Supporting Information for:

Charge Control of the Inverse *trans*-Influence

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General Considerations

All air- and moisture-sensitive experiments were performed under dry nitrogen atmosphere using standard Schlenk techniques or 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. Silver hexafluoroantimonate was purchased from Acros and used without further purification. $[((^{t\text{-Bu}}ArO)_3tacn)U^{V}(NSiMe_3)]$[1] (**1-*t*-Bu**) and $[((^{Ad}ArO)_3tacn)U^{V}(NSiMe_3)]$[2] (**1-Ad**) were synthesized according to literature procedures. ^1H NMR spectra were recorded on a JEOL ECX 400 instrument at a probe temperature of 23 °C. Chemical shifts, δ, are reported relative to residual ^1H resonances of the solvent in ppm, followed by peak multiplicity (s: singlet, d: doublet, q: quintet, m: multiplet), coupling constant in Hertz, integration value and proton assignment. Electronic absorption spectra were recorded from 250 to 2200 nm (Shimadzu, UV-3600) in the indicated solvent at room temperature. Infrared spectra were recorded on a Shimadzu Affinity-1 CE FTIR instrument from 400 to 4000 cm^{-1}. Solid samples of the compounds were homogenized with excess amount of KBr and a pressed pellet was measured at room temperature. The peaks are listed reporting wavenumber [cm^{-1}] and intensity (vw: very weak; w: weak; m: medium; s: strong; vs: very strong; br: broad). Elemental analyses were obtained using Euro EA 3000 (Euro Vector) and EA 1108 (Carlo-Erba) elemental analyzers in the Chair of Inorganic Chemistry at the University Erlangen-Nuremberg (Erlangen, Germany).

Synthetic and Spectroscopic Details

Synthesis of [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ (2-*t*-Bu)

A 20 mL scintillation vial charged with a brown solution of 0.221 g (0.200 mmol) [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{V}(NSiMe$_3$)] (**1-*t*-Bu**) in 10 mL cold methylene chloride. While stirring, a solution of 0.069 g (0.200 mmol, 1.0 eq.) silver hexafluoroantimonate in methylene chloride was added dropwise. The reaction mixture turned black instantaneously and was allowed to stir while warming up to room temperature for 60 minutes. The dark grayish precipitate was filtered off over celite on a glass frit, which was washed with methylene chloride. The volatiles of the filtrate were removed *in vacuo* to give 0.262 g (0.195 mmol, 97 %) of [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ as a deep black-brown powder. Elemental analysis for $C_{54}H_{87}F_6N_4O_3SbSiU \cdot 1/5\ CH_2Cl_2$ calc./found: C: 47.90/47.90; H: 6.48/6.36; N: 4.12/4.12. ^{1}H NMR, benzene-d_6, 400 MHz, δ [ppm]: 7.97 (d, J = 2.6 Hz, 3H, C_{ar}-*H*), 7.58 (d, J = 2.3 Hz, 3H, C_{ar}-*H*), 6.66 (d, J = 7.0 Hz, 3H, benzyl-*H*), 4.88 (d, J = 14.0 Hz, 3H, benzyl-*H*), 3.59 (unres. dd, J = 14.0 H, 3H, tacn-*H*), 3.05-2.90 (m, 3H, tacn-*H*), 2.90-2.75 (m, 3H, tacn-*H*), 2.25-2.05 (m, 3H, tacn-*H*), 1.83 (br s, 27H, *t*-Bu), 1.32 (br s, 27H, *t*-Bu), –0.22 (s, 9H, SiMe$_3$-*H*). IR, $\bar{\nu}$ [cm^{-1}]: 2957 (vs), 2905 (s), 2868 (s), 2112 (w), 2079 (w), 1601 (w), 1472 (s, br), 1443 (s), 1410 (m), 1393 (m), 1362 (m), 1376 (vw), 1362 (m), 1342 (w), 1306 (m), 1233 (vs, br), 1204 (s), 1169 (vs), 1128 (m), 1096 (m), 1059 (w), 1024 (w), 1003 (w), 984 (vw), 947 (vw), 916 (w, br), 881 (m, br), 839 (vs), 810 (m), 779 (w), 746 (s), 660 (vs), 613 (vw), 590 (vw), 538 (m), 507 (vw), 451 (m), 436 (w), 420 (vw).

Synthesis of [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ (2-Ad)

A 20 mL scintillation vial charged with a brown solution of 0.268 g (0.200 mmol) [((^{Ad}ArO)$_3$tacn)U^{V}(NSiMe$_3$)] (**1-Ad**) in 10 mL cold methylene chloride. While stirring, a solution of 0.069 g (0.200 mmol, 1.0 eq.) silver hexafluoroantimonate in methylene chloride was added dropwise. The reaction mixture turned black instantaneously and was allowed to stir while warming up to room temperature for 60 minutes. The dark grayish precipitate was filtered off over celite on a glass frit, which was washed with methylene chloride. The volatiles of the filtrate were removed *in vacuo* to give 0.304 g (0.193 mmol, 96 %) of [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ as a deep black-brown powder. Elemental analysis for $C_{72}H_{105}F_6N_4O_3SbSiU$ calc./found: C: 54.85/55.13; H: 6.71/6.43; N: 3.55/3.75.

^{1}H NMR, benzene-d_6, 400 MHz, δ [ppm]: 8.01 (d, J = 1.9 Hz, 3H, C_{ar}-*H*), 7.73 (unres. d, 3H, Car-H), 5.37 (dd, J = 14 Hz, 3.7 Hz, 3H, benzyl-H), 4.00 (unres. dd, J = 14 Hz, 3H, benzyl-H), 3.67 (br d, J = 10.6 Hz, 3H, tacn-H), 3.3-3.0 (m, 3H, tacn-H), 3.0-2.8 (m, 3H, tacn-H), 2.89 (d, J = 11.9 Hz, 3H, Ad-H), 2.68 (d, J = 11.9 Hz, 3H, Ad-H), 2.15 (br s,9H, Ad-H), 1.81 (d, J = 11.9 Hz, 9H, Ad-H), 1.65 (d, J = 11.9 Hz, 9H, Ad-H), 1.38 (s, 27H, t-Bu), –0.12 (s, 9H, $SiMe_3$-*H*). 3 tacn protons cannot be located due to the fact that they lay under the adamantyl-H-signals between 1.6 and 1.9 ppm. IR, $\tilde{\nu}$ [cm^{-1}]: 2953 (vs), 2901 (vs, br), 2849 (vs), 2077 (m), 1601 (w), 1466 (vs, br), 1450 (vs, br), 1412 (m), 1395 (m), 1362 (m), 1342 (m), 1304 (m, br), 1285 (m), 1244 (s), 1205 (vs, br), 1157 (vw), 1128 (m), 1103 (m), 1094 (m), 1080 (w), 1057 (w), 1024 (vw), 1001 (w), 986 (w), 972 (w), 939 (w), 920 (m), 907 (m), 878 (m), 837 (vs), 804 (s), 772 (s), 750 (m), 729 (s), 660 (vs, br), 640 (m), 608 (vw), 581 (vw), 538 (m), 482 (w), 467 (w), 447 (m), 420 (w).

1-*t*-Bu and 1-Ad IR reference

1-*t*-Bu $\tilde{\nu}$ [cm^{-1}]: 2953 (vs), 2903 (vs), 2866 (vs), 2077 (m), 1603 (w), 1472 (vs, br), 1441 (vs), 1412 (s), 1391 (m), 1377 (w), 1360 (s), 1342 (m), 1306 (vs), 1261 (vs, br), 1238 (vs), 1204 (s), 1169 (s), 1132 (s), 1103 (m), 1063 (w), 1026 (w), 986 (s, br), 935 (m, br), 914 (m), 889 (m), 878 (s), 837 (vs, br), 810 (s), 783 (m), 764 (m), 745 (s), 699 (vw), 679 (vw), 646 (vw), 611 (w), 588 (vw), 532 (s), 444 (s). Only slight differences with **2-*t*-Bu** were visible, the Sb-F-stretch in **2-*t*-Bu** could be assigned at 660 cm^{-1}.

1-Ad $\tilde{\nu}$ [cm^{-1}]: 2951 (s), 2903 (vs), 2847 (s), 2081 (m), 1603 (w), 1466 (s, br), 1412 (m), 1393 (w), 1360 (m), 1343 (m), 1302 (m), 1283 (m), 1261 (s), 1252 (s), 1215 (s), 1182 (w), 1161 (vw), 1132 (m), 1103 (m), 1080 (w), 1063 (w), 1080 (vw), 1001 (w), 974 (w), 988 (m), 928 (m, br), 918 (w), 876 (m, br), 835 (s), 804 (m), 772 (m), 758 (w), 729 (m), 696 (vw), 671 (vw), 652 (vw), 640 (vw), 604 (vw), 532 (m), 480 (vw), 465 (w), 442 (m), 420 (m). Only slight differences with **2-Ad** were visible, the Sb-F-stretch could be assigned in **2-Ad** at 660 cm^{-1}.

