Electronic Supplementary Material (ESI).
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SUPPORTING INFORMATION

Could new U(II) complexes be accessible *via* tuning hybrid heterocalix[4]arene? A theoretical study of redox and structural properties

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Supporting Information

Computational Details

A series of hybrid heterocalix[4]arene macrocycles was designed, see Chart 1 of the main article, H_nL^n (n = 1~3) and H_2L^{2N}. The H_2L^{2N} ligand, *trans*-calix[2]pyrrole[1]pyridine[1]benzene, is analogous to H_2L^2, *trans*-calix[2]pyrrole[2]benzene, which differ in the cyclic ring 3. It is worth noting that H_2L^2 and H_3L^3 were synthesized by the Sessler group,[1] as was calix[1]pyrrole[2]benzene[1]-3-chloropyridine, being an analogue of HL^1. Complexation of both U^{II} and U^{III} ions results in eight complexes, labeled as $[U^mL^n]^z$ (m = II and III, n = 1~3 and 2N, and z = -1 ~ +2). Unrestricted calculations have been performed on the all electron-spin state of each complex. Calculated relative energies are presented in Table S1. Our optimizations of $[U^{II}((^{Ad,Me}ArO)_3mes)]^-$ in all electron-spin states (singlet, triplet and quintet) find that its triplet state is the lowest in energy. For other complexes, it is shown that their highest-spin states are the most stable in energy.

Relativistic density functional theory (DFT) calculations were carried out using the Priroda code, which applies a scalar relativistic all-electron (AE) approach with spin-orbit projected out and neglected from the full Dirac equation.[2] No symmetry constraints were used for structural optimizations of complexes.[3-6] Default convergence criteria for gradients in the geometry optimization (10^{-5} au) and SCF (10^{-6} au) were employed. The GGA-PBE functional[7] was used in the calculations, together with all-electron correlation-consistent double-ς polarized quality basis sets (labeled as B-I).[5] The minimum nature of all the structures was confirmed by analytical frequency calculations. Building on these, zero-point vibration energies and free energies were obtained.

Properties of molecular orbitals in solution were calculated using the ADF 2014 code.[8-10] The default convergence criterion of 10^{-6} au and an integration parameter of 6.0 were applied. The Priroda-optimized structures were used in the ADF calculations. Our previous work[11-15] and others[16-18] have shown that this approximation is reliable, as re-optimizations have only a very slight effect on the structural parameters and molecular properties. Firstly, the scalar relativistic ZORA method of van Lenthe et al.[19-22] was used for electronic structure calculations, together with the PBE functional and Slater-type TZP basis sets (labeled as B-II). With the small-core ZORA basis sets, the core orbitals 1*s*−4*f* for U and 1*s* for C, and N were frozen. The tetrahydrofuran (THF) solvation was taken into account with the Conductor-Like Screening Model, COSMO.[23-24] A dielectric constant of 7.58 was applied with the Esurf type of cavity. The Klamt radii were used for the main group atoms (H = 1.30 Å, C = 2.00 Å and N = 1.83 Å)[25] and for the actinide atoms (U = 1.70 Å)[13, 26-28]. Secondly, spin-orbit coupling (SOC) energies were obtained based on the SOC ZORA Hamiltonian.

The single-electron reduction reactions (eV) of uranium complexes from III to II were theoretically computed. Relative to the reference electrode ferrocene/ferrocenium couple (Fc/Fc^+), we obtained the free energy (Δ_rG) of the following reaction:

$$An^{III}\ compl. + Fc \rightarrow An^{II}\ compl. + Fc^+ \quad (1)$$

$$E^0 = -\Delta_rG/F \quad (2)$$

Then according to Eq. (2) where F is the Faraday constant, 96485 $C\cdot mol^{-1}$, the reduction potential (E^0 in V) was calculated. Notably, Δ_rG was calculated at three levels of theory. The first is Δ_rG(gas), which comes from the Priroda frequency calculations; Δ_rG(sol) is the second level, which is obtained by adding by the solvation energy (G_{sol}) from the ADF calculations; the third is Δ_rG(sol-so) that also includes the SOC energy arising from the SOC-ZORA calculations. See results in Table S2. Herein, we did not consider the multiplet effects of low-valent uranium complexes.[29]

Additionally, E^0 can be obtained entirely from the ADF calculations as seen in Fig. S1. The total bonding energies, E_{TBE}(sol) and E_{TBE}(sol-so), were used to approximately represent the free energy in Eq. 2, for they do not consider the free-energy correction term.

Apart from traditional methods of molecular orbital analysis, an electron density-based approach (quantum theory of atoms in molecule, QTAIM)[30-31] was used to understand U-Ligand bonding. Calculations at the Priroda-optimized geometries were accomplished with the Gaussian09 program.[32] Stuttgart relativistic small-core effective core potentials (RSC-ECPs) and corresponding basis sets were employed for uranium,[33-35] and 6-31G* for other atoms. These combined basis sets were labeled as B-III. The GGA-PBE functional was used. QTAIM parameters [electron density $\rho(r)$, Laplacian of electron density $\nabla^2\rho(r)$ and energy density H(r) at bond critical points (BCPs)], as well as the delocalization index δ(U, N/C) were computed with the Multiwfn 3.3.3 package.[36]

Validation of theoretical approach for calculations of reduction potentials

The computational approach used in this work is reliable for predictions of redox properties of actinides. For example, our current $U^{III/II}$ couples were calculated using solely the ADF code, which gives the same order of E^0 ($L^3 < L^2 < L^{2N} < L^1$; Fig. S1) as in the text; and the experimentally measured trends of $E^0(An^{IV/III})$ (Th < Pa < U < Np < Pu) and $E^0[(An^{VI/V}O_2)^{2+/1+}]$ (U < Pu < Np), were well reproduced by our previous calculations,[37-38] as shown in Fig. S2.

The cyclic voltammetry of $[U^{III}((^{Ad,Me}ArO)_3mes)]$ has revealed a reduction potential at -2.50 V,[39] which deviates from our calculated E^0(sol-so) of -2.95 V for $[U^{II}((^{Ad,Me}ArO)_3mes)]^-$ /$[U^{III}((^{Ad,Me}ArO)_3mes)]$. The difference between experimental and computed values may arise from the following aspects. (i) The multiplet effects were not considered for the calculation of $U^{II/III}$ complexes. Previous configuration interaction calculations found that it contributes about 0.20~0.78 V to neptunyl and plutonyl ions with multiple 5f electrons when comparing them in their VI and V oxidation states.[29]

(ii). Other theoretical approximations would affect the computed E^0 value as well, including methods (different functionals, as well as approaches considering multiple configurations), basis sets, relativity and solvation models. Choices of various functionals were shown to change E^0 values by about 0.4~0.6 V.[40-41] Indeed, the major systematic error source is the single-determinant character of approximate DFT as used here. However, this is, by and large, a systematic error that cancels out in relative values, as these effects would be concentrated on the actinide metals. Another possible systematic error source might be the treatment of solvation. Additionally, choices of basis sets also have a regular effect on E^0 values, for example those calculated in our previous work, as shown in Fig. S3. In brief, the theoretical approach used here does have effects on computed E^0 values of the U^{II}/U^{III} complexes, which leads to differences with experimental values. Notably, the choice of theoretical approach shows an impact on E^0 at a similar magnitude, see for instance Fig. S3, i.e. a relatively constant systematic error that will be strongly reduced in relative values. This is further reflected by those methods affording accurate trends of computed E^0 values for several series of actinide complexes involving $An^{IV/III}$ and $An^{VI/V}$ reductions, in Fig. S2.

Partial discussion of geometrical and electronic structures

Optimized structures of uranium complexes supported by heterocalix[4]arene are shown in Fig.s 2 and S4. The uranium ion, regardless of II or III, is found to reside almost at the center of the macrocyclic ligand. This is firstly reflected by the N1-U-X2 (α1) and X3-U-C4 angles (α2), which were calculated to be approximately linear (170º~178º; Table S3). Secondly, values of around 120º were found for the $Pl1_{cent}$-U-$Cyc3_{cent}$ (β1) and $Cyc3_{cent}$-U-$Ar4_{cent}$ (β2) angles. Thirdly, the dihedral angles (γ1 and γ2) of opposite cyclic planes range from 44º to 56º. See Chart 1 for the numbering of atoms and rings (Cyc); the "cent" subscript refers to the centroid of the ring.

