c = 25.313(2) \text{ \AA}$	$\gamma = 90^\circ$
Volume, Z	$6484.1(8) \text{ \AA}^3$, $Z = 4$	
Calculated density	1.414 mg/m^3	
Absorption coefficient	2.556 mm^{-1}	
F (000)	2860	
Crystal size	0.28 x 0.11 x 0.06 mm	
Theta range for data collection	2.86 to 29.50°	
Limiting indices	$-29 \leq h \leq 29$, $-19 \leq k \leq 19$, $-35 \leq l \leq 35$	
Reflections collected / unique	$194861 / 18030$	$[\text{R(int)} = 0.0704]$
Completeness to theta	99.9 %	
Absorption correction	SADABS	
Max. and min. transmission	0.746 and 0.583	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	$18030 / 0 / 778$	
Goodness-of-fit on F^2	1.119	
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0288$, $wR_2 = 0.0498$	
R indices (all data)	$R_1 = 0.0519$, $wR_2 = 0.0560$	
Largest diff. peak and hole	0.963 and $-0.635 \text{ e\AA}^{-3}$	

DFT

Computational details:

All the structures reported in this study were fully optimized with the Becke's 3-parameter hybrid functional⁹ combined with the non-local correlation functional provided by Perdew/Wang (denoted as B3PW91).¹⁰ The basis set used for uranium atom was the Stuttgart-Dresden small core ECP in combination with its adapted basis set.^{11, 12} However, in order to study the reactions involving bimetallic complexes, the 5*f*-in-large-core ECPs (augmented by a *f* polarization function, $\alpha = 1.0$) were used for fixed oxidation states III and IV. For the rest of the atoms the 6-31G(d,p) basis set was used.¹³⁻¹⁵ In all computations no constraints were imposed on the geometry. All stationary points have been identified for minimum (number of imaginary frequencies $N_{\text{imag}}=0$) or transition states ($N_{\text{imag}}=1$). The vibrational modes and the corresponding frequencies are based on a harmonic force field. Enthalpy energies were obtained at $T = 298.15\text{K}$ within the harmonic approximation. GAUSSIAN09 program suite was used in all calculations.¹⁶

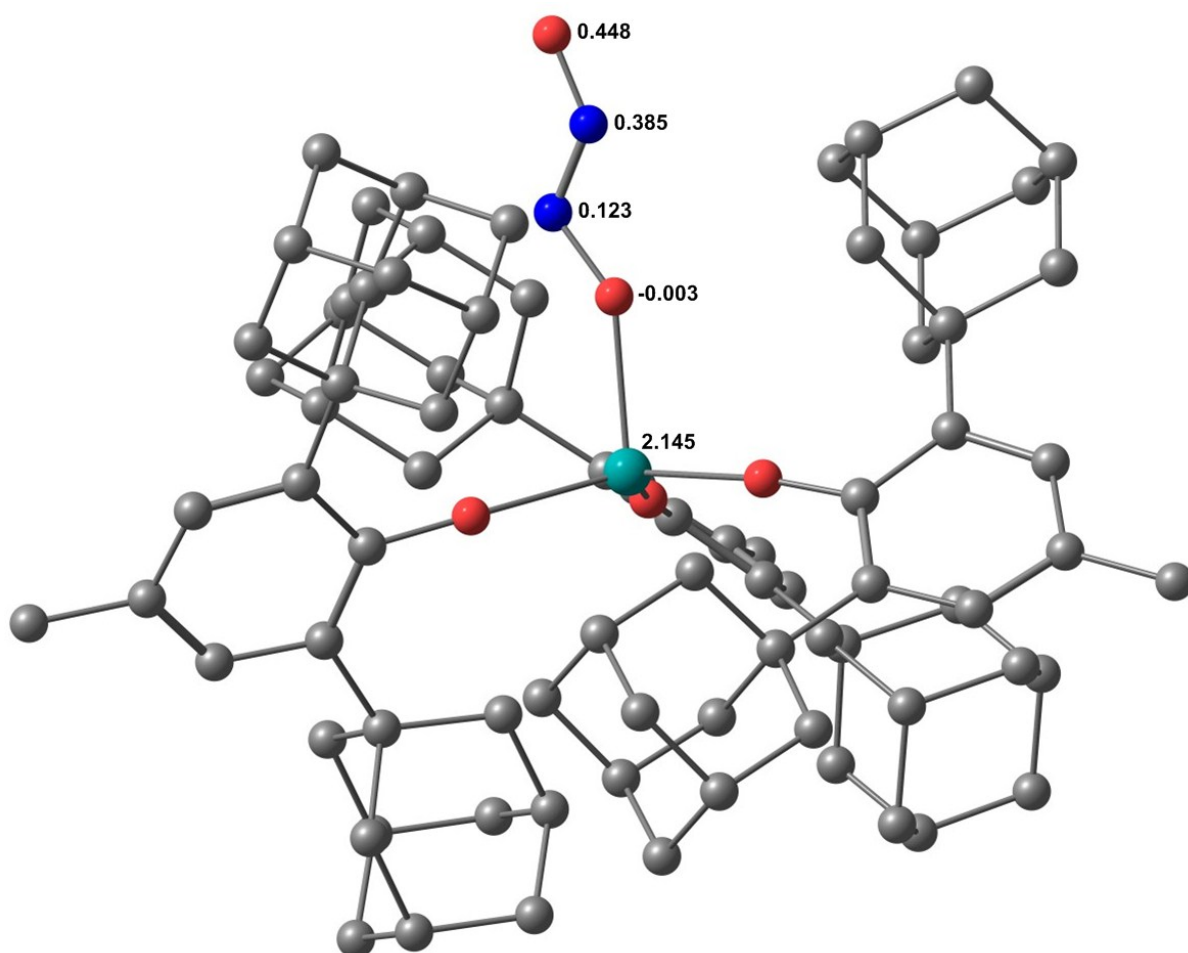


Figure S25: Spin densities of $[(\text{Ad,Ad,MeArO})_3\text{U}^{\text{IV}}(\text{N}_2\text{O}_2)]$

[U(OAr^{Ad,Ad,Me})₃]

scf done: -3406.575260 (LC), -3851.7796202 (SC)

U	12.326961	33.992557	2.358274
O	11.665478	31.899099	2.890805
O	10.907989	35.729684	2.047387
O	14.386069	34.447649	1.580034
C	10.880946	30.806541	2.965475
C	11.001581	29.778209	1.982421
C	10.093112	28.715434	2.024525
H	10.153035	27.932410	1.277616
C	9.101318	28.600065	2.992458
C	9.063156	29.570736	3.988334
H	8.320292	29.453733	4.769070
C	9.932256	30.665662	4.024935
C	12.103336	29.775472	0.905146
C	13.042852	30.950792	-1.155004
H	12.891858	31.805201	-1.827425
C	14.614656	29.870817	0.478425
H	15.591157	29.962590	0.970869
C	13.188628	28.462141	-1.006757
H	13.123456	27.520593	-1.567933
C	11.930260	30.941295	-0.096151
H	10.945400	30.866667	-0.573448
H	11.929921	31.897186	0.449920
C	12.081408	28.476384	0.057938
H	12.196895	27.607377	0.718493
H	11.110952	28.373164	-0.444651
C	14.408957	31.065430	-0.464288
H	14.480054	32.006400	0.095899
H	15.209367	31.095589	-1.214768
C	14.561076	28.568886	-0.330180
H	14.726282	27.705886	0.328811
H	15.359042	28.554233	-1.084797