Absorption Spectroscopy

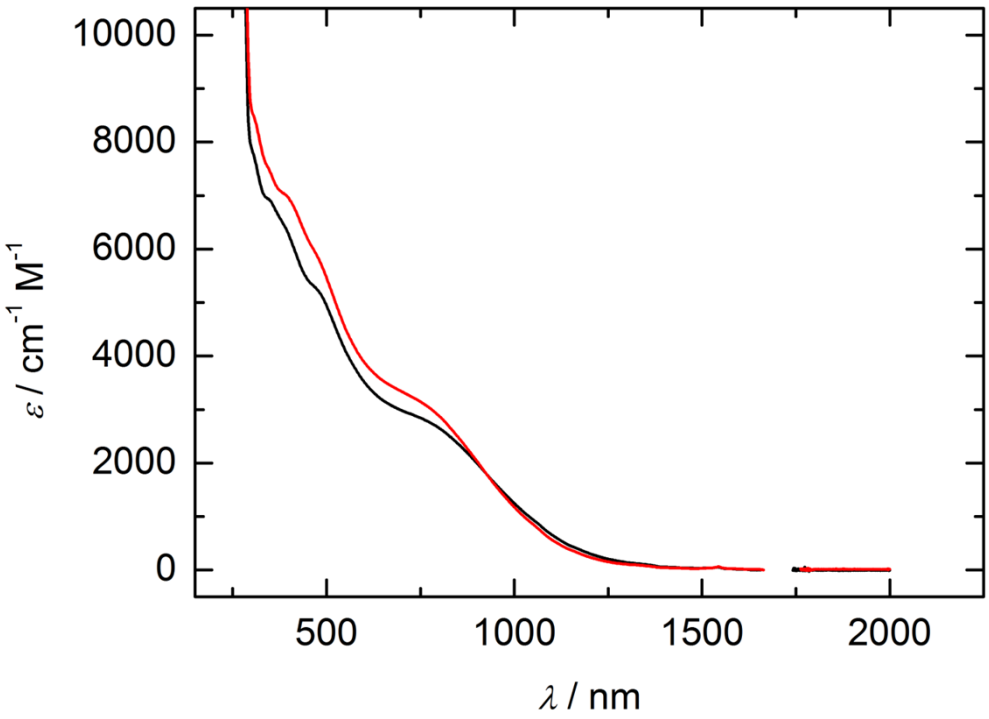


Figure 1: UV/vis/NIR spectra of **2-*t*-Bu** in toluene with c = 2.49·10^{-4} M (black), and **2-Ad** in toluene with c = 2. 42·10^{-4} M (red).

X-Ray Crystal Structure Determinations

CCDC-894627 (for **2-Ad**), CCDC-894628 (for **2- *t*-Bu**), and CCDC-747048 (for **3-Ad**) 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).

Crystallographic Details for [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ (2-*t*-Bu)

Single crystals for X-ray diffraction analysis were obtained by slow diffusion of *n*-hexane into a concentrated solution of [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ and NaSbF$_6$ in dimethoxyethane (DME) as [(($^{t\text{-Bu}}$ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ · 0.5 [Na(DME)$_3$]SbF$_6$ · 1.5 DME in form of violet-brown plates. A suitable single crystal of approximately 0.18 × 0.12 × 0.02 mm³ size was coated with protective perfluoropolyether oil and mounted on a MiTeGen micromount. Intensity data were collected at 100 K on a Bruker Kappa APEX 2 *IμS* duo diffractometer using MoK_α radiation (λ = 0.71073 Å) and QUAZAR focussing Montel optics. Data were corrected for Lorentz and polarization effects. A semi empirical absorption correction was applied on the basis of multiple scans (SADABS 2008/1).[3] The structure was solved by direct methods and refined by full-matrix least-squares procedures on F^2 (SHELXTL NT 6.12).[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to the equivalent isotropic displacement parameter of the corresponding carrier atom by a factor of either 1.2 or 1.5. The asymmetric unit of the crystal structure contained two independent molecules of the complex salt, one molecule of the [Na(DME)$_3$]SbF$_6$ salt and three disordered molecules of DME. The two independent uranium complex cations as well as the solvated [Na(DME)] cation were situated on crystallographic threefold axes. In both of the independent uranium complex cations one of the *t*-Bu groups is disordered. Two preferred orientations were refined in each case with resulting site occupancies of 76.8(9) and 23.2(9) % for c15 – C17 and C15A – C17A and of 76.7(9) and 23.3(9) % for C33 – C35 and C33A – C35A, respectively. The independent SbF$_6$ anion is also disordered with two preferred orientation for the equatorial positions. The refinement resulted in site occupancies of 53(2) and 47(2) % for the affected atoms F13 – F16 and F13A – F16A.

The independent DME solvate molecule is disordered around a threefold axis. Two alternative orientations were refined resulting in site occupancies of 69.8(8) and 30.2(8) % for C201 – C206 and C211 – C216, respectively. SIMU, ISOR, and SAME restraints were applied in the refinement. Crystallographic data, data collection, and refinement details are summarized in Table 1.

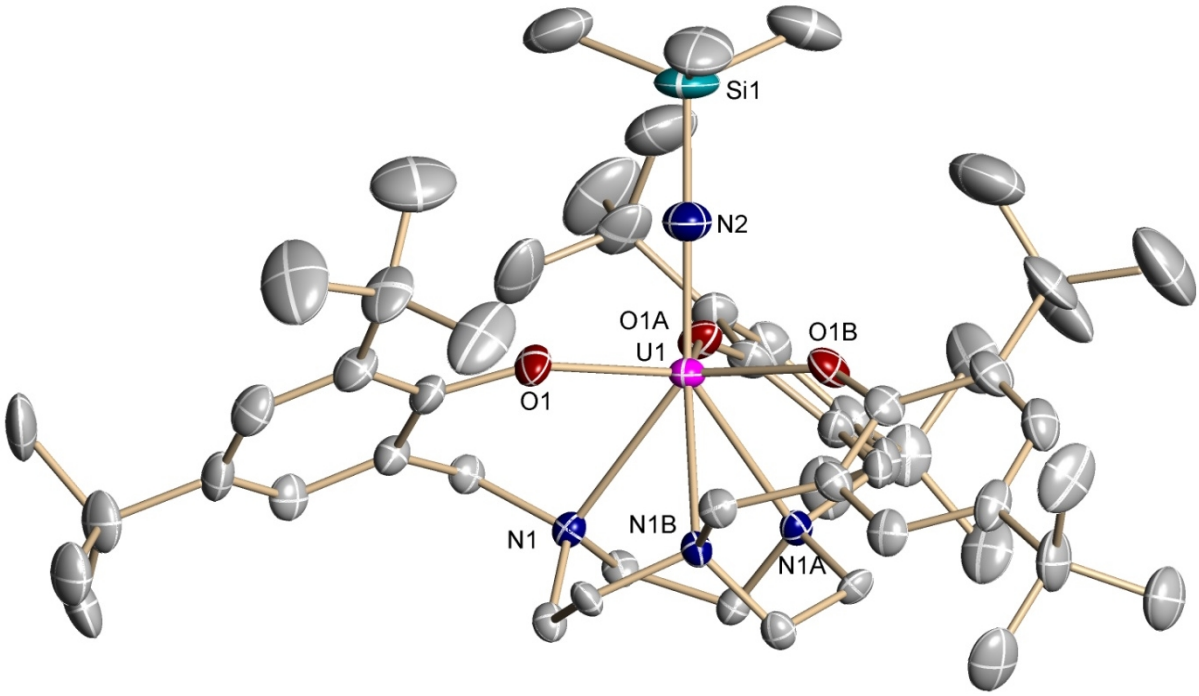


Figure 2: Molecular structure of the cation of $[((^{t\text{-Bu}}ArO)_3tacn)U^{VI}(NSiMe_3)]SbF_6$ (**2-*t*-Bu**) in crystals of $[((^{t\text{-Bu}}ArO)_3tacn)U^{VI}(NSiMe_3)]SbF_6 \cdot 0.5\ [Na(DME)_3]SbF_6 \cdot 1.5$ DME (**2-*t*-Bu · 0.5 [Na(DME)$_3$]SbF$_6$ · 1.5 DME**), counterion, co-crystallized $[Na(DME)_3]SbF_6$ and solvent molecules as well as hydrogen atoms omitted for clarity.