Our theoretically designed and Meyer's experimentally synthesized uranium arene complexes demonstrate U-C/Ar_{cent} contractions upon reducing the U^{III} parent complex to its U^{II} analogue. These differ from previously reported results of cyclopentadienyl complexes of $Ln^{III}\rightarrow Ln^{II}$ (Ln = Y, and La to Lu except for Pm)[42] and $An^{III}\rightarrow An^{II}$ (An = Th, U and Pu). For these systems, an increase in the M-C/Cp_{cent} distances was observed upon reduction, where large differences (0.12~0.16 Å) were attributed to the formation of a $4f^{n+1}$-ground-state Ln^{II} complex and small change (less than 0.04 Å) to a $4f^n5d^1$ Ln^{II} complex;[42] this conclusion is totally accurately applicable for cyclopentadienyl Th and U analogues, but only approximately suitable for Pu complexes, $[Pu^{III}(Cp'')_3]$ and $[Pu^{II}(Cp'')_3]^-$, in that Pu-C/Cp''_{cent} lengthen by 0.05 Å (a small increase) while the $5f^6$ ground state is assigned for the Pu^{II} complex[43]. Obviously, the conclusions drawn from cyclopentadienyl complexes cannot be directly applied to uranium multi- and mono-arene complexes. The ligand difference can, indeed, change the ground-state electronic configuration, as indicated by $5f^4$ for $[U^{II}((^{Ad,Me}ArO)_3mes)]^-$ and $5f^36d^1$ for

$[U(Cp')_3]^-$. More interestingly, the difference would have a significant effect on U-Arene and U-Cp bondings and eventually determine various properties of complexes.

Relative to those of $[U^{II}L^1]^+$, the other three U^{II} complexes show U(5f)-based HOMOs, while their H-1~H-3 do have some differences. For example, $[U^{II}L^2]$ features two δ(U-Ar) orbitals and one less stable π(U-Ar) orbital (Fig. S6 and Table S6); its δ-type orbital, H-2, has contributions from only one Arene ring, which rationalizes it being energetically higher than another δ bonding orbital (H-3) that involves two Arene rings. Generally, these together are responsible for the lower stability of $[U^{II}L^2]$ relative to $[U^{II}L^1]^+$. Calculations reveals that $[U^{II}L^3]^-$ has two nonbonding U(5f) orbitals (HOMO and H-1) and two δ(U-Ar) orbitals (H-3 and H-4). The one additional U(5f) orbital (H-1) may lead to $[U^{II}L^3]^-$ being the least stable.

The U^{III} complexes of heterocalix[4] arene demonstrate electronic structures that are similar to the ones of their U^{II} daughters, except that the former feature a $5f^3$ ground state combined with some Arene participation. (Fig.s S9-S13)

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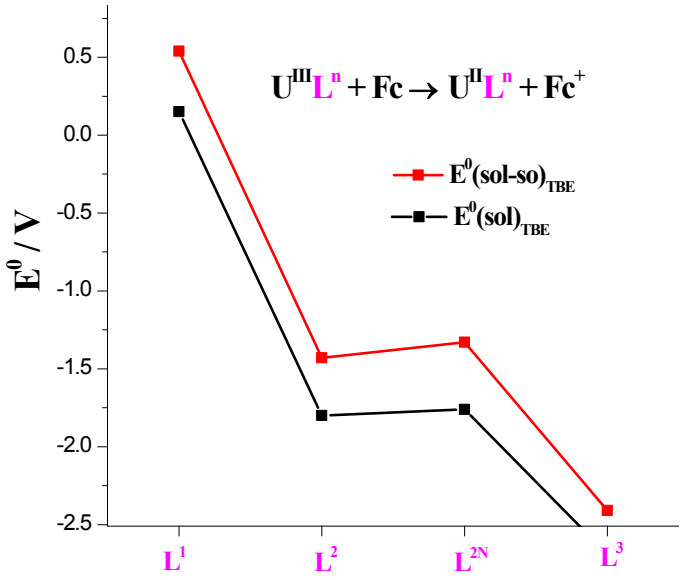

Fig. S1. Reduction potentials (versus Fc/Fc^+ in THF) for various hybrid heterocalix[4]arene uranium complexes reduced from III to II calculated by the ADF code. Noting that $E^0(sol\text{-}so)_{TBE}$ was calculated with the ZORA Hamiltonian including both solvation and spin-orbit coupling effects, where $E^0(sol\text{-}so)_{TBE}$ containing only solvation effect.

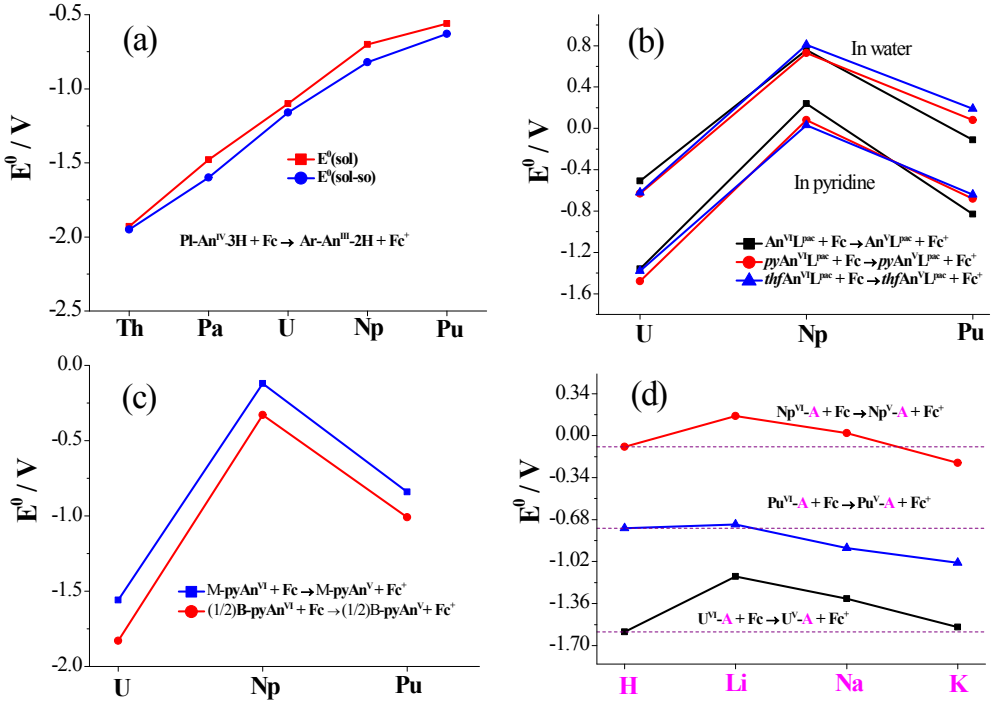

Fig. S2. Calculated single-electron reduction potentials (E^0 in V) of actinide complexes versus Fc/Fc^+ in solution. (a) IV→III: $[(L^2)An^m(\eta\text{-}H)_nBH_{4-n})]^{z+}$ (**BP-An^m-nH**; An = Th, Pa, U, Np and Pu; m = III and IV; n = 2 and 3; and z = 0 and 1); (b) VI→V: $[(Sol)(An^mO_2)(H_2L^{Pac})]^{n-}$ (***Sol*An^{m}L^{Pac}**; Sol = Vac., py and THF; An = U, Np and Pu; m = VI and n = 0, m =V and n = 1); (c) VI→V: $[(py)(An^mO_2)(H_2L^{An})]^{n-}$ (M-**pyAn^m**; m = VI, n =0; m = V, n =1) and $[(py)_2(An^{VI}O_2)_2(L^{An})]^{2n-}$ (B-**pyAn^m**); and (d) VI→V: $[(thf)(An^mO_2)(A_2L^{Pac})]^{n-}$ (**An^m-A**; An = U, Np and Pu; m = VI and n = 0; m = V and n = 1; A = H, Li, Na and K).[38, 44-46]