C	13.511003	29.857511	1.548430
H	13.575045	30.753487	2.173077
H	13.642446	28.996603	2.217276
C	12.987915	29.646145	-1.961055
H	12.021873	29.557915	-2.476231
H	13.766116	29.648889	-2.735717
C	9.877585	31.618668	5.233797
C	8.801940	32.111425	7.503983
H	8.038899	31.751438	8.206664
C	9.515291	34.010530	6.050522
H	9.281551	35.027412	5.711612
C	11.235049	32.560236	7.176144
H	12.225524	32.547893	7.650558
C	8.819379	31.181874	6.280916
H	7.821412	31.175258	5.823403
H	9.029279	30.157236	6.613040
C	11.245039	31.618798	5.963081
H	11.474713	30.593601	6.281334
H	12.032203	31.909955	5.259132
C	8.463245	33.541133	7.063435
H	8.441770	34.213841	7.931363
H	7.463989	33.573352	6.609661
C	10.900500	33.985487	6.714481
H	11.665611	34.336444	6.005273
H	10.926300	34.679423	7.565453
C	9.508417	33.067870	4.838745
H	10.210877	33.438511	4.083561
H	8.523357	33.077406	4.356803
C	10.176854	32.094006	8.184293
H	10.173995	32.747892	9.066910
H	10.413260	31.081140	8.536321
C	8.108452	27.467255	2.966855
H	7.191450	27.744954	2.430808

H	7.811647	27.169271	3.977889
H	8.519889	26.584929	2.466290
C	9.836463	36.413071	2.497136
C	8.526417	36.113486	2.011936
C	7.440472	36.740660	2.630303
H	6.434330	36.508382	2.300379
C	7.577899	37.670270	3.657208
C	8.870132	38.030195	4.025176
H	8.977876	38.801772	4.778941
C	10.013103	37.451107	3.462381
C	8.271161	35.204653	0.793525
C	8.827235	34.867024	-1.672981
H	9.420270	35.267068	-2.506005
C	8.440355	32.864115	-0.205954
H	8.753431	31.836357	0.015945
C	6.528665	34.329255	-0.862997
H	5.457735	34.359749	-1.103811
C	9.059984	35.737331	-0.429220
H	10.125232	35.771729	-0.185113
H	8.747869	36.770996	-0.627557
C	6.775137	35.189074	0.385797
H	6.165338	34.796750	1.210497
H	6.435733	36.214669	0.192189
C	9.262278	33.424113	-1.377141
H	9.125658	32.795490	-2.267428
H	10.334861	33.398322	-1.136839
C	6.952182	32.882797	-0.579238
H	6.352407	32.464559	0.240041
H	6.774244	32.252104	-1.460597
C	8.663595	33.729755	1.043800
H	8.089768	33.331173	1.889188
H	9.718789	33.672991	1.337743
C	7.338749	34.882407	-2.042837

H	7.160332	34.277723	-2.942345
H	7.018524	35.906822	-2.275178
C	11.400227	37.996145	3.853780
C	12.677894	39.803491	5.143268
H	12.537921	40.678850	5.791069
C	13.573434	38.988510	2.961816
H	14.102203	39.268100	2.041698
C	13.638468	37.506404	4.986432
H	14.204438	36.728680	5.516264
C	11.296730	39.236523	4.781175
H	10.700819	40.012923	4.285011
H	10.772580	38.970652	5.708549
C	12.245024	36.963648	4.636711
H	11.706435	36.660646	5.542590
H	12.361954	36.052661	4.027476
C	13.424465	40.216850	3.868860
H	14.410087	40.629823	4.123116
H	12.870786	41.007504	3.345424
C	14.374075	37.903253	3.698146
H	15.379546	38.271998	3.940526
H	14.507271	37.027168	3.048951
C	12.183176	38.447377	2.594377
H	12.271006	37.607879	1.899557
H	11.600286	39.223223	2.081181
C	13.486511	38.736105	5.891029
H	14.475460	39.126225	6.165569
H	12.979190	38.460454	6.825430
C	6.373052	38.274107	4.330568
H	6.010170	37.643874	5.153026
H	5.540569	38.397841	3.630020
H	6.600920	39.257477	4.754185
C	15.663897	34.228199	1.221909
C	16.106401	34.658430	-0.072499

C	17.389939	34.302807	-0.484137
H	17.736173	34.596213	-1.468629
C	18.276036	33.585384	0.319716
C	17.853813	33.271165	1.601493
H	18.562743	32.767095	2.253059
C	16.577709	33.579935	2.098797
C	15.239873	35.538146	-0.993423
C	13.096881	35.716630	-2.361668
H	12.193783	35.168793	-2.662486
C	13.962886	37.738831	-1.150941
H	13.674993	38.634747	-0.585313
C	15.152189	36.880892	-3.169234
H	15.744314	37.155571	-4.052351
C	13.964277	34.806167	-1.478618
H	14.256202	33.904037	-2.031740
H	13.385113	34.469164	-0.611260
C	16.003863	35.971528	-2.270996
H	16.924466	36.499373	-1.989785
H	16.303037	35.086484	-2.848238
C	12.700024	36.974057	-1.573373
H	12.117004	36.700101	-0.684819
H	12.056328	37.616262	-2.189255
C	14.754834	38.146796	-2.398896
H	14.151880	38.806237	-3.037775
H	15.651971	38.710981	-2.110472
C	14.831003	36.840362	-0.258035
H	14.290055	36.584593	0.656906
H	15.741169	37.374618	0.045777
C	13.889569	36.128056	-3.609323
H	13.273251	36.764104	-4.258759
H	14.162413	35.239749	-4.194997
C	16.380642	33.248114	3.598928
C	17.360434	33.794907	5.905165

H	18.097192	34.424822	6.420537
C	16.680876	31.436166	5.383533
H	16.932272	30.377175	5.525958
C	14.946349	33.193975	5.721413
H	13.936981	33.402330	6.098936
C	17.379681	34.126397	4.407390
H	17.132539	35.184307	4.245995
H	18.391073	33.983337	4.013048
C	14.980288	33.500235	4.210859
H	14.686373	34.545128	4.037070
H	14.263608	32.813127	3.728043
C	17.712329	32.313609	6.109176
H	18.719911	32.110298	5.722262
H	17.726983	32.071568	7.180236
C	15.283847	31.715463	5.950414
H	15.250321	31.484328	7.023202
H	14.539301	31.074250	5.461102
C	16.699828	31.752912	3.879924
H	17.681445	31.491597	3.473531
H	15.969519	31.126317	3.350876
C	15.960494	34.073084	6.463162
H	15.711370	35.135519	6.340662
H	15.921527	33.858113	7.539215
C	19.636632	33.183967	-0.186576
H	20.302020	32.901161	0.634917
H	20.117429	33.997909	-0.740210
H	19.576426	32.325136	-0.867275