Crystallographic Details for [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ (2-Ad)

Single crystals for X-ray diffraction analysis were obtained by slow diffusion of *n*-hexane into a concentrated solution of [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]SbF$_6$ in toluene as [((^{Ad}ArO)$_3$tacn)U^{VI}-(NSiMe$_3$)]SbF$_6$ · 2.5 toluene · 0.5 *n*-hexane in form of black prisms. A suitable single crystal of approximately 0.18 × 0.12 × 0.06 mm³ size was coated with protective perfluoropolyether oil and mounted on a glass fibre. Intensity data were collected at 150 K on a Bruker Nonius KappaCCD diffractometer using graphite monochromatized MoK_α radiation (λ = 0.71073 Å). Data were corrected for Lorentz and polarization effects. A semi empirical absorption correction was applied on the basis of multiple scans (SADABS 2.10).[3] The structure was solved by direct methods and refined by full-matrix least-squares procedures on F^2 (SHELXTL NT 6.12).[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to the equivalent isotropic displacement parameter of the corresponding carrier atom by a factor of either 1.2 or 1.5. Part of the ligand is subjected to disorder. Two alternative orientations of one of the *t*-BuPh moieties were refined resulting in site occupancies of 64.7(7) % for C50 – C55, C66 – C69 and 35.3(7) % for C50A – C55A, C66A – C69A, respectively. Another *t*-Bu-group of the ligand shows rotational disorder. Two alternative orientations of this group were refined with site occupancies of 66(2) % for C46 – C48 and 34(2) % for C46A – C48A. The compound crystallized with a total of 2.5 molecules of toluene and 0.5 molecules of *n*-hexane. 1.5 toluene molecules were disordered over three alternative sites with occupancies of 62.9(9) % for C201 – C207, 38.0(9) % for C211 – C217 and 49.1(9) % for C301 – C307. The *n*-hexane molecule is situated on a crystallographic inversion centre. SIMU, ISOR, SAME, FLAT, and DFIX restraints were applied in the refinement. Crystallographic data, data collection, and refinement details are summarized in Table 1.

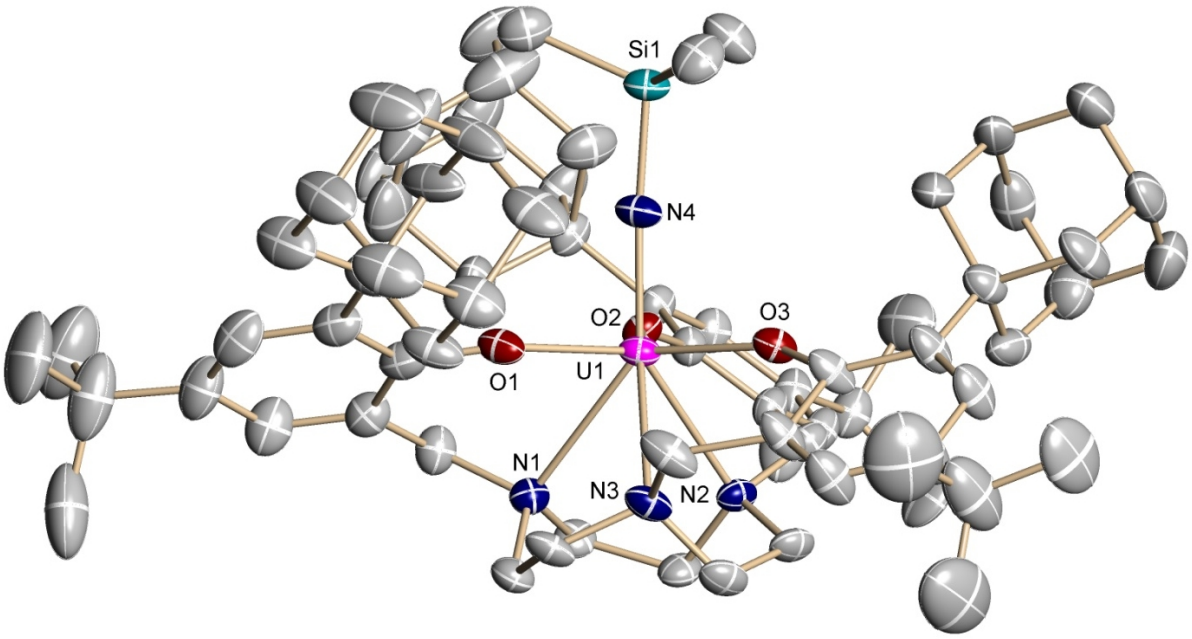


Figure 3: Molecular structure of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]SbF_6$ (**2-Ad**) in crystals of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]SbF_6 \cdot 2.5$ toluene $\cdot$ 0.5 *n*-hexane (**2-Ad · 2.5 toluene · 0.5 *n*-hexane**), co-crystallized solvent molecules and hydrogen atoms omitted for clarity.

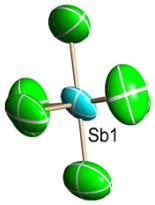


Figure 4: Molecular structure of the SbF_6^--counterion of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]SbF_6$ (**2-Ad**).

Crystallographic Details for [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)]BPh$_4$ (3-Ad)

The oxidation of [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)] (**1-Ad**) was also achieved by reaction with 1 equiv. of AgBPh$_4$ in cold toluene. Single crystals for X-ray diffraction analysis were obtained by slow diffusion of *n*-pentane into a concentrated solution of [((^{Ad}ArO)$_3$tacn)U^{VI}-(NSiMe$_3$)]BPh$_4$ in methylene chloride and acetonitrile as [((^{Ad}ArO)$_3$tacn)U^{VI}(NSiMe$_3$)] BPh$_4$ · CH$_2$Cl$_2$ · 0.5 C$_5$H$_{12}$ in form of dark brown to black blocks. A suitable single crystal of approximately 0.23 × 0.18 × 0.18 mm³ size was coated with protective perfluoropolyether oil and mounted on a glass fibre. Intensity data were collected at 150 K on a Bruker-Nonius KappaCCD diffractometer using graphite monochromatized MoK_α radiation. Data were corrected for Lorentz and polarization effects. A semi empirical absorption correction was applied on the basis of multiple scans (SADABS 2.10).[3] The structure was solved by direct methods and refined using blocked matrix least-squares procedures on F^2 (SHELXTL NT 6.12).[4] All non-hydrogen atoms were refined anisotropically. The compound crystallized with one molecule of methylene chloride and half a molecule of *n*-pentane in the unit. This solvent molecule is located on an inversion centre and disordered with 50% occupancy. DFIX, SIMU, and ISOR restraints were applied in the refinement of the disorder. According to a PLATON-analysis, additional voids in the structure are accessible for further solvent molecules. A following SQUEEZE treatment resulted only in three remaining electrons per unit cell, which allows for the conclusion that co-crystallized solvent already evaporated from these positions in the structure. Hydrogen atoms were placed in positions of optimized geometry, their isotropic displacement parameters were tied to the equivalent isotropic displacement parameter of the corresponding carrier atom by a factor of either 1.2 or 1.5. Crystallographic data, data collection, and refinement details are summarized in Table 1.

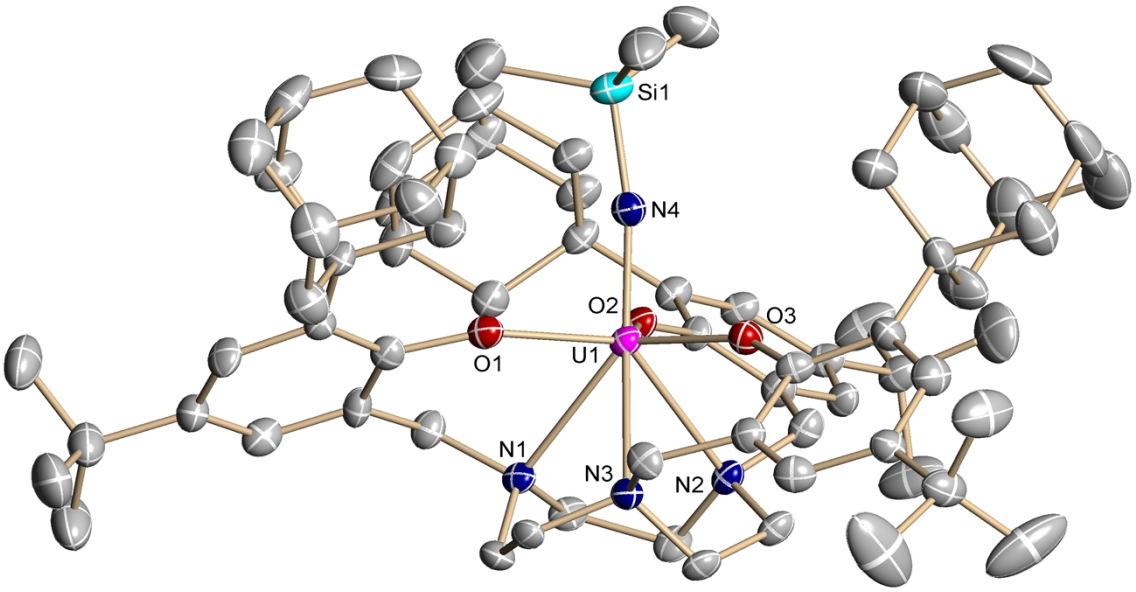


Figure 5: Molecular structure of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]BPh_4$ (**3-Ad**) in crystals of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]BPh_4 \cdot CH_2Cl_2 \cdot 0.5\ C_5H_{12}$ (**3-Ad · CH_2Cl_2 · 0.5 C_5H_{12}**), counterion, co-crystallized solvent molecules and hydrogen atoms omitted for clarity.