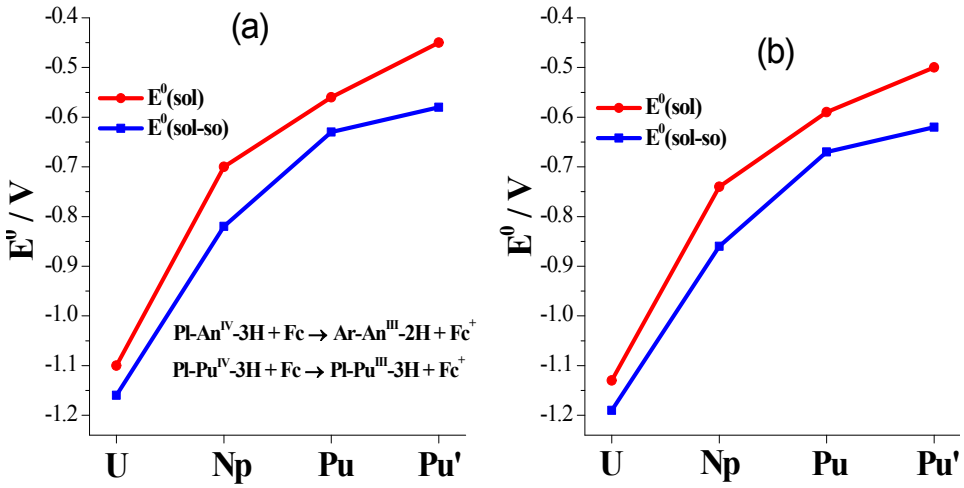

Fig. S3. Calculated single-electron reduction potentials (E^0 in V) of $[(\mathbf{BP}\text{-L})An^m(\eta\text{-H})_nBH_{4-n})]^{z+}$ (**BP** = **Ar** and **Pl**; An = U, Np and Pu; m = III and IV; n = 2 and 3; and z = 0 and 1; labeled as **BP-An^m-nH**) versus Fc/Fc^+ in THF: (a) calculated with TZP basis sets, and (b) with DZP.[44]

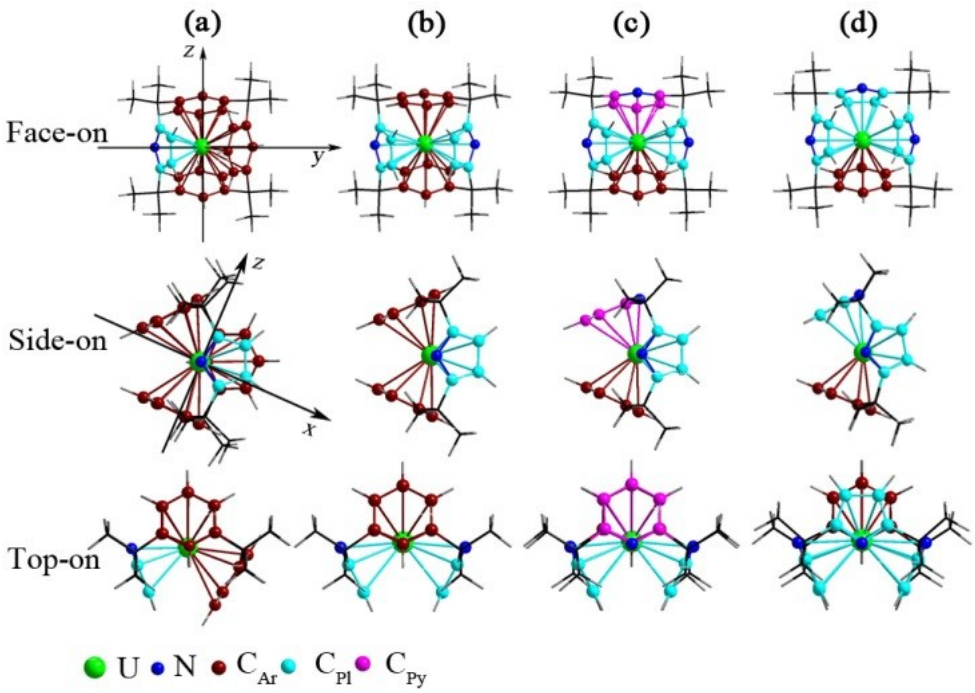

Fig. S4. Structures of optimized uranium complexes of L^1 (a), L^2 (b), L^{2N} (c) and L^3 (d).

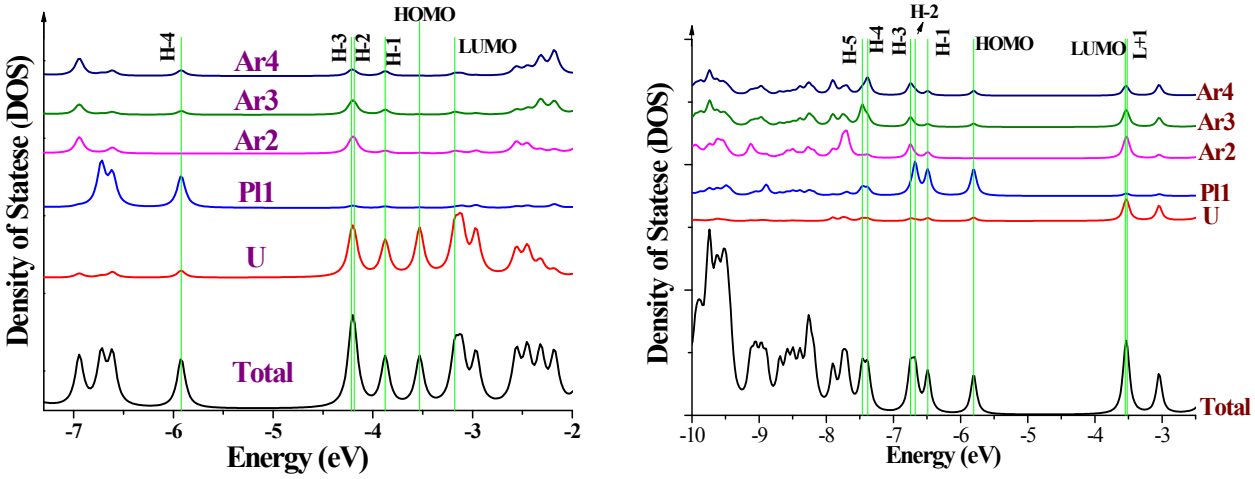

Fig. S5. The α-spin (left) and β-spin (right) density of states (DOS) of $[U^{II}L^{1}]^{+}$.

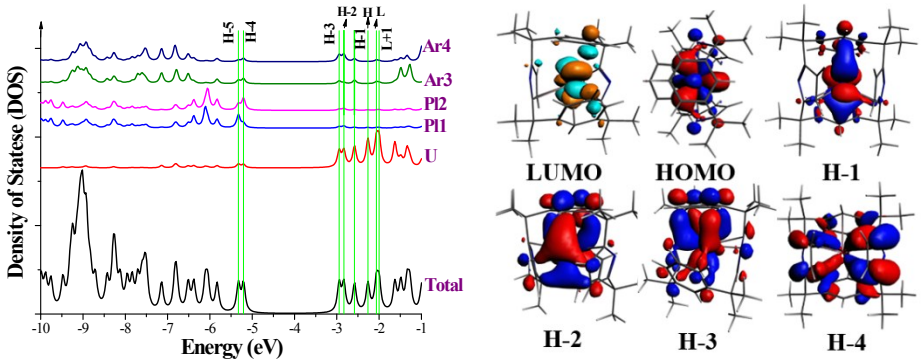

Fig. S6. The α-spin density of states (left) and frontier orbitals (right) for $[U^{II}L^{2}]$.

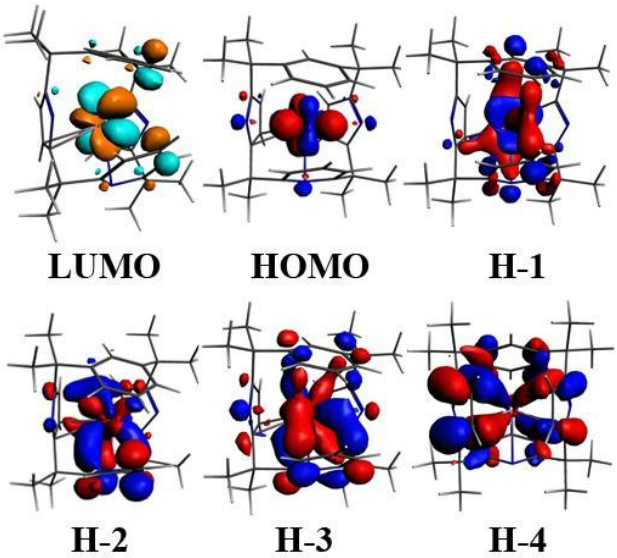

Fig. S7. Characteristic α-spin orbitals of $[U^{II}L^{2N}]$.