[(Ad,Ad,MeArO)₃U(NO)] N-Bonded. N–O stretching frequency: 1751 cm⁻¹

192

scf done: -3542.082498 (LC), -3981.6491019 (SC)

C	-6.892073	4.340180	21.733776
C	-5.936260	3.548780	22.631632
C	-6.347132	2.067907	22.633565

C	-6.284561	1.516797	21.200630
C	-7.237178	2.314376	20.302102
C	-6.806564	3.785856	20.306862
C	-4.502853	3.683991	22.097346
C	-4.365743	3.121157	20.652681
C	-4.850063	1.642389	20.667621
C	-5.364286	3.912506	19.780030
C	-2.870244	3.165517	20.240386
C	-2.253534	3.842285	19.150417
C	-0.830919	3.762493	18.969749
C	-0.095200	3.003771	19.879881
C	-0.668595	2.320868	20.949466
C	-2.039254	2.424475	21.097093
O	-2.999700	4.558317	18.268166
U	-4.132335	5.766107	16.857042
O	-5.762581	6.786647	17.887604
C	-6.821942	7.217364	18.616565
C	-8.147503	6.869746	18.215750
C	-9.195170	7.196170	19.084511
C	-9.008981	7.875578	20.281310
C	-7.717497	8.287322	20.589529
C	-6.604521	8.004121	19.790798
C	-8.497846	6.205354	16.867139
C	-7.971684	7.064043	15.690165
C	-8.322783	6.431646	14.334538
C	-7.717596	5.023033	14.249062
C	-8.286682	4.148737	15.375421
C	-7.943401	4.767088	16.740328
C	-9.846045	6.337395	14.184273
C	-10.402029	5.465662	15.315766
C	-10.034235	6.085962	16.670782
C	-9.810360	4.054524	15.225613
C	-10.169469	8.212574	21.180475

C	-5.243339	8.609147	20.202827
C	-5.385547	9.547726	21.431943
C	-4.048356	10.187457	21.830581
C	-3.496297	11.010424	20.659141
C	-3.306332	10.084337	19.450745
C	-4.663820	9.475705	19.059068
C	-3.056429	9.081365	22.210162
C	-2.862072	8.158715	21.001594
C	-4.205912	7.531373	20.596803
C	-2.309758	8.976163	19.826905
C	-0.059238	4.462670	17.831137
C	-0.232078	5.999577	17.888243
C	0.516284	6.690261	16.737233
C	0.005571	6.151883	15.392806
C	0.245469	4.639080	15.304613
C	-0.509037	3.940258	16.445491
C	2.018013	6.406102	16.854373
C	2.239928	4.890033	16.779677
C	1.468954	4.198567	17.913692
C	1.747141	4.356744	15.428683
C	0.176163	1.510583	21.897003
O	-3.898122	5.240095	14.738549
C	-3.685879	4.697261	13.509025
C	-3.606985	3.285571	13.343808
C	-3.208603	2.795030	12.090234
C	-2.937685	3.601025	10.999264
C	-3.136822	4.969526	11.162754
C	-3.520286	5.556465	12.369128
C	-3.975025	2.167227	14.350547
C	-2.760414	1.224042	14.578047
C	-3.132994	0.016020	15.449658
C	-3.611959	0.502082	16.822825
C	-4.840906	1.399167	16.627664

C	-4.456834	2.605617	15.750863
C	-5.966748	0.591680	15.973724
C	-5.491968	0.112100	14.599389
C	-4.254039	-0.782477	14.766739
C	-5.137337	1.329573	13.735101
C	-3.750879	7.084096	12.376363
C	-2.673466	7.816071	13.204514
C	-2.924814	9.332971	13.234680
C	-4.312202	9.621715	13.828800
C	-5.391089	8.945840	12.970309
C	-5.148786	7.428741	12.942189
C	-2.864175	9.891156	11.806973
C	-3.945003	9.206151	10.958932
C	-3.695360	7.690324	10.948780
C	-5.331782	9.501217	11.543436
C	-2.463346	3.032708	9.688253
N	-3.118720	7.796445	16.515373
O	-2.308841	8.675110	16.549328
H	-10.209004	6.917488	18.826367
H	-7.584379	8.858291	21.499641
H	-7.912663	7.057518	13.533891
H	-7.850084	3.143512	15.318962
H	-11.496135	5.413230	15.241450
H	-8.406342	8.069234	15.764547
H	-6.886726	7.195977	15.774930
H	-10.464607	5.466228	17.467959
H	-10.492527	7.079791	16.749423
H	-7.944070	4.572835	13.273770
H	-6.622871	5.074746	14.318616
H	-10.067933	3.591644	14.263945
H	-10.231382	3.415233	16.013147
H	-6.851948	4.764623	16.881719
H	-8.349032	4.147186	17.549395

H	-10.294132	7.339162	14.222745
H	-10.106131	5.907170	13.207842
H	-11.008241	7.527230	21.025073
H	-10.540504	9.228653	20.994872
H	-9.886264	8.161470	22.236792
H	-4.220193	10.843217	22.694495
H	-2.915311	10.656473	18.599834
H	-2.159950	7.354078	21.254805
H	-6.113334	10.338919	21.210052
H	-5.769288	8.984253	22.292582
H	-4.607730	6.931335	21.423061
H	-4.038592	6.840975	19.762444
H	-2.541322	11.475530	20.938050
H	-4.189811	11.824875	20.410174
H	-1.344848	9.423158	20.101504
H	-2.117329	8.323222	18.969828
H	-4.564377	8.875912	18.150598
H	-5.378044	10.275394	18.821765
H	-3.435118	8.512627	23.070252
H	-2.094508	9.516709	22.512316
H	0.978583	2.929468	19.764487
H	-2.492107	1.898037	21.931572
H	0.330551	7.769190	16.794662
H	-0.130478	4.261505	14.345493
H	3.308296	4.665530	16.898357
H	-1.292921	6.266991	17.846345
H	0.139228	6.364267	18.855007
H	1.855468	4.556491	18.876670
H	1.665718	3.119540	17.865696
H	0.509554	6.665228	14.563397
H	-1.065170	6.360861	15.280970
H	1.938795	3.277690	15.354385
H	2.294074	4.836672	14.606163

H	-0.341145	2.855812	16.405943
H	-1.586536	4.089534	16.312784
H	2.567336	6.911293	16.048549
H	2.405966	6.799633	17.803529
H	-0.430729	1.062373	22.689117
H	0.945518	2.126681	22.377017
H	0.695964	0.696734	21.377531
H	-6.571729	0.456807	21.200760
H	-5.971802	3.942421	23.656166
H	-7.464905	4.373096	19.657832
H	-4.783652	1.230443	19.653081
H	-4.184984	1.032150	21.287455
H	-5.088835	4.970206	19.767261
H	-5.331440	3.537283	18.747321
H	-7.363227	1.959250	23.036013
H	-5.680696	1.489945	23.288328
H	-7.922547	4.261270	22.105092
H	-6.635443	5.406546	21.737067
H	-4.192836	4.736522	22.099746
H	-3.817880	3.161028	22.772793
H	-7.217190	1.912215	19.279581
H	-8.271045	2.220529	20.660878
H	-2.983484	5.597895	10.294729
H	-3.113184	1.721371	11.957237
H	-2.156315	9.808142	13.856755
H	-6.381371	9.140507	13.403785
H	-3.892627	9.574183	9.925545
H	-2.671728	7.416924	14.219484
H	-1.684572	7.603132	12.776898
H	-2.708369	7.512473	10.503392
H	-4.436957	7.199966	10.303947
H	-4.361571	9.252645	14.858902
H	-4.485221	10.705890	13.863849