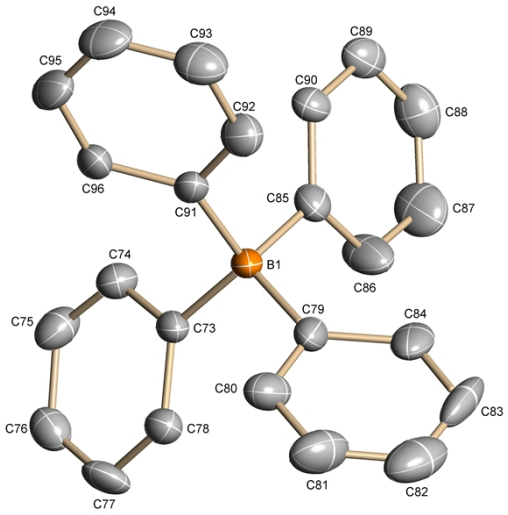


Figure 6: Structure of the BPh_4^--counterion of $[((^{Ad}ArO)_3tacn)U^{VI}(NSiMe_3)]BPh_4$ (**3-Ad**), hydrogen atoms omitted for clarity.

Table 1: Crystallographic data, data collection, and refinement details for **2-*t*-Bu · 0.5 [Na(DME)$_3$]SbF$_6$ · 1.5 DME**, **2-Ad · 2.5 toluene · 0.5 *n*-hexane**, and **3-Ad · CH_2Cl_2 · 0.5 C_5H_{12}**.

	2-*t*-Bu	**2-Ad**	**3-Ad**
Empirical formula	$C_{66}H_{117}F_9N_4Na_{0.5}O_9Sb_{1.5}SiU$	$C_{92.50}H_{132}F_6N_4O_3SbSiU$	$C_{99.50}H_{133}BCl_2N_4O_3SiU$
Mol. weight	1741.88	1849.89	1780.93
Crystal size [mm^3]	0.18×0.12×0.02	0.18×0.12×0.06	0.23×0.18×0.18
Wavelength [Å]	0.71073	0.71073	0.71073
Temperature [K]	100	150	150
Crystal system	trigonal	monoclinic	triclinic
Space group	*R*3 (no. 146)	$P2_1/c$ (no. 14)	*P*–1 (No. 2)
a [Å]	14.928(2)	19.293(4)	16.1844(7)
b [Å]	14.928(2)	16.638(3)	17.476(3)
c [Å]	63.398(11)	28.095(5)	19.116(3)
α [°]	90	90	94.215(13)
β [°]	90	101.198(11)	95.920(6)
γ [°]	120	90	111.501(5)
V [Å^3]	12234(3)	8847(3)	4967(2)
Z	6	4	2
ρ_{calc} [g/cm^3]	1.419	1.389	1.191
μ [mm^{-1}]	2.563	2.209	1.746
F (000)	5292	3800	1854
2θ interval [°]	$5.4 \le 2\theta \le 54.2$	$6.3 \le 2\theta \le 54.2$	$6.9 \le 2\theta \le 54.0$
Limiting Indices	$-19 \le h \le 18$ $-19 \le k \le 19$ $-81 \le l \le 81$	$-24 \le h \le 24$ $-21 \le k \le 21$ $-36 \le l \le 36$	$-20 \le h \le 20$ $-22 \le k \le 22$ $-24 \le l \le 24$
Completeness to	θ = 27.09°: 99.9 %	θ = 27.10°: 99.8 %	θ = 27.00°: 99.6 %
Collected reflections	65892	139819	104736
Independent reflections; R_{int}	12037; 0.0768	19494; 0.0661	21620; 0.1335
No. restraints/ refined parameters	274 / 721	616 / 1170	61 / 1036
wR_2 (all data)	0.0734	0.1136	0.1246
R_1 [$I \ge 2\sigma(I)$]	0.0346	0.0480	0.0560
GooF on F^2	1.019	1.084	0.985
$\Delta\rho_{max/min}$ [e.Å^3]	0.783 / –0.872	1.967 / –1.816	1.648 / –0.964

Computational Details

General Method

In order to investigate possible ITI effects (or their absence) in **2-*t*-Bu** and **2-Ad**, restricted geometry optimisations were performed for the cationic, uranium-containing full models of **2-*t*-Bu** and **2-Ad** with axial (**2-*t*-Bu$_{ax}$** and **2-Ad$_{ax}$**) and equatorial (**2-*t*-Bu$_{eq}$** and **2-Ad$_{eq}$**) isomers using coordinates derived from the X-ray crystal structures as a start point. Despite exhaustive attempts, **2-Ad$_{eq}$** suffered extensive convergence problems and could not be converged. We suggest this reflects the sterically highly unfavourable environment resulting from the bulky adamantyl groups. No constraints were imposed on the structures during the geometry optimisations. The calculations were performed using the Amsterdam Density Functional (ADF) suite version 2010.01.[5,6] The DFT geometry optimisations employed Slater type orbital (STO) triple-ζ-plus polarisation all-electron basis sets (from the ZORA/TZP database of the ADF suite). Scalar relativistic approaches were used within the ZORA Hamiltonian for the inclusion of relativistic effects and the local density approximation (LDA) with the correlation potential due to Vosko *et al.*[7] was used in all of the calculations. Gradient corrections were performed using the functionals of Becke[8] and Perdew.[9] MOLEKEL[10] was used to prepare the three-dimensional plots of the electron density.

Table 2: Calculated bond lengths and Nalewajski-Mrozek bond indices for **2-*t*-Bu$_{ax}$**, **2-*t*-Bu$_{eq}$**, and **2-Ad$_{ax}$**.

Entry	Calculated bond lengths and Nalewajski-Mrozek bond indices in parentheses						
	U=N	U–O	U–O	U–O	U–N	U–N	U–N
2-*t*-Bu$_{ax}$	1.9122	2.1677	2.1677	2.1675	2.7248	2.7244	2.7250
	(2.71)	(1.30)	(1.30)	(1.30)	(0.44)	(0.44)	(0.44)
2-*t*-Bu$_{eq}$	1.9294	2.1327*	2.1100	2.1757	2.7078	2.6505	2.8246
	(2.67)	(1.41)	(1.41)	(1.27)	(0.41)	(0.41)	(0.39)
2-Ad$_{ax}$	1.9143	2.1637	2.1611	2.1722	2.7219	2.7112	2.6829
	(2.70)	(1.30)	(1.30)	(1.28)	(0.44)	(0.44)	(0.45)

* Trans to the imido group.

Although data for the hypothetical **2-Ad$_{eq}$** could not be obtained, the geometry optimized structures of **2-*t*-Bu$_{ax}$** and **2-*t*-Bu$_{eq}$** provide an opportunity to assess any possible ITI effects. The calculated parameters closely match those where experimental data are available, Table 2, and we thus conclude that the calculations provide qualitative models. Notably, in **2-*t*-Bu$_{eq}$** the $O_{aryloxide}$–U–N_{imido} angle is calculated to be 150.3°, which would be expected to disfavour any ITI effects on the basis of data obtained for related oxo-complexes.[11] Furthermore, there is no discernible trend regarding U=N and U–O bond lengths with respect to an axial or equatorial isomer as was the case with related oxo-complexes.[11]

Table 3: Calculated Mulliken charges for **2-*t*-Bu$_{ax}$**, **2-*t*-Bu$_{eq}$**, and **2-Ad$_{ax}$**.