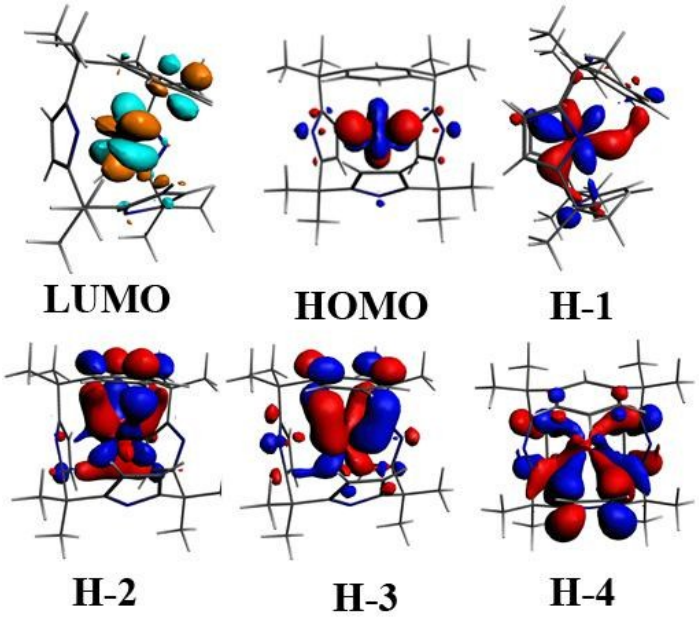

Fig. S8. Characteristic α-spin orbitals of $[U^{II}L^{3}]^{-}$.

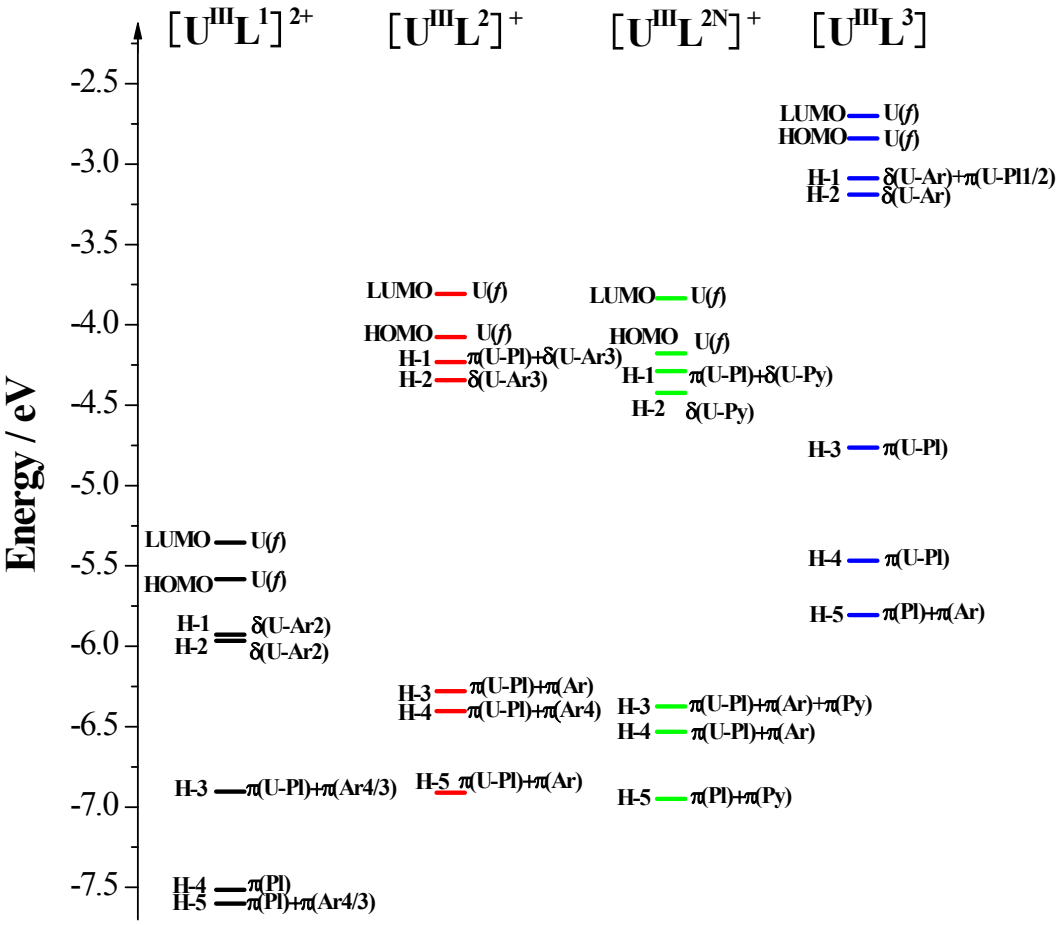

Fig. S9. Energy levels of α-spin orbitals and character for the trivalent uranium complexes of different polypyrrolic ligands.

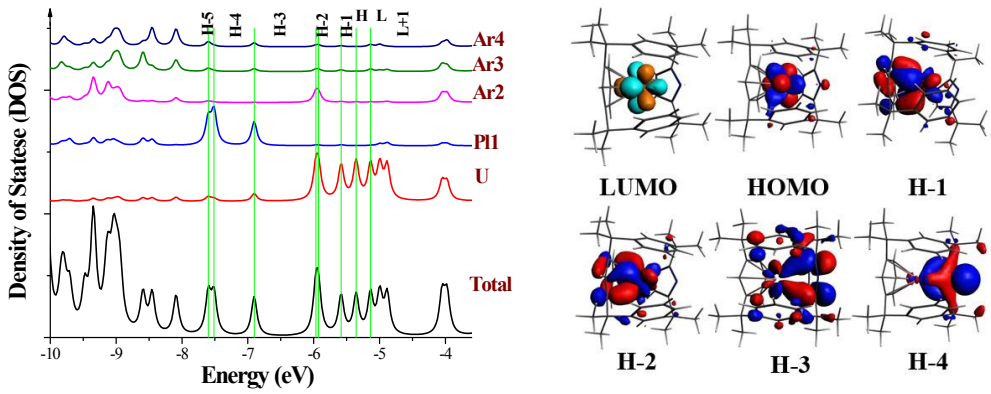

Fig. S10. The α-spin density of states (left) and frontier orbitals (right) for $[U^{III}L^{1}]^{2+}$.

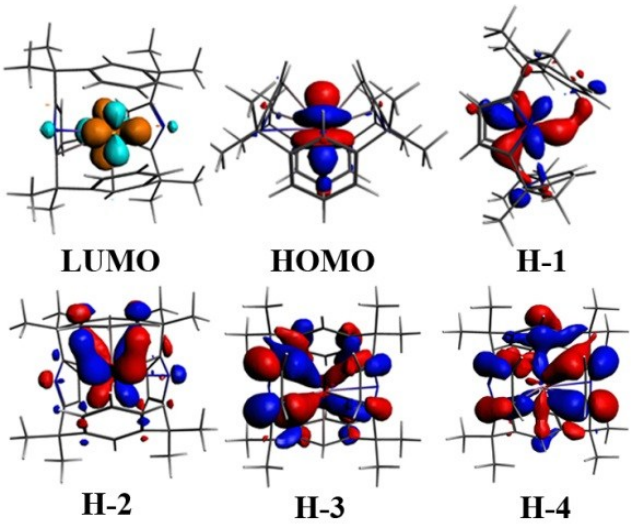

Fig. S11. Characteristic α-spin orbitals of $[U^{III}L^{2}]^{+}$.