H	-6.110513	9.039547	10.920971
H	-5.521575	10.583018	11.545816
H	-5.909628	6.932773	12.324899
H	-5.245425	7.023656	13.953380
H	-3.020235	10.978324	11.816598
H	-1.872478	9.713809	11.368865
H	-2.966566	3.506915	8.838762
H	-2.647277	1.955810	9.627726
H	-1.385858	3.188418	9.550941
H	-2.247055	-0.620822	15.570379
H	-6.292283	-0.453498	14.104271
H	-5.178594	1.772131	17.600497
H	-2.373689	0.868099	13.617636
H	-1.949080	1.793938	15.046580
H	-3.638502	3.127890	16.267202
H	-5.324562	3.275157	15.649555
H	-3.915854	-1.145998	13.786944
H	-4.506808	-1.668071	15.365073
H	-6.234323	-0.261373	16.611197
H	-6.870822	1.205647	15.868059
H	-6.014587	1.978654	13.610668
H	-4.863139	0.990708	12.731329
H	-2.815140	1.057384	17.333546
H	-3.867854	-0.351947	17.463699

[(^{Ad},^{Ad},^{Me}ArO)₃U(NO)] O-Bonded, N–O stretching frequency: 1453 cm⁻¹

192

scf done: -3542.052119 (LC), -3981.6307974 (SC)

C	-3.511373	0.490474	16.776785
C	-3.108090	0.016493	15.375670
C	-2.781310	1.231916	14.496138
C	-4.005832	2.177857	14.339676
C	-4.410186	2.604266	15.768607
C	-4.747057	1.390655	16.655377

C	-4.265192	-0.774872	14.746646
C	-5.508848	0.122161	14.653294
C	-5.199086	1.346251	13.780439
C	-5.907963	0.590390	16.055771
C	-3.684324	3.301677	13.323526
C	-3.739297	4.710575	13.504667
C	-3.588809	5.582662	12.373748
C	-3.269626	5.004664	11.144816
C	-3.113598	3.633768	10.955250
C	-3.350222	2.819217	12.047690
O	-3.921141	5.241154	14.746668
U	-4.099875	5.747863	16.863285
O	-2.987917	7.692368	16.589607
C	-3.772033	7.114827	12.417704
C	-2.663004	7.792252	13.251702
C	-2.870041	9.313767	13.327529
C	-4.241792	9.623107	13.945376
C	-5.349824	9.006449	13.079663
C	-5.154647	7.484822	13.003656
C	-2.806449	9.908465	11.915304
C	-3.914220	9.277758	11.059893
C	-3.712482	7.755226	11.005964
C	-5.285371	9.599166	11.667510
C	-2.714949	3.072424	9.616192
O	-5.750183	6.786378	17.830775
C	-6.815704	7.201899	18.567755
C	-8.135226	6.825337	18.174765
C	-9.186843	7.134086	19.045574
C	-9.010675	7.822124	20.238241
C	-7.726954	8.260690	20.538222
C	-6.609404	7.997890	19.737108
C	-8.481754	6.154948	16.827861
C	-7.985621	7.028852	15.649308

C	-8.335729	6.393643	14.294479
C	-7.699646	4.999474	14.197035
C	-8.237640	4.109129	15.326181
C	-7.895636	4.730736	16.690026
C	-9.857705	6.265100	14.158268
C	-10.383203	5.376780	15.291360
C	-10.016858	6.000500	16.644833
C	-9.760310	3.980014	15.191286
C	-10.174372	8.139866	21.140440
C	-5.261712	8.634541	20.151741
C	-5.431394	9.566152	21.382918
C	-4.113913	10.238270	21.791109
C	-3.579273	11.079614	20.624887
C	-3.357454	10.162157	19.415976
C	-4.695691	9.516342	19.011907
C	-3.098507	9.154135	22.173700
C	-2.872692	8.242468	20.962151
C	-4.198503	7.582376	20.547417
C	-2.329949	9.084457	19.800640
O	-2.976908	4.553620	18.278445
C	-2.238415	3.834470	19.166892
C	-0.817486	3.739492	18.986152
C	-0.090968	2.984927	19.907372
C	-0.671966	2.322851	20.985948
C	-2.041825	2.439942	21.130473
C	-2.864398	3.176262	20.261806
C	-0.036183	4.420394	17.841217
C	-0.187179	5.960381	17.883089
C	0.578321	6.630042	16.731252
C	0.064914	6.089891	15.388661
C	0.279232	4.572271	15.313977
C	-0.490238	3.894696	16.458176
C	2.074415	6.323439	16.856185

C	2.273349	4.803701	16.792794
C	1.487946	4.134191	17.929694
C	1.775714	4.266740	15.445106
C	0.165295	1.520629	21.946821
C	-4.362456	3.144487	20.665380
C	-4.852238	1.667484	20.692546
C	-6.291087	1.552247	21.215378
C	-6.362141	2.117674	22.642171
C	-5.945672	3.596944	22.628611
C	-4.507978	3.722624	22.103159
C	-7.233372	2.343878	20.300932
C	-6.798546	3.814087	20.295152
C	-5.352114	3.930954	19.777707
C	-6.892041	4.382553	21.715955
H	-10.195518	6.833779	18.792034
H	-7.603043	8.837348	21.445542
H	-7.948100	7.032363	13.492662
H	-7.779284	3.114046	15.262179
H	-11.476475	5.299606	15.227061
H	-8.441523	8.023930	15.731586
H	-6.903111	7.182133	15.725750
H	-10.425996	5.369032	17.444007
H	-10.496701	6.983425	16.730124
H	-7.927301	4.547441	13.222884
H	-6.606255	5.075076	14.255500
H	-10.016004	3.513531	14.230874
H	-10.158938	3.329177	15.981079
H	-6.802100	4.756609	16.819288
H	-8.275857	4.098034	17.501610
H	-10.328333	7.256143	14.205195
H	-10.117371	5.832996	13.182537
H	-10.994972	7.429639	21.000096
H	-10.574479	9.142594	20.943189