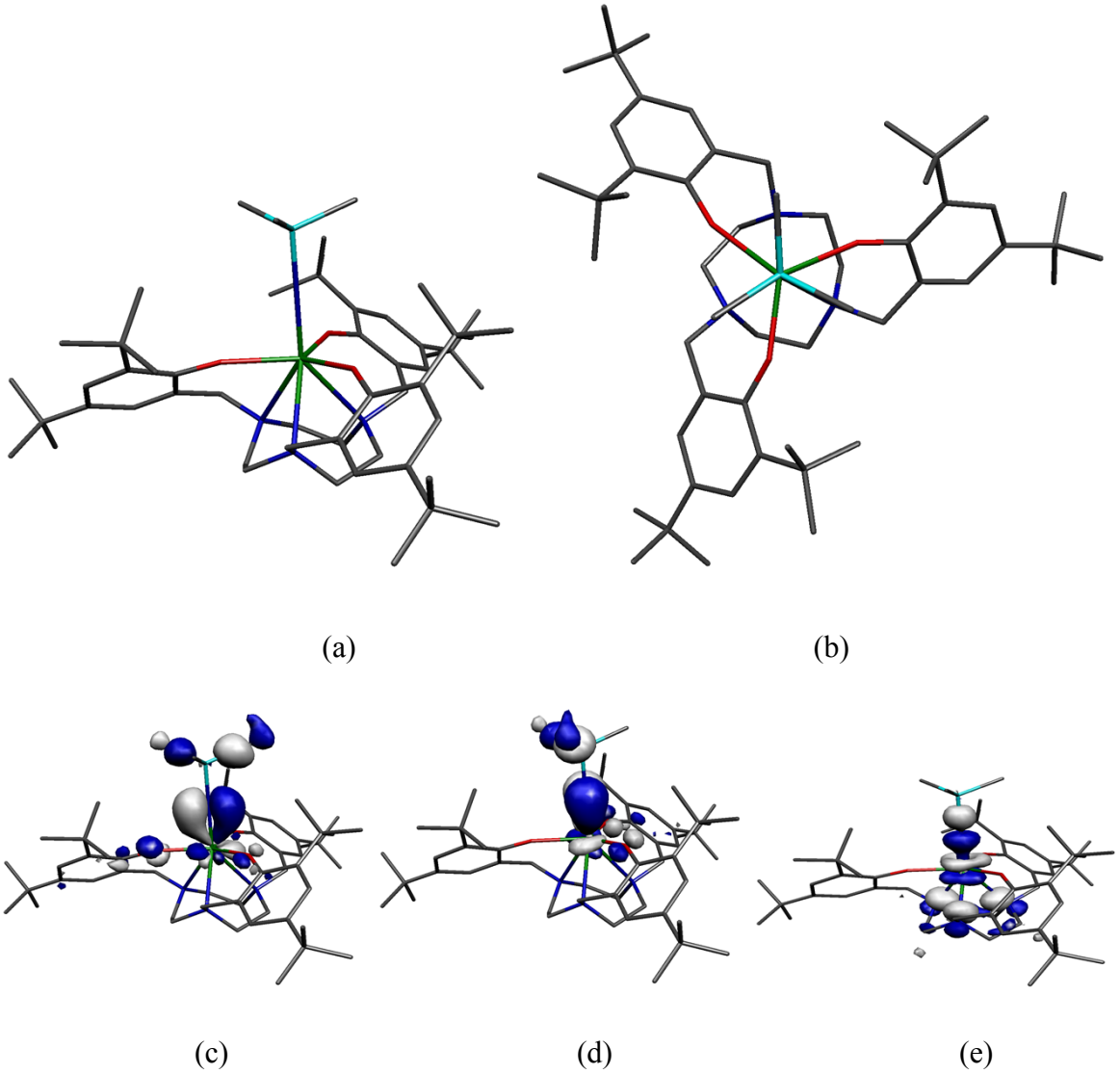
Entry	Calculated Mulliken charges							
	U	$TMSN^{2-}_{imido}$	O	O	O	N	N	N
2-*t*-Bu$_{ax}$	+2.61	–0.52	−0.76	−0.76	−0.76	−0.75	−0.75	−0.75
2-*t*-Bu$_{eq}$	+2.58	–0.57	−0.72*	−0.72	−0.77	−0.75	−0.80	−0.73
2-Ad$_{ax}$	+2.68	–0.65	−0.79	−0.78	−0.78	−0.75	−0.76	−0.77

* Trans to the imido group.

The calculated charges, Table 3, also show little variation, and certainly no systematic variation that might be anticipated from any ITI effects. The calculations reveal that **2-*t*-Bu$_{ax}$** is more stable than **2-*t*-Bu$_{eq}$** by ~11 kcal mol^{-1}, which is entirely in line with the observation that only **2-*t*-Bu$_{ax}$** can be isolated experimentally. The convergence issues for **2-Ad$_{eq}$** suggest that the axial isomer is more stable than the equatorial congener by at least ~11 kcal mol^{-1} and most likely by a substantially larger value. Thus, the calculations entirely reproduce the experimentally observed outcomes. The calculated charge for the $TMSN^{2-}$ is the sum for the constituent atoms in the corresponding molecule.

Final Geometry and Selected Kohn Sham Molecular Orbitals for 2-*t*-Bu$_{ax}$

(Hydrogen atoms omitted for clarity)



(a) (b)

(c) (d) (e)

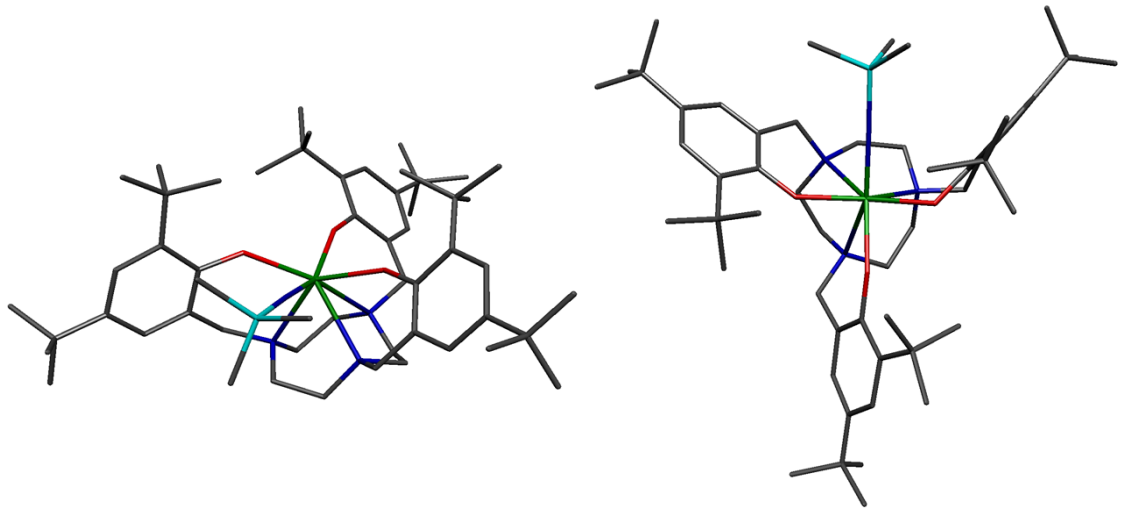
(a) Optimised structure – side view; (b) Optimised structure – top view;

(c) HOMO–6 (–8.218 eV); (d) HOMO–7 (–8.220 eV); (e) HOMO–8 (–8.720 eV).

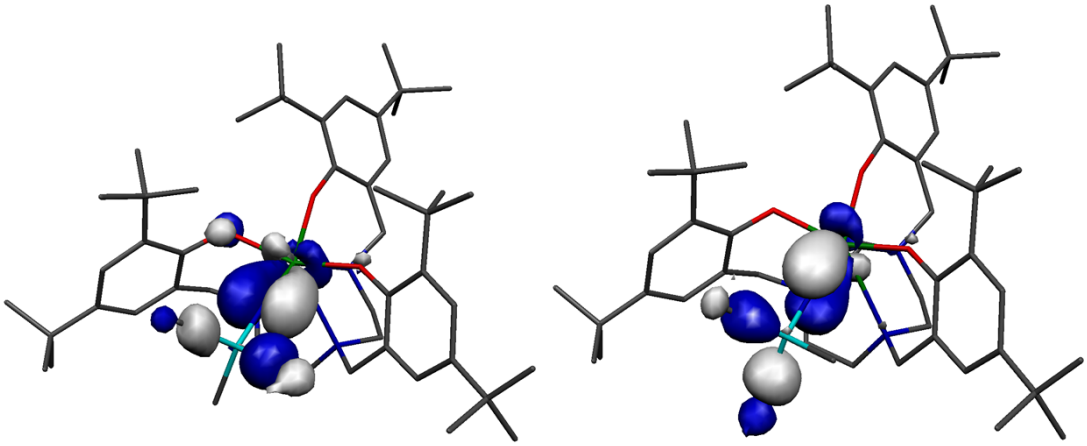
HOMOs –6 and –7 are quasi-degenerate. The U=N σ-bond is delocalised over several MOs, but is most clearly visualised in HOMO–8.

Final Geometry and Selected Kohn Sham Molecular Orbitals for 2-*t*-Bu$_{eq}$

(Hydrogen atoms omitted for clarity)



(a) (b)



(c) (d)

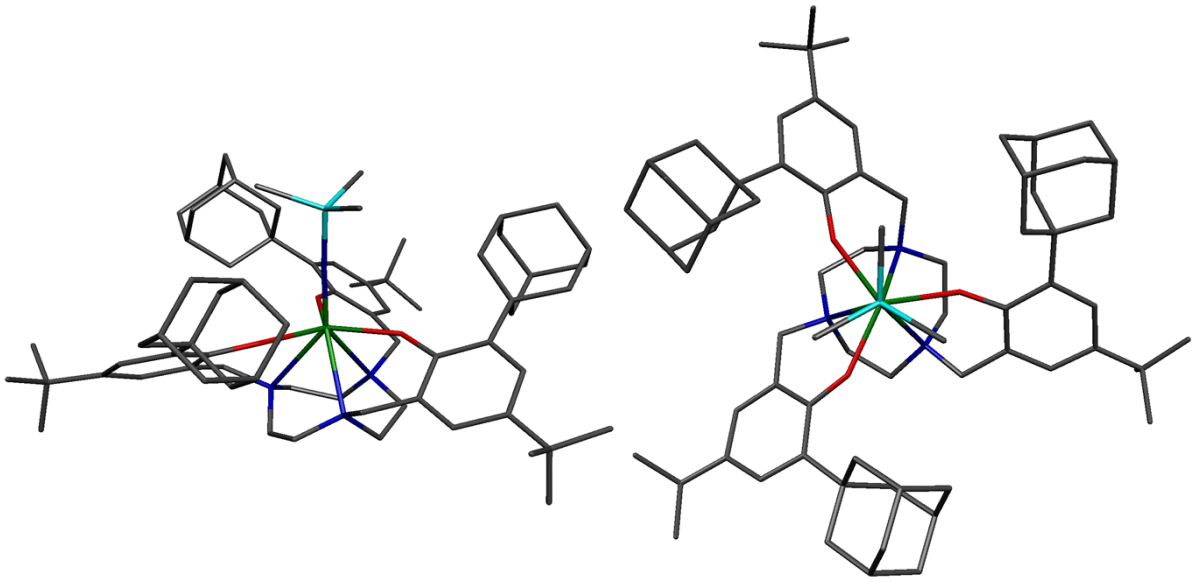
(a) Optimised structure – side view; (b) Optimised structure – top view;

(c) HOMO–6 (–8.260 eV); (d) HOMO–7 (–8.732 eV).