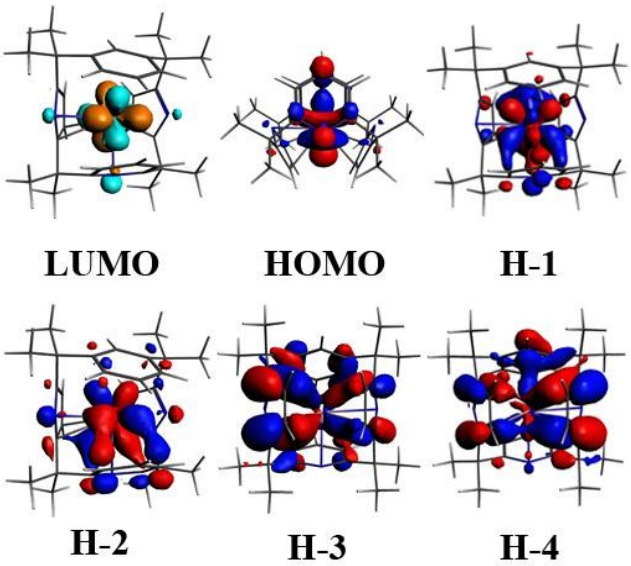

Fig. S12. Characteristic α-spin orbitals of $[U^{III}L^{2N}]^{+}$.

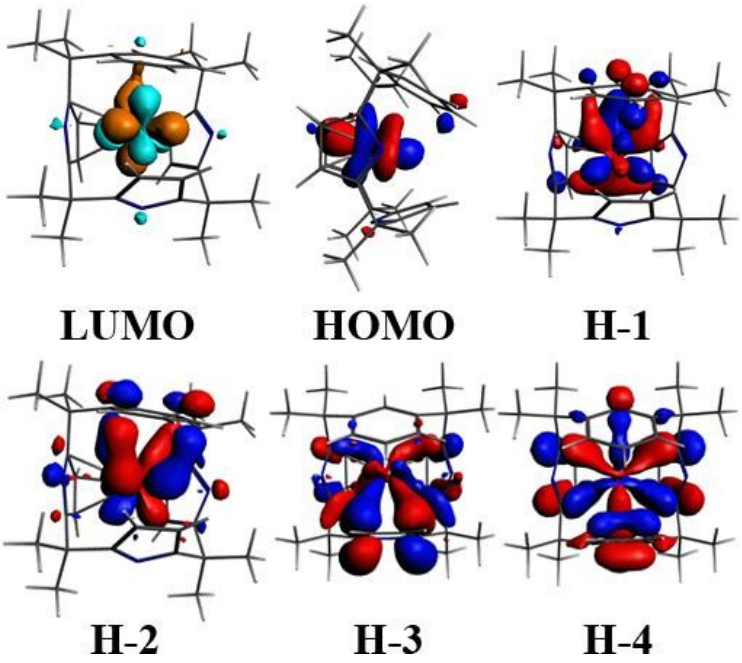

Fig. S13. Characteristic α-spin orbitals of [$U^{III}L^{3}$].

Table S1. Calculated relative energies (kcal/mol) of di and trivalent uranium complexes in various electron-spin state (ESS).

Complexes	ESS	ΔE [a]	ΔE_0 [a]	ΔG [a]
$[U^{II}((^{Ad,Me}ArO)_3mes)]^-$	Singlet	7.09	6.96	6.56
	Triplet	0.00	0.00	0.00
	Quintet	1.52	1.81	1.71
$[U^{III}((^{Ad,Me}ArO)_3mes)]$	Doublet	7.49	6.70	5.98
	Quartet	0.00	0.00	0.00
$[U^{II}L^2]$	Singlet	11.71	11.71	11.14
	Triplet	2.67	2.67	2.18
	Quintet	0.00	0.00	0.00
$[U^{III}L^2]^+$	Doublet	7.91	7.91	7.67
	Quartet	0.00	0.00	0.00
$[U^{II}L^1]^+$	Singlet	11.12	10.89	11.07
	Triplet	4.18	3.68	3.61
	Quintet	0.00	0.00	0.00
$[U^{II}L^3]^-$	Singlet	7.99	7.69	7.92
	Triplet	2.91	2.50	2.57
	Quintet	0.00	0.00	0.00

[a] The total energy (E), the total energy including zero-point vibrational energy (E_0) and the free energy correction (G); and ΔE, ΔE_0 and ΔG (in kcal/mol) denote the relative energy with respect to the lowest-energy isomer.

Table S2. Energies (eV) of the single-electron reduction reactions of uranium complexes from III to II calculated by the Priroda and ADF codes, together with reduction potential E^0 (V, versus Fc^+/Fc) in THF.

Reduction reaction	Δ_rE [a]	Δ_rE_0[a]	Δ_rG [a]	Δ_rG(sol) [b]	Δ_rG(sol-so) [b]	E^0(sol)[c]	E^0(sol-so)[c]
$[U^{III}L^1]^{2+} + e = [U^{II}L^1]^+$	-8.22	-8.26	-8.26	-4.76	-4.72	-0.64	-0.68
$[U^{III}L^2]^+ + e = [U^{II}L^2]$	-4.54	-4.62	-4.61	-3.53	-3.50	-1.87	-1.90
$[U^{III}L^{2N}]^+ + e = [U^{II}L^{2N}]$	-4.67	-4.74	-4.74	-3.64	-3.61	-1.76	-1.79
$[U^{III}L^3] + e = [U^{II}L^3]^-$	-0.82	-0.94	-0.95	-2.24	-2.22	-3.16	-3.18

[a] The total energy (Δ_rE), total energy including zero-point vibrational energy (Δ_rE_0) and free energy (Δ_rG) in the gas phase for the single-electron reduction reactions of uranium complexes.

[b] The solvation energy is included in Δ_rG(sol), and both solvation and spin-orbit energies are added in Δ_rG(sol-so). These energies were calculated by the ADF code.

[c] The free energies, both Δ_rG(sol) and Δ_rG(sol-so), for the reference electrode of Fc/Fc^+ were calculated to be -5.40 eV. Thus, reduction potentials, E^0(sol) and E^0(sol-so), were obtained according to Eq. (2) in Computational Details.

Table S3. Optimized bond angles (α in degree) and interplanar cyclic (arene, pyridine and pyrrolide) angles (β) for the uranium complexes of different polypyrrolic ligands.

Complexes	Approaches	α1 [a]	α2 [a]	β1 [b]	β2 [b]	γ1 [c]	γ2 [c]
$[U^{II}L^{1}]^{+}$	Calc.	171.9	176.0	115.5	117.7	55.4	52.7
$[U^{II}L^{2}]$	Calc.	170.4	176.7	118.1	123.6	55.3	49.9
$[U^{II}L^{2N}]$	Calc.	169.9	175.8	117.1	122.9	55.1	46.6
$[U^{II}L^{3}]^{-}$	Calc.	175.6	176.6	124.0	126.8	50.7	47.6
$[U^{III}L^{1}]^{2+}$	Calc.	170.9	175.0	114.0	119.2	50.0	51.0
$[U^{III}L^{2}]^{+}$	Calc.	171.9	177.7	117.9	123.2	50.0	48.7
$[U^{III}L^{2N}]^{+}$	Calc.	171.5	177.2	117.0	122.2	49.8	44.6
$[U^{III}L^{3}]$	Calc.	176.4	177.9	125.4	126.1	47.7	47.2
$[U^{III}L^{2}(BH_4)]$	Calc.[d]	119.8	119.1	119.6	178.2	76.6	8.0
$[U^{III}L^{2}(BH_4)]$	Expt.[d]	118.9	122.0	117.4	174.7	81.5	14.2
$[U^{III}L^{2}(I)]$	Expt.[d]	118.3	121.4	117.0	170.7	82.2	16.4
$[U^{III}L^{2}(I)(THF)]$	Expt.[d]	115.2	118.6	125.0	171.6	48.3	18.0

[a] α1 and α2 denote the N1-U-X2 and X3-U-C4 angles, respectively. The atom numbers are marked in Chart 1(a).

[b] β1 and β2 are the $Pl1_{cent}$-U-$Cyc2_{cent}$ and $Cyc3_{cent}$-U-$Ar4_{cent}$ angles, respectively where the respective cycle (arene, pyridine and pyrrolide) is denoted as Cyc, the number of each cycle is marked in Chart 1(a), and the subscript "cent" stands for the centroid of the cycle.