H	-9.883384	8.111237	22.195448
H	-4.307657	10.885737	22.656685
H	-2.976900	10.744692	18.567424
H	-2.152087	7.454854	21.217244
H	-6.176992	10.339928	21.159048
H	-5.805260	8.991689	22.240634
H	-4.587700	6.968651	21.369886
H	-4.009677	6.897408	19.712270
H	-2.638871	11.570384	20.909075
H	-4.294747	11.874938	20.375955
H	-1.387891	9.564653	20.097991
H	-2.086803	8.451560	18.940106
H	-4.572200	8.921000	18.104841
H	-5.428307	10.298311	18.771276
H	-3.470440	8.573330	23.028866
H	-2.149110	9.610184	22.484520
H	0.982014	2.897954	19.794742
H	-2.500678	1.928745	21.971086
H	0.401110	7.709953	16.783128
H	-0.099170	4.192121	14.356630
H	3.337456	4.562330	16.916648
H	-1.242503	6.246655	17.832039
H	0.181882	6.329681	18.848782
H	1.877107	4.495154	18.890368
H	1.667588	3.051761	17.892169
H	0.583281	6.586503	14.557923
H	-1.000373	6.319979	15.268817
H	1.950452	3.184140	15.380503
H	2.331991	4.730978	14.619937
H	-0.343261	2.806872	16.426196
H	-1.564710	4.063448	16.321226
H	2.634221	6.814933	16.049140
H	2.465332	6.717437	17.803925

H	-0.448555	1.072507	22.733552
H	0.925538	2.142908	22.433381
H	0.695574	0.707842	21.436595
H	-6.581795	0.493289	21.223828
H	-5.987032	4.001064	23.648763
H	-7.450190	4.397339	19.636031
H	-4.779479	1.242962	19.683585
H	-4.193724	1.062430	21.324289
H	-5.072706	4.988052	19.757677
H	-5.314817	3.543500	18.749137
H	-7.381580	2.017078	23.038065
H	-5.702987	1.543497	23.307511
H	-7.925503	4.311145	22.080122
H	-6.631664	5.447875	21.710054
H	-4.195039	4.774342	22.097079
H	-3.829053	3.204608	22.788428
H	-7.205533	1.931518	19.282583
H	-8.270589	2.256842	20.651381
H	-3.134325	5.642483	10.280552
H	-3.278692	1.745879	11.898197
H	-2.086288	9.747365	13.959902
H	-6.330245	9.218432	13.527172
H	-3.861779	9.672038	10.036230
H	-2.655198	7.365817	14.254103
H	-1.687608	7.564198	12.801422
H	-2.737193	7.555023	10.544184
H	-4.478134	7.308282	10.357604
H	-4.285297	9.230691	14.967593
H	-4.382460	10.709945	14.017181
H	-6.084779	9.179853	11.041336
H	-5.440612	10.685886	11.701694
H	-5.933073	7.031561	12.375693
H	-5.261652	7.048979	14.001299

H	-2.931364	10.998977	11.954485
H	-1.823989	9.714826	11.463560
H	-3.262659	3.554189	8.799033
H	-2.906881	1.996783	9.559168
H	-1.646254	3.225126	9.420146
H	-2.217800	-0.622269	15.442390
H	-6.335625	-0.438402	14.197663
H	-5.030391	1.756054	17.647871
H	-2.446550	0.884232	13.513563
H	-1.945974	1.798333	14.925514
H	-3.565074	3.123081	16.243829
H	-5.284835	3.272350	15.720556
H	-3.980408	-1.130240	13.747100
H	-4.487164	-1.665180	15.350051
H	-6.140828	-0.268536	16.698836
H	-6.815522	1.206162	16.005801
H	-6.080981	1.996505	13.706126
H	-4.977678	1.015246	12.761179
H	-2.687437	1.039929	17.249429
H	-3.734888	-0.368357	17.423260
N	-2.165274	8.611134	16.610374

[(^{Ad,Ad,Me}ArO)₃U(NO)] Isomerization NO η^2 Bonded

192

scf done: -3542.042397 (LC), -3981.621076 (SC)

C	-6.726968	4.365206	21.834719
C	-5.805982	3.432262	22.627008
C	-6.336411	1.993062	22.538428
C	-6.380993	1.553199	21.067023
C	-7.301000	2.491875	20.278104
C	-6.747393	3.918225	20.367744
C	-4.388735	3.498643	22.039402
C	-4.356201	3.035570	20.553484
C	-4.965589	1.607398	20.475510

C	-5.321218	3.965970	19.785176
C	-2.879699	2.987194	20.079494
C	-2.250599	3.720354	19.036818
C	-0.846583	3.561184	18.788247
C	-0.146194	2.639048	19.565964
C	-0.734929	1.890208	20.582441
C	-2.083071	2.094455	20.815721
O	-2.976651	4.562281	18.256381
U	-4.169320	5.858582	16.986292
O	-5.818445	6.889633	17.987933
C	-6.859886	7.276006	18.765633
C	-8.192377	6.928808	18.393592
C	-9.217583	7.212162	19.303800
C	-8.998672	7.831982	20.527518
C	-7.703536	8.251951	20.808495
C	-6.616502	8.027169	19.956032
C	-8.567646	6.299146	17.035750
C	-8.057179	7.170586	15.860532
C	-8.427351	6.550710	14.503337
C	-7.828735	5.140381	14.395971
C	-8.384607	4.256872	15.521414
C	-8.014890	4.862998	16.883998
C	-9.952907	6.463164	14.373340
C	-10.495998	5.583267	15.505315
C	-10.106636	6.186115	16.862595
C	-9.910766	4.170681	15.394291
C	-10.121569	8.054898	21.506376
C	-5.267560	8.697064	20.303798
C	-5.352847	9.491784	21.634902
C	-4.041577	10.217779	21.965263
C	-3.712982	11.210412	20.841685
C	-3.576142	10.439138	19.522696
C	-4.899300	9.723041	19.200319

C	-2.911016	9.193133	22.109793
C	-2.774234	8.424295	20.789865
C	-4.094663	7.702812	20.473239
C	-2.441740	9.414384	19.664351
C	-0.054989	4.379350	17.746437
C	-0.086754	5.883404	18.113427
C	0.685584	6.726610	17.085497
C	0.091030	6.515388	15.686444
C	0.180595	5.035643	15.292068
C	-0.587145	4.176541	16.307930
C	2.158342	6.295135	17.071758
C	2.235966	4.811714	16.686968
C	1.443323	3.975790	17.703414
C	1.654480	4.609701	15.282613
C	0.075475	0.921603	21.403131
O	-4.054586	5.194682	14.911562
C	-3.506575	4.689951	13.774060
C	-3.228045	3.294733	13.670737
C	-2.382240	2.879430	12.634771
C	-1.822334	3.746992	11.705902
C	-2.256612	5.066317	11.744380
C	-3.151286	5.562989	12.700033
C	-3.864036	2.139247	14.484096
C	-2.788702	1.132370	14.978571
C	-3.422852	-0.109962	15.620683
C	-4.246505	0.315781	16.840237
C	-5.342909	1.285972	16.381847
C	-4.703445	2.524585	15.723856
C	-6.266199	0.574045	15.384998
C	-5.444980	0.146946	14.163664
C	-4.331455	-0.814498	14.602443
C	-4.823239	1.389271	13.511684
C	-3.668035	7.000118	12.435924