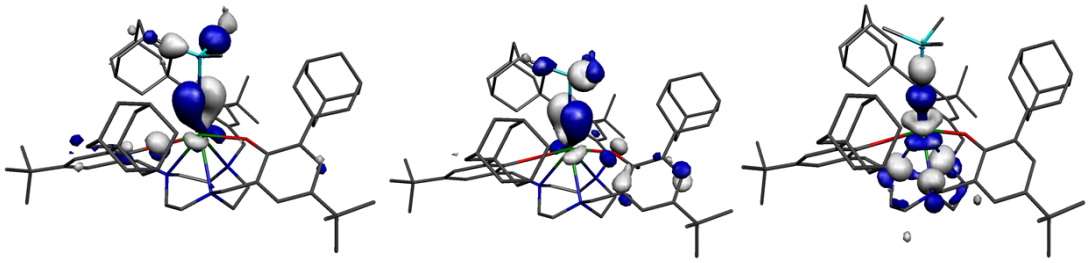
HOMOs –6 and –7 are no-longer quasi-degenerate. The U=N σ-bond is delocalised over several MOs to such an extent that no one MO visualises it clearly.

Final Geometry and Selected Kohn Sham Molecular Orbitals for 2-Ad_{ax}

(Hydrogen atoms omitted for clarity)



(a) (b)



(c) (d) (e)

(a) Optimised structure – side view; (b) Optimised structure – top view;

(c) HOMO–6 (–8.082 eV); (d) HOMO–7 (–8.101 eV); (e) HOMO–17 (–8.634 eV).

HOMOs –6 and –7 are quasi-degenerate. The U=N σ-bond is delocalised over several MOs, but is most clearly visualised in HOMO–17.

Final Calculated Coordinates and Single Point Energy for Geometry Optimized 2-*t*-Bu$_{ax}$

Atom	X	Y	Z [Å]
1.H	-4.763159	-5.025428	-3.348553
2.H	-1.970742	6.638300	-3.347555
3.H	6.733489	-1.612569	-3.347902
4.H	-0.844453	-0.864152	-3.679055
5.H	-0.326342	1.162991	-3.679559
6.H	1.171709	-0.299579	-3.679032
7.H	-6.045292	-6.159926	-2.881682
8.H	-2.311625	8.315934	-2.880359
9.H	8.357096	-2.156108	-2.881456
10.H	-2.626721	0.611187	-3.197580
11.H	0.783997	-2.579642	-3.198397
12.H	1.843364	1.968742	-3.196660
13.H	-4.426920	6.082990	-2.685916
14.H	-3.053719	-6.875251	-2.685331
15.H	7.482151	0.791485	-2.685954
16.H	-1.702135	-2.249760	-3.009311
17.H	-1.097343	2.598582	-3.009792
18.H	2.800196	-0.349226	-3.008418
19.C	-5.381525	-5.368928	-2.506224
20.C	-1.958788	7.345437	-2.505103
21.C	7.340264	-1.976673	-2.505875
22.H	-4.609446	7.807318	-2.279568
23.H	-4.455596	-7.895838	-2.278925
24.H	9.066363	0.087072	-2.278642
25.C	-0.755371	1.583074	-2.760559
26.C	-0.993700	-1.445828	-2.760095
27.C	1.749568	-0.137956	-2.759737
28.H	-6.020796	-4.535878	-2.181088
29.H	-0.917689	7.481995	-2.179943
30.H	6.938145	-2.946742	-2.180908
31.C	-4.321528	6.823776	-1.879905
32.C	-3.748233	-7.154115	-1.879482
33.C	8.070398	0.329639	-1.879604
34.C	-1.966880	0.766839	-2.322692
35.C	0.319389	-2.086926	-2.322935
36.C	1.647782	1.319458	-2.321987
37.H	-4.364885	-3.173739	-1.887643
38.H	-0.567204	5.366978	-1.888567
39.H	4.931291	-2.194120	-1.887292
40.C	7.386610	-0.953932	-1.354690
41.C	-4.518693	-5.920291	-1.355000
42.C	-2.868138	6.873784	-1.354396
43.H	2.728957	-2.656029	-1.788609
44.H	-3.664170	-1.035629	-1.788427
45.H	0.934484	3.690617	-1.789409
46.N	-1.587828	-0.540523	-1.723740
47.N	0.325477	1.644800	-1.723976
48.N	1.262306	-1.105238	-1.723624
49.H	-2.543694	1.320281	-1.573410
50.H	0.129117	-2.863885	-1.574238
51.H	2.414913	1.542649	-1.572192
52.H	-5.038209	6.567914	-1.088027
53.H	-3.168539	-7.646112	-1.087000
54.H	8.206758	1.078037	-1.087518
55.C	4.847101	-1.354654	-1.197232
56.C	-3.595751	-3.520616	-1.197591
57.C	-1.251682	4.874518	-1.197923
58.H	-6.156779	-7.129120	-0.558351
59.H	-3.096900	8.896427	-0.556942
60.H	9.252564	-1.767552	-0.557752
61.C	-2.813535	-1.142025	-1.093951
62.C	0.417122	3.007417	-1.094627
63.C	2.395919	-1.866291	-1.093995
64.C	-2.448983	5.491752	-0.825987
65.C	-3.531446	-4.866270	-0.826267
66.C	5.980184	-0.625929	-0.825934
67.C	-2.683833	-2.584630	-0.701695
68.C	-0.896895	3.616835	-0.702130
69.C	3.580575	-1.032996	-0.701433
70.C	-5.454946	-6.358768	-0.204070
71.C	-2.780301	7.903429	-0.203135
72.C	8.234295	-1.545607	-0.203767
73.H	-6.040880	-5.508096	0.173709
74.H	-1.750672	7.985612	0.174781
75.H	7.790792	-2.478697	0.173544
76.H	-3.046970	-0.517556	-0.217140
77.H	1.074658	2.897808	-0.217776
78.H	1.971720	-2.380648	-0.217249
79.C	5.786838	0.424100	0.090475
80.C	-3.261440	4.799560	0.090795
81.C	-2.525416	-5.223877	0.090186
82.H	-4.886825	-6.778766	0.637565
83.H	-3.428075	7.620654	0.638253
84.H	8.313150	-0.843800	0.638110
85.H	-4.184753	5.278537	0.408525
86.H	-2.478503	-6.262980	0.407804
87.H	6.663203	0.984556	0.407758
88.H	-4.915576	1.587838	0.228441
89.H	1.083213	-5.051956	0.228126
90.H	3.831748	3.462820	0.227998
91.C	-1.753595	2.927136	0.184970
92.C	-1.657681	-2.981819	0.184719
93.C	3.411452	0.054218	0.185038
94.U	0.000020	0.000262	0.423521
95.C	-2.967556	3.536687	0.624510
96.C	-1.578523	-4.338033	0.623824
97.C	4.546190	0.801093	0.624226
98.O	-1.366677	1.677695	0.555775
99.O	-0.768467	-2.022320	0.555645
100.O	2.135961	0.343885	0.555959
101.H	-5.760429	3.914093	1.081094
102.H	-0.508166	-6.945154	1.081316
103.H	6.268820	3.031621	1.080253
104.C	-4.413486	1.516213	1.204908
105.C	0.894332	-4.580075	1.203992
106.C	3.518998	3.063693	1.204534
107.H	2.484112	2.710918	1.132778
108.H	-3.590511	0.796476	1.132703
109.H	1.106341	-3.507586	1.130389
110.C	-3.898053	2.894276	1.675495
111.C	-0.556887	-4.822222	1.674851
112.C	4.454820	1.928429	1.674979
113.H	-5.140284	1.121111	1.930448
114.H	1.599796	-5.011070	1.930089
115.H	3.540491	3.890685	1.930084
116.C	-5.132462	3.769097	1.971792
117.C	-0.697200	-6.328463	1.971621