[c] γ1 is the interplanar angles between Pl1 and Cyc2, and γ2 is between Cyc3 and Ar4. See the cycle numbers in Chart 1(a).

[d] The complex $[U^{III}L^{2}(BH_4)]$ was optimized with the same approach as in this work, compared with experimental values for $[U^{III}L^{2}(X)]$ (X = BH_4, I and I/THF) from Refs. (P. L. Arnold, C. J. Stevens, J. H. Farnaby, M. G. Gardiner, G. S. Nichol, J. B. Love, *J. Am. Chem. Soc.* **2014**, *136*, 10218-10221 and P. L. Arnold, J. H. Farnaby, R. C. White, N. Kaltsoyannis, M. G. Gardiner, J. B. Love, *Chem. Sci.* **2014**, *5*, 756-765).

Table S4. Optimized bond lengths (Å) for the uranium complexes of different polypyrrolic ligands.

Complexes	Approaches	U-N1[a]	U-X2[a]	U-X3[a]	U-C4[a]	Dis.1[b]	Dis.2[b]	Dis.3[b]	Dis.4[b]
$[U^{II}L^{1}]^{+}$	Calc.	2.624	2.828	2.812	2.812	2.486	2.530	2.541	2.541
$[U^{II}L^{2}]$	Calc.	2.715	2.715	2.786	2.786	2.530	2.530	2.484	2.484
$[U^{II}L^{2N}]$	Calc.	2.692	2.692	2.649	2.788	2.515	2.515	2.458	2.489
$[U^{II}L^{3}]^{-}$	Calc.	2.747	2.747	2.728	2.742	2.545	2.545	2.545	2.408
$[U^{III}L^{1}]^{2+}$	Calc.	2.461	2.878	2.815	2.815	2.458	2.600	2.547	2.547
$[U^{III}L^{2}]^{+}$	Calc.	2.608	2.608	2.803	2.803	2.486	2.486	2.517	2.517
$[U^{III}L^{2N}]^{+}$	Calc.	2.584	2.584	2.639	2.801	2.470	2.470	2.509	2.509
$[U^{III}L^{3}]$	Calc.	2.682	2.682	2.640	2.838	2.500	2.500	2.462	2.533
$[U^{III}L^{2}(BH_4)]$	Calc.[c]	2.448	2.448	2.807	2.807	3.652	3.652	2.507	2.507
$[U^{III}L^{2}(BH_4)]$	Expt.[c]	2.476	2.452	2.844	2.846	3.665	3.648	2.601	2.580
$[U^{III}L^{2}(I)]$	Expt.[c]	2.463	2.470	2.857	2.860	3.668	3.658	2.631	2.610
$[U^{III}L^{2}(I)(THF)]$	Expt.[c]	2.529	2.502	3.105	2.949	3.682	3.692	2.672	2.666

[a] The atom numbers are marked in Chart 1(a).

[b] The distance (Dis.) is determined between the uranium and the centroid of planar arene (Ar), pyridine (Py) or pyrrolide (Pl), where the cycle numbers are marked in Chart 1(a).

[c] The complex $[U^{III}L^{2}(BH_4)]$ was optimized with the same approach as in this work, compared with experimental values for $[U^{III}L^{2}(X)]$ (X = BH_4, I and I/THF) from Refs. (P. L. Arnold, C. J. Stevens, J. H. Farnaby, M. G. Gardiner, G. S. Nichol, J. B. Love, *J. Am. Chem. Soc.* **2014**, *136*, 10218-10221 and P. L. Arnold, J. H. Farnaby, R. C. White, N. Kaltsoyannis, M. G. Gardiner, J. B. Love, *Chem. Sci.* **2014**, *5*, 756-765).

Table S5. Contributions (%) to the α-spin orbitals of $[U^{II}L^{1}]^{+}$.[a~f]

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Ar2	Ar3	Ar4	
LUMO	-3.178	81.22(f_{z^2x},f_{z^2y})		1.56(p_y)	2.25(p_x)	2.56(p_z)	U(f)
HOMO	-3.532	95.67(f_x,f_{z^3})					U(f)
H-1	-3.876	70.53(f_z,f_{xyz})		2.14(p_y)	6.80(p_x,p_z)	9.32(p_z)	δ(U-Ar)
H-2	-4.187	53.40(f_{z^3},f_x)		18.68(p_y,p_x)	12.04(p_x,p_z)	2.47(p_z)	δ(U-Ar)
H-3	-4.215	53.31(f_{xyz},f_{z^2y})		11.22(p_y,p_x)	12.07(p_x,p_z)	6.10(p_z)	δ(U-Ar)
H-4	-5.922	11.52(f_{z^2y},f_y)	57.81(p_y, p_x)		1.97(p_x)	9.58(p_z)	π(U-Pl)+π(Ar4/3)
H-5	-6.612	7.44(f_y,f_{z^2y})	56.72(p_y,p_z,p_x)	6.66(p_y,p_x)	2.02(p_x)	9.21(p_z)	π(U-Pl)+π(U-Ar2)

[a] The sum of contributions for each orbital is less than 100%, for the output of SFO contributions smaller than 1% in the calculations is suppressed.

[b] The coordinate orientation is shown in Fig.s 2 and S4.

[c] Major character of metal and ligand are listed. Only the two largest compositions of uranium are given. With respect to uranium components, f_x, f_y and f_z denote $f_{x(x^2-3y^2)}$, $f_{y(3x^2-y^2)}$ and $f_{z(x^2-y^2)}$, respectively.

[d] See the labeling of the aromatic rings in Chart 1.

[f] In the assignment, that the cyclic ring is not numbered denotes that all rings of the same type are included.

Table S6. Contributions (%) to the α-spin orbitals of $[U^{II}L^{2}]$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Ar3	Ar4	
LUMO	-2.064	83.55(f_{z^2x},f_z)		1.02(p_y)	2.40(p_x)	4.98(p_z)	U(f)
HOMO	-2.265	93.69(f_x,f_{z^3})	1.09(p_y)	1.13(p_y)			U(f)
H-1	-2.583	69.79(f_z,f_{z^3})		1.08(p_y)	3.97(p_x)	11.72(p_z)	π(U-Ar)
H-2	-2.834	54.01(f_{z^3},f_z)	3.91(p_y)	4.44(p_y)	23.02(p_z,p_x)	2.79(p_z)	δ(U-Ar3)+π(U-Pl)
H-3	-2.945	54.79(f_{xyz},f_{z^2y})	1.57(p_y)	1.89(p_y)	22.04(p_x,p_z)	9.40(p_z)	δ(U-Ar)
H-4	-5.206	10.69(f_y,d_{yz})	38.53(p_y,p_z,p_x)	12.07(p_y,p_x)	9.06(p_x,p_z)	16.30(p_z)	π(U-Pl)+π(Ar)
H-5	-5.326	8.94(f_{z^2x},f_z)	15.63(p_y,p_x)	40.93(p_y,p_x)	1.81(p_x)	10.22(p_z)	π(U-Pl)

Table S7. Contributions (%) to the α-spin orbitals of $[U^{II}L^{2N}]$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Py3	Ar4	
LUMO	-2.263	83.22(f_{z^2x}, f_{z^3})			3.9(p_x, p_z)	5.04(p_z)	U(f)
HOMO	-2.350	92.11(f_x,f_{z^3})	1.14(p_y)	1.21(p_y)	1.30(p_z)		U(f)
H-1	-2.735	66.42(f_z,f_{z^2x})	1.15(p_y)	1.24(p_y)	9.48(p_x,p_z)	11.44(p_z)	π(U-Ar/Py)
H-2	-2.942	48.65(f_x,f_{z^3})	4.07(p_y)	4.24(p_y)	31.34(p_x,p_z)	1.65(p_z)	δ(U-Py)+π(U-Pl)
H-3	-3.035	57.74(f_{xyz},f_{z^2y})	1.55(p_y)	3.09(p_y)	19.55(p_x,p_z)	9.47(p_z)	δ(U-Py/Ar)
H-4	-5.309	10.71(f_y,f_{z^2y})	39.25(p_y, p_x,p_z)	10.72(p_y, p_x)	9.91(p_x,p_z)	16.07(p_z)	π(U-Pl)+π(Ar)+π(Py)
H-5	-5.472	13.16(f_{z^2x},f_z)	16.51(p_y,p_x)	43.54(p_y, p_x,p_z)		8.47(p_z)	π(U-Pl)