C	-2.554737	8.044608	12.699893
C	-3.024551	9.462566	12.334956
C	-4.253481	9.830414	13.178294
C	-5.385164	8.833494	12.885469
C	-4.923757	7.407972	13.235188
C	-3.396714	9.518177	10.846052
C	-4.541057	8.531422	10.568269
C	-4.084284	7.111753	10.935249
C	-5.766873	8.911565	11.403839
C	-0.823916	3.273051	10.683282
O	-3.635045	8.108665	16.183150
N	-2.662313	7.746615	16.854379
H	-10.237594	6.942436	19.059684
H	-7.547435	8.785882	21.737302
H	-8.024834	7.183098	13.702330
H	-7.953106	3.250772	15.450904
H	-11.591228	5.535360	15.445455
H	-8.492796	8.174314	15.949941
H	-6.972146	7.300891	15.931888
H	-10.526302	5.554911	17.656328
H	-10.560665	7.179951	16.965176
H	-8.071372	4.700872	13.419328
H	-6.733540	5.187805	14.455104
H	-10.184804	3.716814	14.432806
H	-10.322586	3.526329	16.182604
H	-6.920751	4.866023	17.000573
H	-8.401690	4.235808	17.696658
H	-10.396841	7.466056	14.426957
H	-10.228841	6.041650	13.397389
H	-9.985449	8.983678	22.069754
H	-10.183867	7.239633	22.238510
H	-11.090214	8.109502	20.999703
H	-4.172598	10.760385	22.910865

H	-3.341903	11.135334	18.707063
H	-1.975121	7.676995	20.875010
H	-6.156547	10.235722	21.570639
H	-5.604210	8.811860	22.460060
H	-4.334511	6.983565	21.266907
H	-3.964306	7.115772	19.556924
H	-2.781575	11.746770	21.067676
H	-4.506308	11.965798	20.761406
H	-1.497115	9.929159	19.886504
H	-2.284451	8.883560	18.715371
H	-4.834362	9.219689	18.231731
H	-5.711667	10.456802	19.116561
H	-3.130463	8.501130	22.934003
H	-1.965976	9.695412	22.355273
H	0.911154	2.487808	19.387773
H	-2.543322	1.525004	21.617853
H	0.605620	7.785450	17.361196
H	-0.259841	4.887799	14.298966
H	3.282850	4.480373	16.705146
H	-1.119661	6.231542	18.184387
H	0.355289	6.010426	19.110825
H	1.895212	4.110466	18.694422
H	1.537303	2.912548	17.445013
H	0.620332	7.136457	14.951641
H	-0.956074	6.851466	15.672108
H	1.741727	3.556592	14.983141
H	2.218437	5.200249	14.548154
H	-0.492774	3.116637	16.040837
H	-1.656180	4.404285	16.250205
H	2.728677	6.903136	16.356550
H	2.609542	6.455098	18.060352
H	0.661470	0.248282	20.767561
H	-0.565056	0.304532	22.040029

H	0.784945	1.443688	22.056970
H	-6.753998	0.522477	21.001219
H	-5.769166	3.747153	23.678394
H	-7.378652	4.604804	19.794245
H	-4.982518	1.284379	19.427704
H	-4.330235	0.891493	21.006422
H	-4.960712	4.998715	19.832768
H	-5.364301	3.654116	18.729381
H	-7.339255	1.933462	22.982195
H	-5.692046	1.315081	23.114672
H	-7.745114	4.342031	22.245381
H	-6.380592	5.403476	21.907295
H	-3.998825	4.523369	22.101290
H	-3.717198	2.876914	22.640765
H	-7.359426	2.168628	19.229396
H	-8.322546	2.456970	20.679716
H	-1.886327	5.740075	10.977781
H	-2.146469	1.823672	12.541853
H	-2.210753	10.170887	12.538934
H	-6.256892	9.079213	13.506510
H	-4.795670	8.553094	9.500134
H	-2.257398	8.008682	13.754751
H	-1.662799	7.785149	12.114902
H	-3.253031	6.843393	10.277200
H	-4.885528	6.388154	10.734723
H	-3.998722	9.811122	14.244355
H	-4.582220	10.851402	12.941221
H	-6.598616	8.227278	11.187277
H	-6.108923	9.923750	11.148603
H	-5.728342	6.691663	13.029197
H	-4.725889	7.361859	14.304585
H	-3.700945	10.537132	10.571216
H	-2.524377	9.267838	10.226835

H	-0.914758	3.828350	9.744293
H	-0.955711	2.210059	10.457868
H	0.206463	3.403147	11.037901
H	-2.622372	-0.791907	15.935823
H	-6.096862	-0.350314	13.433227
H	-5.929340	1.617725	17.248762
H	-2.147786	0.810184	14.152487
H	-2.136403	1.634844	15.702688
H	-4.050106	3.002051	16.470716
H	-5.488955	3.231662	15.433708
H	-3.745442	-1.136502	13.730837
H	-4.765912	-1.720220	15.046398
H	-6.730337	-0.299494	15.862089
H	-7.082762	1.238170	15.072795
H	-5.609292	2.082219	13.182834
H	-4.272646	1.096182	12.610765
H	-3.595503	0.796505	17.581328
H	-4.696212	-0.560335	17.326447

[(^{Ad},^{Ad},^{Me}ArO)₃U(NO)] TS radical coupling *estimated*

194

SCF Done: -3671.983631

C	-5.329424	9.762681	11.918875
C	-5.363620	9.147969	13.322967
C	-4.218649	9.729025	14.166295
C	-2.872060	9.404238	13.500982
C	-2.841436	10.019912	12.096785
C	-3.984425	9.423376	11.266200
C	-5.201097	7.624559	13.214356
C	-3.841839	7.236687	12.589453
C	-2.697584	7.879300	13.403093
C	-3.808554	7.899393	11.185944
C	-3.681480	5.702391	12.514024
C	-3.832532	4.803110	13.624139

C	-3.772825	3.398699	13.407683
C	-3.450959	2.949878	12.116001
C	-3.225244	3.789184	11.041408
C	-3.373600	5.154208	11.268417
O	-4.028586	5.304862	14.879974
U	-4.028788	5.848118	16.986805
O	-2.848111	7.687814	16.905293
N	-1.691076	8.214831	16.482066
N	-1.580608	9.982560	16.802898
O	-0.668955	10.743584	16.536856
C	-4.062916	2.238613	14.394006
C	-2.821634	1.306797	14.488930
C	-3.107985	0.057231	15.333385
C	-3.485977	0.477689	16.758290
C	-4.737885	1.360610	16.694736
C	-4.443855	2.611851	15.844229
C	-4.266264	-0.731258	14.703235
C	-5.525183	0.148214	14.667876
C	-5.253697	1.406195	13.830526
C	-5.899169	0.560953	16.094489
C	-2.843695	3.260652	9.684212
O	-2.775170	4.611333	18.247667
C	-2.076496	3.874975	19.157883
C	-2.725679	3.296346	20.282863
C	-1.926358	2.606655	21.210041
C	-0.559812	2.444041	21.082261
C	0.036647	2.984039	19.945923
C	-0.665647	3.689811	18.969077
C	-4.233338	3.275376	20.647346
C	-4.437098	3.902467	22.056559
C	-5.889545	3.768559	22.539041
C	-6.818789	4.502474	21.568141
C	-6.667467	3.889221	20.171295