118.C	5.829669	2.560044	1.971034	135.H	3.841138	2.120755	3.761030
119.H	-4.856666	4.755734	2.369307	136.H	-3.757500	2.266873	3.761503
120.H	-1.689776	-6.582824	2.368647	137.H	-0.084217	-4.386082	3.760903
121.H	6.546314	1.827727	2.367986	138.Si	-0.000094	0.000131	4.117067
122.H	5.706127	3.343463	2.731647	139.H	-0.439156	2.457947	4.354825
123.H	-5.749195	3.269965	2.732078	140.H	-1.905728	-1.612207	4.359575
124.H	0.042933	-6.612460	2.732521	141.H	2.349559	-0.843680	4.361364
125.N	-0.000553	0.002287	2.335681	142.H	-2.492959	0.066907	4.356142
126.H	-2.241280	2.067425	2.845065	143.H	1.308093	2.122604	4.358964
127.H	-0.670118	-2.973688	2.844076	144.H	1.188920	-2.191955	4.354090
128.H	2.910151	0.907568	2.844474	145.C	-1.690084	-0.593895	4.710373
129.C	-3.110863	2.717599	2.993346	146.C	0.331928	1.760619	4.709430
130.C	-0.797861	-4.051941	2.992531	147.C	1.359279	-1.166773	4.709973
131.C	3.908144	1.335321	2.992919	148.H	-1.721540	-0.602564	5.813118
132.H	-2.760687	3.688909	3.372349	149.H	0.335593	1.793002	5.812204
133.H	-1.814130	-4.234685	3.371344	150.H	1.380491	-1.191351	5.812722
134.H	4.573863	0.546223	3.371994				

Energy: -861.14418218 eV

Final Calculated Coordinates and Single Point Energy for Geometry Optimized 2-*t*-Bu$_{eq}$

Atom	X	Y	Z [Å]	39.H	1.430320	7.939188	5.534592
1.U	3.064702	4.063745	5.685788	40.H	0.324913	7.221293	4.383623
2.O	3.965623	3.557672	7.525434	41.H	4.210483	6.541447	3.873613
3.O	1.303412	3.010043	6.265322	42.H	3.311253	8.066831	3.997415
4.O	2.381709	3.385678	3.734487	43.H	3.552269	8.209977	6.354224
5.N	4.184167	6.239968	6.844579	44.H	5.111270	7.776847	5.685251
6.N	2.238142	6.274689	4.480185	45.H	6.055283	6.874200	7.615276
7.N	1.357880	5.675302	7.256710	46.H	6.125492	5.762942	6.242058
8.C	3.500643	6.581060	8.124097	47.H	1.562953	4.397194	8.895659
9.C	2.021049	6.819067	7.944657	48.H	0.186842	5.505992	9.023044
10.C	0.394559	6.151537	6.233388	49.H	0.849300	5.489772	3.133644
11.C	1.082091	6.974893	5.141891	50.H	1.668562	6.953180	2.543260
12.C	3.488733	7.090278	4.489450	51.C	-2.368705	2.649871	8.307575
13.C	4.099724	7.387826	5.872872	52.C	-1.454820	3.675308	8.577422
14.C	5.612692	5.956157	7.187502	53.H	-1.681495	4.426014	9.337273
15.C	5.891196	4.820535	8.159320	54.H	-2.696732	0.931850	7.079037
16.C	7.055966	4.918780	8.926064	55.H	4.454822	2.757879	-0.287887
17.C	7.488420	3.881478	9.763352	56.H	3.095759	6.683345	0.768675
18.C	6.671257	2.744192	9.848139	57.H	7.652438	5.829445	8.841016
19.C	5.474302	2.587033	9.135670	58.H	6.977285	1.938525	10.508403
20.C	5.107849	3.646303	8.262415	59.C	-0.554438	0.771609	5.448285
21.C	0.726281	4.836648	8.331150	60.C	3.478486	1.317852	1.790066
22.C	-0.233058	3.764672	7.908618	61.C	4.613589	1.312940	9.292498
23.C	-2.001610	1.731406	7.315702	62.C	4.446000	0.624213	0.806472
24.C	-0.800253	1.779392	6.585755	63.H	4.134606	0.746914	-0.239742
25.C	0.104508	2.825913	6.912628	64.H	5.477947	0.987727	0.909380
26.C	1.826348	5.986367	3.051075	65.H	4.450130	-0.455226	1.013486
27.C	2.725131	5.129032	2.198618	66.C	3.873689	0.879597	3.219729
28.C	3.240796	5.627308	0.997673	67.H	3.982047	-0.214664	3.248061
29.C	3.898527	4.788354	0.091502	68.H	4.826019	1.321949	3.534124
30.C	3.971121	3.423657	0.423598	69.H	3.102804	1.154791	3.945580
31.C	3.465189	2.854560	1.601449	70.C	2.053764	0.791911	1.492648
32.C	2.871434	3.761218	2.523614	71.H	2.022524	-0.300516	1.628787
33.H	3.670483	5.744511	8.812794	72.H	1.318974	1.243325	2.169146
34.H	3.965952	7.477473	8.577798	73.H	1.757078	1.017073	0.458105
35.H	1.567238	6.986004	8.935027	74.C	4.503106	0.563944	7.942747
36.H	1.843150	7.740349	7.379511	75.H	4.006473	1.172640	7.178400
37.H	-0.408179	6.767239	6.683712	76.H	5.496280	0.279220	7.566574
38.H	-0.091464	5.267965	5.795178	77.H	3.912525	-0.354931	8.074721

78.C	5.225703	0.328366	10.309582	115.H	8.210770	2.831400	12.279076
79.H	6.217583	-0.028709	9.998492	116.C	9.977701	3.912077	9.478679
80.H	5.311528	0.769818	11.312417	117.H	10.951708	3.980816	9.986658
81.H	4.571091	-0.550821	10.391243	118.H	9.916492	4.733328	8.750233
82.C	3.199968	1.681169	9.802978	119.H	9.946744	2.963971	8.922413
83.H	3.256816	2.198224	10.771887	120.C	8.917359	5.330112	11.270691
84.H	2.667892	2.322541	9.091377	121.H	9.872533	5.391455	11.812635
85.H	2.604470	0.766569	9.941570	122.H	8.101992	5.429446	12.001524
86.C	-0.607453	1.540722	4.107840	123.H	8.871413	6.191542	10.590187
87.H	-1.569009	2.065015	4.003249	124.C	4.525491	5.295286	-1.219084
88.H	0.203741	2.274823	4.030051	125.C	4.023041	4.451536	-2.413904
89.H	-0.518355	0.835499	3.268845	126.H	4.464777	4.824134	-3.350055
90.C	0.806502	0.063553	5.618639	127.H	2.928734	4.505344	-2.505051
91.H	1.635232	0.776888	5.648074	128.H	4.303437	3.394146	-2.317495
92.H	0.825954	-0.522348	6.548956	129.C	4.175022	6.769324	-1.490722
93.H	0.977317	-0.625406	4.778607	130.H	4.624506	7.086425	-2.441976
94.C	-1.633800	-0.329414	5.397029	131.H	4.563804	7.436032	-0.707217
95.H	-1.691839	-0.895860	6.337366	132.H	3.088507	6.921069	-1.569595
96.H	-2.630888	0.071457	5.167301	133.C	6.064118	5.164741	-1.123117
97.H	-1.377664	-1.039525	4.598130	134.H	6.535682	5.509387	-2.055982
98.C	-3.700742	2.569571	9.074983	135.H	6.367999	4.121814	-0.955865
99.C	-4.585980	1.410320	8.583448	136.H	6.461359	5.770118	-0.295063
100.H	-4.101497	0.434113	8.726906	137.N	4.825265	4.077343	4.896488
101.H	-4.846466	1.516392	7.520519	138.Si	6.485071	4.152788	4.198141
102.H	-5.525079	1.398190	9.154305	139.C	7.802593	3.758534	5.494455
103.C	-3.412674	2.361228	10.580706	140.H	8.757598	3.626799	4.959230
104.H	-2.820204	3.187522	10.998401	141.H	7.581190	2.816633	6.017599
105.H	-2.858946	1.426867	10.752002	142.H	7.956041	4.532714	6.257180
106.H	-4.357106	2.308329	11.143280	143.C	6.820770	2.945986	2.791224
107.C	-4.485425	3.890314	8.891105	144.H	7.807660	3.215155	2.378783
108.H	-3.923174	4.755727	9.269121	145.H	6.084643	3.012544	1.981234
109.H	-5.435538	3.845122	9.444232	146.H	6.885121	1.905774	3.138781
110.H	-4.715137	4.070374	7.830776	147.C	6.775585	5.897176	3.502574
111.C	8.828138	3.986914	10.512462	148.H	7.807942	5.949127	3.121176
112.C	9.014536	2.845195	11.528871	149.H	6.668294	6.705008	4.241358
113.H	9.966510	2.979610	12.061017	150.H	6.102907	6.105215	2.656828
114.H	9.051285	1.860822	11.041350				

Energy: -860.66386683 eV

Final Calculated Coordinates and Single Point Energy for Geometry Optimized 2-Ad_{ax}