Table S8. Contributions (%) to the α-spin orbitals of $[U^{II}L^3]^-$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Pl3	Ar4	
LUMO	-0.700	81.31(f_{z^2x},f_{z^3})	1.36(p_y)			7.31(p_z)	U(f)
HOMO	-1.108	92.00(f_x,f_{z^3})	1.38(p_y)	1.43(p_y)			U(f)
H-1	-1.266	80.68(f_{z^3},f_x)	1.13(p_y)	1.25(p_y)	2.20(p_z)	3.89(p_z)	U(f)
H-2	-1.693	52.88(f_z,f_x)	3.68(p_y)	3.8(p_y)		31.04(p_z)	δ(U-Ar)+π(U-Pl1/2)
H-3	-1.727	54.57(f_{xyz},f_{z^2y})	3.96(p_y)	4.29(p_y)	2.21(p_x)	27.53(p_z)	δ(U-Ar)
H-4	-3.878	10.11(f_y,f_{xyz})	15.65(p_y,p_x)	14.02(p_y,p_x)	44.66(p_x,p_z)	3.27(p_z)	π(U-Pl)
H-5	-4.404	8.00(f_{z^2x},f_z)	29.09(p_y,p_x,p_z)	28.3(p_y,p_x)	7.48(p_x)	3.55(p_z)	π(U-Pl)

Table S9. Contributions (%) to the α-spin orbitals of $[U^{III}L^1]^{2+}$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Ar2	Ar3	Ar4	
LUMO	-5.355	94.58(f_{z^3}, f_x)					U(f)
HOMO	-5.583	86.99(f_{xyz},f_z)	1.02(p_x)				U(f)
H-1	-5.928	69.56(f_x,f_{z^3})		14.67(p_y,p_x)	1.04(p_x)	1.55(p_z)	δ(U-Ar2)
H-2	-5.966	66.19(f_z,f_{xyz})		16.53(p_x,p_y,p_z)	1.24(p_x)	1.25(p_z)	δ(U-Ar2)
H-3	-6.903	16.45(f_y,f_{z^2x})	54.77(p_y,p_x)		3.19(p_x)	8.24(p_z)	π(U-Pl)+π(Ar4/3)
H-4	-7.515	3.26(f_y,p_y)	76.74(p_y,p_x,p_z,s)				π(Pl)
H-5	-7.600	8.2(f_y,f_{z^2y})	56.14(p_x,p_y,p_z,s)	1.32(p_y)	5.51(p_x)	10.65(p_z)	π(Pl)+π(Ar4/3)

Table S10. Contributions (%) to the α-spin orbitals of $[U^{III}L^2]^+$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Ar3	Ar4	
LUMO	-3.808	93.35(f_x,f_{z^3})					U(f)
HOMO	-4.075	84.12(f_z,f_{z^3})			1.79(p_x)	1.05(p_z)	U(f)
H-1	-4.231	72.83(f_x,f_z)	3.69(p_y)	4.21(p_y)	7.04(p_x,p_z)	1.01(p_z)	π(U-Pl)+δ(U-Ar3)
H-2	-4.344	71.74(f_{xyz},f_{z^2y})	1.29(p_y)	1.58(p_y)	11.08(p_z,p_x)	3.01(p_z)	δ(U-Ar3)
H-3	-6.280	13.06(f_{z^2y},f_y)	36.37(p_y, p_z,p_x)	7.69(p_y)	7.90(p_x,p_z)	18.85(p_z)	π(U-Pl)+π(Ar)
H-4	-6.403	12.72(f_{z^2x},f_z)	11.88(p_y)	40.41(p_y, p_x,p_z)	1.64(p_x)	11.91(p_z)	π(U-Pl)+π(Ar4)
H-5	-6.910	7.59(f_y,f_{z^2y})	27.55(p_x,p_y,p_z,s)	19.49(p_x,p_y,p_z)	10.33(p_x,p_z)	17.86(p_z)	π(U-Pl)+π(Ar)

Table S11. Contributions (%) to the α-spin orbitals of $[U^{III}L^{2N}]^{+}$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Py3	Ar4	
LUMO	-3.834	91.28(f_z^3,f_x)			1.98(p_z)		U(f)
HOMO	-4.178	78.37(f_z,$f_z^2{}_x$)			9.72(p_x,p_z)		U(f)
H-1	-4.288	72.05(f_x,f_z)	4.16(p_y)	4.25(p_y)	5.64(p_z,p_x)	1.20(p_z)	π(U-Pl)+δ(U-Py)
H-2	-4.424	71.89(f_{xyz},$f_z^2{}_y$)	1.25(p_y)	1.64(p_y)	8.55(p_x, p_z)	3.12(p_z)	δ(U-Py)
H-3	-6.374	12.93($_z^2{}_y$,f_y)	35.02(p_y,p_x, p_z)	9.39(p_y,p_x)	6.55(p_x, p_z)	19.11(p_z)	π(U-Pl)+π(Ar)+π(Py)
H-4	-6.532	13.24($f_z^2{}_x$,f_z)	14.99(p_y)	38.83(p_y,p_x, p_z)		9.52(p_z)	π(U-Pl)+π(Ar)
H-5	-6.950		23.63(p_x,p_y,s,p_z)	11.22(p_x,p_y,s,p_z)	32.84(p_z,p_x)		π(Pl)+π(Py)

Table S12. Contributions (%) to the α-spin orbitals of $[U^{III}L^{3}]$. (See footnotes to Table S5.)

Orbitals	Energy	Contributions (%)					Assignment
	eV	U	Pl1	Pl2	Pl3	Ar4	
LUMO	-2.700	90.75(f_z^3, f_x)				1.23(p_z)	U(f)
HOMO	-2.839	85.96(f_x,f_z^3)				2.09(p_z)	U(f)
H-1	-3.089	71.52(f_z,f_x)	4.36(p_y)	4.04(p_y)		12.53(p_z)	δ(U-Ar)+π(U-Pl1/2)
H-2	-3.190	71.50(f_{xyz},$f_z^2{}_y$)	1.13(p_y)	1.45(p_y)		15.37(p_z)	δ(U-Ar)
H-3	-4.763	14.33(f_y,f_{xyz})	11.24(p_y,p_x)	8.72(p_y,p_x)		52.87(p_x,p_z)	π(U-Pl)
H-4	-5.467	12.40($f_z^2{}_x$,f_z)	23.97(p_y)	21.87(p_y,p_x)	18.74(p_x,p_z)	2.75(p_z)	π(U-Pl)
H-5	-5.806	7.95($f_z^2{}_y$,d_{yz})	21.5(p_y,p_x,p_z)	17.12(p_y,p_x,p_z)	12.42(p_x,p_z)	23.5(p_z)	π(Pl)+π(Ar)

Table S13. QTAIM data (au.) for the U-X bonds in uranium complexes, where X denotes N or C atoms of the six-membered rings (**Arene** or **Pyridine**). The electron density (ρ), Laplacian ($\nabla^2\rho$), and energy density (H(r) at bond critical points (BCPs), together with the delocalization index δ(U, X), are included.

Complexes	**Ar/Py**	U-X	ρ(*r*)	$\nabla^2\rho(r)$	H(*r*)	δ
$[U^{II}L^1]^+$	Ar2	C	—	—	—	0.263
		C	0.041	0.105	-0.004	0.255
	Ar3	C	0.026	0.075	—	0.181
		C	0.026	0.069	-0.001	0.163
	Ar4	C	0.044	0.123	-0.005	0.290
$[U^{II}L^2]$	Ar3	C	0.051	0.131	-0.008	0.357
	Ar4	C	0.024	0.072	—	0.182
$[U^{II}L^{2N}]$	Py3 [a]	N [a]	0.054	0.183	-0.005	0.438
	Ar4	C	0.026	0.078	—	0.193
$[U^{II}L^3]^-$	Ar4	C	0.034	0.097	-0.002	0.297
$[U^{III}L^1]^{2+}$	Ar2	C	0.060	0.142	-0.012	0.354
		C	0.060	0.144	-0.012	0.333
	Ar3	C	—	—	—	0.183
	Ar4	C	—	—	—	0.228
$[U^{III}L^2]^+$	Ar3	C	0.048	0.127	-0.006	0.301
	Ar4	C	0.024	0.067	—	0.155
$[U^{III}L^{2N}]^+$	Py3 [a]	N [a]	0.055	0.177	-0.005	0.424
	Ar4	C	0.026	0.073	—	0.163
$[U^{III}L^3]$	Ar4	C	0.037	0.111	-0.003	0.262

[a] Six-membered pyridine ring includes one N atoms.