C	-5.205107	4.013988	19.700029
C	-7.078177	2.412852	20.214420
C	-6.156516	1.670676	21.189032
C	-6.282370	2.283783	22.591881
C	-4.703393	1.792057	20.711078
C	0.130751	4.217218	17.756267
C	0.165494	5.762954	17.729259
C	0.944016	6.279407	16.506805
C	0.297878	5.750954	15.217899
C	0.324227	4.216583	15.211848
C	-0.455055	3.688512	16.425765
C	2.397065	5.792353	16.575057
C	2.407054	4.258693	16.577837
C	1.611077	3.748798	17.788070
C	1.776846	3.731463	15.283473
C	0.256423	1.713950	22.115744
O	-5.831565	6.826129	17.751885
C	-6.917327	7.191761	18.493081
C	-8.220448	6.746377	18.102315
C	-9.286447	6.995767	18.972089
C	-9.151893	7.695257	20.163833
C	-7.897232	8.207423	20.457693
C	-6.762462	8.005022	19.659206
C	-8.545069	6.067261	16.754581
C	-8.092755	6.971084	15.581789
C	-8.416635	6.328874	14.223840
C	-7.714886	4.966644	14.118009
C	-8.213460	4.046066	15.240972
C	-7.897046	4.671592	16.609025
C	-9.930995	6.132936	14.088852
C	-10.414110	5.215805	15.217664
C	-10.072437	5.846007	16.574610
C	-9.728435	3.849278	15.106773

C	-10.335102	7.941206	21.062928
C	-5.459545	8.722306	20.092653
C	-5.708935	9.662323	21.305614
C	-4.442508	10.409588	21.742169
C	-3.917244	11.259845	20.579528
C	-3.616945	10.337285	19.392910
C	-4.903737	9.613754	18.954747
C	-3.385301	9.385091	22.172441
C	-3.079184	8.468482	20.983214
C	-4.356116	7.735323	20.539257
C	-2.551254	9.314957	19.818937
H	-10.276059	6.639483	18.716638
H	-7.810002	8.795888	21.360611
H	-8.061208	6.990363	13.425154
H	-7.712462	3.072658	15.170321
H	-11.503066	5.090108	15.155389
H	-8.596927	7.942139	15.671932
H	-7.019545	7.169809	15.659562
H	-10.452045	5.190115	17.368734
H	-10.596171	6.805667	16.667072
H	-7.920061	4.509861	13.140900
H	-6.627598	5.091823	14.184410
H	-9.964093	3.378625	14.143165
H	-10.096524	3.175339	15.892217
H	-6.808994	4.747612	16.742878
H	-8.256750	4.017420	17.413577
H	-10.445050	7.101963	14.142750
H	-10.174028	5.695399	13.111169
H	-10.955025	7.044111	21.165478
H	-10.981853	8.735489	20.669305
H	-10.019006	8.245210	22.065228
H	-4.697372	11.057471	22.591380
H	-3.240317	10.927307	18.548300

H	-2.326194	7.723288	21.270866
H	-6.489982	10.389825	21.050584
H	-6.072229	9.082005	22.163567
H	-4.737557	7.110078	21.356219
H	-4.104251	7.051669	19.717670
H	-3.010947	11.801568	20.881559
H	-4.664111	12.014083	20.297451
H	-1.631246	9.834528	20.118007
H	-2.296180	8.662201	18.980159
H	-4.703298	9.010380	18.066121
H	-5.669413	10.349583	18.674811
H	-3.751833	8.799481	23.026679
H	-2.468888	9.892835	22.501222
H	1.102813	2.837279	19.831257
H	-2.402236	2.167377	22.081307
H	0.914700	7.375323	16.506148
H	-0.150677	3.843963	14.295273
H	3.439661	3.894732	16.662838
H	-0.851619	6.163038	17.720042
H	0.632834	6.123861	18.655274
H	2.098636	4.116408	18.699938
H	1.655511	2.651883	17.813906
H	0.834874	6.139274	14.342157
H	-0.733243	6.115032	15.136698
H	1.813775	2.633722	15.263100
H	2.341679	4.087810	14.411652
H	-0.430852	2.590653	16.444949
H	-1.507417	3.975587	16.337583
H	2.968157	6.175899	15.718931
H	2.884212	6.175198	17.482081
H	-0.380787	1.250606	22.874654
H	0.946514	2.391432	22.633024
H	0.864123	0.922734	21.662282

H	-6.430331	0.607910	21.225188
H	-5.972042	4.208384	23.541676
H	-7.305780	4.438285	19.472134
H	-4.585169	1.332465	19.722244
H	-4.055526	1.224788	21.387022
H	-4.947930	5.079736	19.671592
H	-5.122822	3.595710	18.684861
H	-7.312207	2.180228	22.958818
H	-5.636287	1.743702	23.297262
H	-7.862737	4.421781	21.897757
H	-6.581573	5.572016	21.534427
H	-4.142104	4.958916	22.023220
H	-3.773466	3.422275	22.782436
H	-7.010557	1.963864	19.213876
H	-8.125553	2.323658	20.532095
H	-3.241007	5.812442	10.419735
H	-3.380086	1.881086	11.938716
H	-2.053028	9.821551	14.097722
H	-6.325398	9.370473	13.803741
H	-3.954289	9.831183	10.247029
H	-2.667721	7.442960	14.402837
H	-1.738426	7.637361	12.926838
H	-2.848211	7.695359	10.695946
H	-4.596213	7.471934	10.551189
H	-4.248237	9.313956	15.182331
H	-4.337746	10.816229	14.264800
H	-6.156047	9.368472	11.312359
H	-5.461820	10.851593	11.973386
H	-6.002761	7.202288	12.595186
H	-5.299129	7.169259	14.203279
H	-2.944189	11.111640	12.158219
H	-1.875930	9.816181	11.614524
H	-3.408926	3.755036	8.886729

H	-3.027561	2.184900	9.606983
H	-1.779761	3.427116	9.474291
H	-2.206170	-0.568397	15.358133
H	-6.353222	-0.409799	14.211367
H	-5.006501	1.684869	17.705604
H	-2.505430	0.996167	13.488206
H	-1.984894	1.870673	14.916519
H	-3.603472	3.137192	16.320161
H	-5.329286	3.263505	15.836508
H	-3.998076	-1.047103	13.685967
H	-4.461284	-1.645256	15.279915
H	-6.101299	-0.324385	16.711933
H	-6.818015	1.161745	16.088602
H	-6.147392	2.042702	13.794255
H	-5.047951	1.111590	12.796891
H	-2.659467	1.025002	17.229172
H	-3.680678	-0.405654	17.380831

[(Ad,Ad,MeArO)₃U(N₂O₂)]