Atom	X	Y	Z [Å]	19.H	2.249103	8.488405	-2.925477
1.H	-0.983119	-0.532802	-4.443912	20.H	-0.708265	7.664378	-3.138914
2.H	0.439481	1.069787	-4.408954	21.C	-7.336444	-2.682731	-3.014112
3.H	1.132908	-0.942859	-4.329181	22.C	6.193491	-4.635280	-2.949980
4.H	-1.885266	1.602334	-4.067291	23.C	1.668722	-1.019428	-3.373645
5.H	1.738022	6.935663	-3.615595	24.C	-1.276311	1.472019	-3.152418
6.H	6.516848	-3.680057	-3.388766	25.C	2.017563	7.442677	-2.680355
7.H	-0.267255	-2.756303	-3.890182	26.H	-0.050528	9.182700	-2.479185
8.H	-2.380212	-1.379555	-3.780315	27.C	-0.511279	-2.105777	-3.028759
9.H	-7.002705	-1.775877	-3.537729	28.C	2.196082	0.351662	-2.954077
10.H	-6.806688	-3.542018	-3.450045	29.H	-3.623638	0.644858	-2.748610
11.H	2.681166	0.829271	-3.826593	30.H	2.941879	6.985110	-2.299166
12.H	0.360673	2.709177	-3.764256	31.C	-0.336850	8.151225	-2.225562
13.H	-8.411459	-2.804557	-3.214455	32.H	-1.584314	2.245859	-2.441503
14.H	6.926193	-5.406497	-3.230923	33.N	-1.564172	0.151545	-2.526636
15.C	-1.396793	-0.959124	-3.519891	34.H	-5.432084	-0.607507	-2.423596
16.H	5.231085	-4.909784	-3.404465	35.H	-1.056962	-2.714916	-2.301998
17.C	0.193542	1.651042	-3.510489	36.H	2.098787	4.975231	-2.358059
18.H	2.529810	-1.682464	-3.546615	37.N	1.122849	1.232345	-2.414819

38.H	3.436342	-4.406659	-2.123579	100.C	-1.048120	4.417011	-0.066213
39.N	0.740002	-1.634246	-2.370731	101.C	-3.478601	-3.087998	-0.089853
40.H	2.575507	2.794846	-2.377831	102.H	0.015159	-6.210551	0.042846
41.H	2.958160	0.240780	-2.177310	103.H	5.409316	3.261065	0.067708
42.H	1.311255	-3.692106	-2.275873	104.H	0.558997	8.135360	0.402926
43.C	-2.957437	0.226179	-1.974363	105.C	4.961543	1.140917	-0.011384
44.H	-1.167358	8.205979	-1.509063	106.H	-2.152675	-7.454822	0.207916
45.C	0.879079	7.394069	-1.644195	107.O	2.104177	-0.608183	-0.124270
46.C	6.092288	-4.531912	-1.409519	108.C	-3.409835	3.485940	0.082528
47.C	-4.908448	-1.302673	-1.764029	109.C	4.449513	-1.329136	0.108055
48.C	1.220146	4.843099	-1.726837	110.H	-4.105161	-5.799046	0.291893
49.H	4.663784	-6.200172	-1.235965	111.H	-3.177636	6.208692	0.354551
50.C	-7.088680	-2.590037	-1.490885	112.H	7.553176	2.015252	0.430955
51.H	8.196231	-4.996450	-1.152829	113.H	-5.529072	5.232954	0.479714
52.H	6.370246	-6.678739	-1.109873	114.H	-5.414201	2.728344	0.414890
53.H	-7.536379	-0.433138	-1.400125	115.C	-0.793158	-5.813631	0.679693
54.C	3.736320	-3.561353	-1.500858	116.H	7.085957	-0.468057	0.607396
55.H	7.875754	-3.254941	-1.247240	117.C	5.427001	2.397520	0.753548
56.H	-8.717206	-3.952945	-1.047276	118.C	-2.735096	-4.148755	0.739160
57.H	-8.939394	-1.486246	-1.115256	119.C	-2.290317	4.263269	0.830839
58.C	1.768879	2.405554	-1.733989	120.C	-1.733779	-6.959742	1.100566
59.H	-7.151640	-4.770425	-1.206212	121.C	-4.653339	3.294612	0.976791
60.C	1.360407	-2.794722	-1.637079	122.C	4.943023	-0.110842	0.913473
61.C	-3.571450	-1.046248	-1.461859	123.C	-3.655214	-5.321410	1.177864
62.C	0.487357	5.949635	-1.291687	124.C	6.860877	2.177491	1.274846
63.C	5.643458	-5.897863	-0.839412	125.C	-2.890323	5.633875	1.250565
64.C	7.491325	-4.207578	-0.855240	126.C	-5.217761	4.671486	1.377190
65.C	-5.587385	-2.397700	-1.215351	127.H	-1.173630	-7.726327	1.661622
66.C	5.054747	-3.458452	-1.037381	128.C	6.392811	-0.294078	1.446265
67.C	0.866974	3.544509	-1.349264	129.H	7.212231	3.074391	1.811814
68.C	-7.860961	-1.371649	-0.928488	130.H	3.450549	2.831313	1.581635
69.C	-7.644024	-3.863053	-0.828585	131.H	-2.132157	6.224352	1.791056
70.H	-2.914231	0.975002	-1.168635	132.H	0.497702	-4.335597	1.642456
71.C	2.777095	-2.604450	-1.175278	133.H	-4.481381	-4.937969	1.799421
72.H	1.638963	9.149060	-0.582365	134.N	-0.065578	-0.094367	1.596816
73.H	-2.030975	-5.225857	-1.023686	135.H	-6.115084	4.546414	2.005983
74.H	5.627495	0.946060	-0.869665	136.C	-2.866269	-6.384133	1.975710
75.H	-3.679682	4.028450	-0.840063	137.C	4.478650	2.655893	1.943219
76.C	1.352757	8.110490	-0.356777	138.C	-0.188233	-5.149758	1.934917
77.H	2.258451	1.996555	-0.835279	139.H	-1.472754	-2.689248	1.766658
78.C	-0.623750	5.692180	-0.469130	140.H	-1.507908	2.512223	1.873518
79.H	0.701401	-2.994799	-0.775133	141.H	2.994233	0.305968	1.812490
80.C	-2.855510	-1.907796	-0.595130	142.H	-3.557707	-7.192370	2.263323
81.C	-0.262196	3.316474	-0.529115	143.H	-3.872382	1.513978	1.969650
82.C	-4.836426	-3.267293	-0.411025	144.C	-4.134352	5.452982	2.147597
83.H	-0.925559	-3.960570	-0.452462	145.H	6.441984	-1.179644	2.101971
84.C	5.360210	-2.343766	-0.244797	146.C	6.871159	0.956282	2.217663
85.H	-1.196780	6.545848	-0.116740	147.C	-2.121931	-3.534969	2.029343
86.H	3.951787	1.303784	-0.413211	148.C	-1.936207	3.489901	2.133012
87.H	2.223439	7.601003	0.081534	149.H	-4.519255	6.449013	2.419317
88.H	5.568420	-5.863155	0.256990	150.C	4.033983	0.180515	2.140844
89.H	7.496724	-4.158782	0.242818	151.C	-4.256666	2.510862	2.245560
90.H	-7.708782	-1.274871	0.156281	152.H	4.786066	3.568002	2.481127
91.C	3.113655	-1.488086	-0.367681	153.H	0.411258	-5.882381	2.500101
92.H	-3.016565	2.503585	-0.213651	154.H	7.896993	0.775267	2.576506
93.H	6.377364	-2.248714	0.120526	155.H	-1.161699	4.053770	2.679807
94.U	0.007878	-0.072346	-0.315909	156.H	-2.941015	-3.136891	2.651760
95.O	-1.576022	-1.546271	-0.301740	157.H	-5.142616	2.347443	2.881410
96.H	-7.531985	-3.836516	0.264615	158.C	-1.324854	-4.594513	2.818959
97.C	-1.594239	-4.766327	-0.120146	159.H	4.059470	-0.692075	2.814720
98.H	-5.334809	-4.141529	-0.004148	160.C	4.508491	1.441060	2.894752
99.O	-0.539208	2.016859	-0.236695	161.C	-3.183619	3.302800	3.022049

162.C	-2.260887	-5.743365	3.239893	175.H	6.284357	2.114498	3.971005
163.C	-3.747837	4.679018	3.423787	176.H	-2.996367	5.244342	4.000713
164.C	5.941118	1.225346	3.415985	177.H	-2.240576	-1.285994	3.721206
165.Si	-0.047068	-0.117729	3.377871	178.H	-2.893567	2.744834	3.926973
166.H	-1.702719	-6.498531	3.818464	179.H	-4.629027	4.556337	4.075464
167.H	2.057626	-1.457130	3.561736	180.H	5.965613	0.376393	4.119826
168.H	-0.897091	-4.121461	3.717535	181.C	1.028066	-1.565233	3.928949
169.H	0.634541	-2.522123	3.559182	182.C	0.674601	1.507312	4.005596
170.H	3.832304	1.623274	3.745406	183.C	-1.811192	-0.319385	4.015518
171.H	-3.060502	-5.360573	3.896119	184.H	1.061686	-1.614948	5.029323
172.H	0.042138	2.361933	3.731240	185.H	0.751651	1.480078	5.104663
173.H	-2.468897	0.474597	3.635396	186.H	-1.816415	-0.264392	5.116199
174.H	1.680367	1.685263	3.600989				

Energy: -1086.27984249 eV

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