194

scf done: -3671.983631

C	-6.818789	4.502474	21.568140
C	-5.889545	3.768559	22.539041
C	-6.282370	2.283783	22.591881
C	-6.156516	1.670676	21.189032
C	-7.078177	2.412851	20.214420
C	-6.667467	3.889220	20.171295
C	-4.437098	3.902467	22.056559
C	-4.233338	3.275376	20.647346
C	-4.703393	1.792057	20.711078
C	-5.205107	4.013988	19.700029
C	-2.725679	3.296346	20.282863
C	-2.076496	3.874975	19.157883
C	-0.665647	3.689812	18.969077

C	0.036647	2.984040	19.945923
C	-0.559812	2.444042	21.082261
C	-1.926358	2.606655	21.210041
O	-2.775170	4.611333	18.247667
U	-4.028788	5.848118	16.986805
O	-5.831565	6.826129	17.751885
C	-6.917327	7.191761	18.493081
C	-8.220448	6.746377	18.102316
C	-9.286447	6.995767	18.972090
C	-9.151893	7.695257	20.163834
C	-7.897232	8.207423	20.457694
C	-6.762462	8.005022	19.659206
C	-8.545069	6.067261	16.754582
C	-8.092755	6.971084	15.581790
C	-8.416636	6.328874	14.223841
C	-7.714887	4.966644	14.118010
C	-8.213461	4.046066	15.240973
C	-7.897046	4.671592	16.609026
C	-9.930996	6.132936	14.088853
C	-10.414110	5.215805	15.217665
C	-10.072437	5.846007	16.574611
C	-9.728436	3.849278	15.106774
C	-10.335101	7.941206	21.062929
C	-5.459545	8.722306	20.092653
C	-5.708934	9.662322	21.305615
C	-4.442507	10.409587	21.742169
C	-3.917244	11.259845	20.579528
C	-3.616945	10.337285	19.392910
C	-4.903737	9.613754	18.954747
C	-3.385300	9.385090	22.172441
C	-3.079184	8.468481	20.983213
C	-4.356116	7.735322	20.539257
C	-2.551254	9.314957	19.818937

C	0.130751	4.217219	17.756266
C	0.165493	5.762955	17.729258
C	0.944015	6.279407	16.506804
C	0.297877	5.750954	15.217898
C	0.324227	4.216583	15.211848
C	-0.455055	3.688512	16.425765
C	2.397064	5.792354	16.575056
C	2.407053	4.258694	16.577836
C	1.611077	3.748799	17.788069
C	1.776845	3.731463	15.283473
C	0.256423	1.713951	22.115744
O	-4.028586	5.304862	14.879974
C	-3.832532	4.803110	13.624139
C	-3.772825	3.398699	13.407683
C	-3.450959	2.949878	12.116001
C	-3.225244	3.789184	11.041408
C	-3.373600	5.154208	11.268417
C	-3.681480	5.702391	12.514024
C	-4.062916	2.238613	14.394006
C	-2.821634	1.306797	14.488930
C	-3.107985	0.057231	15.333386
C	-3.485977	0.477689	16.758291
C	-4.737885	1.360610	16.694737
C	-4.443855	2.611851	15.844229
C	-5.899169	0.560953	16.094490
C	-5.525183	0.148214	14.667877
C	-4.266264	-0.731258	14.703236
C	-5.253697	1.406195	13.830527
C	-3.841839	7.236687	12.589453
C	-2.697584	7.879300	13.403093
C	-2.872060	9.404238	13.500982
C	-4.218649	9.729025	14.166295
C	-5.363620	9.147969	13.322967

C	-5.201097	7.624559	13.214356
C	-2.841436	10.019912	12.096785
C	-3.984425	9.423376	11.266200
C	-3.808554	7.899393	11.185944
C	-5.329424	9.762681	11.918875
C	-2.843695	3.260652	9.684212
O	-2.848111	7.687814	16.905293
N	-1.682890	8.218560	16.479071
H	-10.276059	6.639483	18.716639
H	-7.810001	8.795888	21.360612
H	-8.061209	6.990363	13.425155
H	-7.712463	3.072658	15.170322
H	-11.503066	5.090108	15.155390
H	-8.596927	7.942139	15.671933
H	-7.019545	7.169809	15.659563
H	-10.452045	5.190115	17.368735
H	-10.596171	6.805667	16.667073
H	-7.920062	4.509861	13.140901
H	-6.627599	5.091823	14.184410
H	-9.964094	3.378625	14.143166
H	-10.096524	3.175339	15.892218
H	-6.808994	4.747612	16.742878
H	-8.256750	4.017420	17.413578
H	-10.445051	7.101963	14.142751
H	-10.174029	5.695399	13.111170
H	-10.955024	7.044111	21.165480
H	-10.981852	8.735489	20.669307
H	-10.019005	8.245209	22.065229
H	-4.697371	11.057470	22.591381
H	-3.240317	10.927307	18.548300
H	-2.326194	7.723287	21.270865
H	-6.489981	10.389824	21.050585
H	-6.072228	9.082004	22.163568

H	-4.737557	7.110077	21.356219
H	-4.104251	7.051669	19.717669
H	-3.010946	11.801567	20.881559
H	-4.664111	12.014083	20.297452
H	-1.631246	9.834528	20.118006
H	-2.296180	8.662201	18.980158
H	-4.703298	9.010380	18.066121
H	-5.669413	10.349583	18.674812
H	-3.751832	8.799480	23.026679
H	-2.468887	9.892834	22.501222
H	1.102813	2.837280	19.831256
H	-2.402236	2.167377	22.081307
H	0.914699	7.375323	16.506147
H	-0.150677	3.843963	14.295273
H	3.439661	3.894733	16.662837
H	-0.851620	6.163038	17.720041
H	0.632833	6.123862	18.655273
H	2.098636	4.116409	18.699937
H	1.655511	2.651884	17.813906
H	0.834873	6.139274	14.342156
H	-0.733244	6.115032	15.136697
H	1.813775	2.633722	15.263100
H	2.341678	4.087810	14.411652
H	-0.430852	2.590653	16.444949
H	-1.507417	3.975587	16.337583
H	2.968156	6.175900	15.718930
H	2.884211	6.175199	17.482080
H	-0.380786	1.250607	22.874654
H	0.946514	2.391433	22.633024
H	0.864123	0.922735	21.662282
H	-6.430330	0.607910	21.225188
H	-5.972042	4.208384	23.541676
H	-7.305780	4.438284	19.472133

H	-4.585169	1.332465	19.722244
H	-4.055525	1.224788	21.387022
H	-4.947930	5.079736	19.671591
H	-5.122822	3.595709	18.684861
H	-7.312207	2.180228	22.958818
H	-5.636286	1.743702	23.297262
H	-7.862737	4.421781	21.897756
H	-6.581573	5.572016	21.534426
H	-4.142104	4.958916	22.023219
H	-3.773466	3.422275	22.782436
H	-7.010557	1.963863	19.213876
H	-8.125553	2.323657	20.532095
H	-3.241007	5.812442	10.419735
H	-3.380086	1.881086	11.938716
H	-2.053028	9.821551	14.097722
H	-6.325398	9.370473	13.803741
H	-3.954289	9.831183	10.247029
H	-2.667721	7.442960	14.402837
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194

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191

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H	-2.566679	-0.461316	16.974193

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