Table S14. Total and averaged values of QTAIM data (au.) for the U-X bonds in uranium complexes, where X denotes N or C atoms of the six-membered rings (**Arene** or **Pyridine**).

Complexes	U-X	ρ(*r*)	□^{2}ρ(*r*)	H(*r*)	δ
$[U^{II}L^1]^+$	Total	0.137	0.372	-0.010	1.152
	Averaged [a]	0.0076	0.0207	-0.0006	0.0640
$[U^{II}L^2]$	Total	0.075	0.203	-0.008	0.539
	Averaged [a]	0.0063	0.0169	-0.0007	0.0449
$[U^{II}L^{2N}]$	Total	0.080	0.261	-0.005	0.631
	Averaged [a]	0.0067	0.0218	-0.0004	0.0526
$[U^{II}L^3]^-$	Total	0.034	0.097	-0.002	0.297
	Averaged [a]	0.0057	0.0162	-0.0003	0.0495
$[U^{III}L^1]^{2+}$	Total	0.120	0.286	-0.024	1.098
	Averaged [a]	0.0067	0.0159	-0.0013	0.0610
$[U^{III}L^2]^+$	Total	0.072	0.194	-0.006	0.456
	Averaged [a]	0.0060	0.0162	-0.0005	0.0380
$[U^{III}L^{2N}]^+$	Total	0.081	0.250	-0.005	0.587
	Averaged [a]	0.0068	0.0208	-0.0004	0.0489
$[U^{III}L^3]$	Total	0.037	0.111	-0.003	0.262
	Averaged [a]	0.0062	0.0185	-0.0005	0.0437

[a] The averaged value was obtained by dividing C/N numbers in six-numbered rings (Arene/Pyrine) of ligand. L^1, L^2/L^{2N} and L^3 include 3, 2 and 1 six-numbered rings, respectively, and thus correspond to 18, 12 and 6 C/N atoms.

Table S15. QTAIM data (au.) for the U-X bonds in uranium complexes, where X denotes N or C atoms of the five-membered rings (**Pyrrole**). The electron density (ρ), Laplacian ($\nabla^2\rho$), and energy density (H(r) at bond critical points (BCPs), together with the delocalization index δ(U, X), are included.

Complexes	**Pl**	U-X	ρ(*r*)	$\nabla^2\rho(r)$	H(*r*)	δ
$[U^{II}L^1]^+$	Pl1	N	0.037	0.120	-0.001	0.286
		C	0.039	0.095	-0.005	0.207
$[U^{II}L^2]$	Pl1	N	—	—	—	0.288
		C	0.051	0.136	-0.007	0.310
	Pl2	N	—	—	—	0.272
		C	0.049	0.129	-0.006	0.298
$[U^{II}L^{2N}]$	Pl1	N	—	—	—	0.280
		C	0.054	0.143	-0.008	0.308
	Pl2	N	—	—	—	0.306
		C	0.050	0.133	-0.007	0.295
$[U^{II}L^3]^-$	Pl1	N	0.035	0.128	0.001	0.252
		C	0.040	0.114	-0.003	0.259
		C	0.042	0.116	-0.004	0.248
	Pl2	N	—	—	—	0.243
		C	0.039	0.111	-0.003	0.252
		C	0.040	0.113	-0.003	0.243
	Pl3	N	0.039	0.134	-0.001	0.285
$[U^{III}L^1]^{2+}$	Pl1	N	0.034	0.090	-0.001	0.300
		C	0.033	0.077	-0.003	0.208
$[U^{III}L^2]^+$	Pl1	N	0.050	0.165	-0.003	0.336
		C	0.052	0.124	-0.008	0.310
		C	0.055	0.127	-0.011	0.256
	Pl2	N	0.045	0.151	-0.002	0.359
		C	0.049	0.116	-0.007	0.297
		C	0.051	0.120	-0.009	0.243
$[U^{III}L^{2N}]^+$	Pl1	N	0.048	0.155	-0.002	0.347
		C	0.045	0.126	-0.005	0.279
		C	0.057	0.131	-0.011	0.270
	Pl2	N	0.052	0.171	-0.004	0.376
		C	0.042	0.114	-0.004	0.209
$[U^{III}L^3]$	Pl1	N	0.038	0.131	—	0.280
		C	0.049	0.122	-0.007	0.301
		C	0.047	0.126	-0.006	0.283
	Pl2	N	0.041	0.142	-0.001	0.297
		C	0.047	0.117	-0.006	0.300
		C	0.045	0.121	-0.005	0.274
	Pl3	N	0.035	0.108	-0.001	0.269

Cartesian coordinates of optimized complexes

$[U^{II}L^{1}]^{+}$

C	1.38807994	-0.16248813	-0.74873077
C	0.98771953	-1.34114651	-1.65973429
C	1.13409026	1.21371412	-1.38879005
C	2.87484705	-0.19432181	-0.34640033
C	-0.04540226	-1.21051202	-2.61175613
C	1.46945865	-2.64154815	-1.36899998
H	1.78694177	1.34084823	-2.26628550
H	1.37489079	2.00677014	-0.66395460
H	0.10001314	1.37729622	-1.72229742
H	3.49949994	-0.02512390	-1.23718357
H	3.20430858	-1.13912016	0.10645610
H	3.08132325	0.60925893	0.37766060
C	-3.37948481	-0.22846396	1.04791818
C	-3.65100017	-1.40450051	0.08739424
C	-3.79014701	-2.71384027	0.61064716
C	0.91203297	-3.80100184	-1.95251513
N	-1.21835574	-5.35101562	-0.63071974
C	-0.56048691	-2.34994525	-3.24880471
H	-0.42746797	-0.22664423	-2.88698817
H	2.28172594	-2.75895821	-0.65414052
C	-3.64447735	1.14815609	0.41322144
C	-4.22999599	-0.29387876	2.33077664
C	-3.50530804	-1.25644237	-1.30818911
H	-3.92642377	-2.84519031	1.68245089
C	-3.72825208	-3.86407486	-0.20709340
C	1.18573539	-5.18140624	-1.33587985
C	-0.11811887	-3.63516276	-2.90505140
C	-1.96933957	-5.20889178	0.51481627
C	0.09749601	-5.18043335	-0.26208502
H	-1.31866686	-2.23327067	-4.02581260
H	-4.71680759	1.25141120	0.18557105
H	-3.09160038	1.33473602	-0.51780387
H	-3.36667382	1.94108969	1.12483152
H	-5.29095750	-0.14769253	2.07523535
H	-3.92679977	0.51033960	3.01921281
H	-4.15583837	-1.24274280	2.87888622
C	-3.51056357	-2.38812837	-2.13804589
H	-3.42331483	-0.26579490	-1.75720754
C	-3.58568250	-3.68094167	-1.60069640
C	-3.49499032	-5.24566857	0.42339291
C	0.97821305	-6.33589321	-2.33239016
C	2.58911928	-5.30563121	-0.72359236
H	-0.57121180	-4.50593202	-3.37886316
C	-1.14637023	-4.85195937	1.60355808
C	0.18696019	-4.83362602	1.10236713
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H	-3.53661557	-4.54424629	-2.26427642
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C	-4.14427449	-5.39902687	1.80715272
H	1.19695398	-7.29194548	-1.83194728
H	1.65934031	-6.22923459	-3.19177409
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H	2.70413771	-6.30353078	-0.27363967
H	2.79228690	-4.56844207	0.06781965
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H	-3.42447624	-6.43540442	-1.42838075
H	-5.04857366	-6.31993963	-0.67144165
H	-3.79341856	-4.66049183	2.54370327
H	-3.91062835	-6.39566424	2.21165390
H	-5.23902170	-5.30796694	1.72650922
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H	0.16117892	-2.55738448	3.13263601
H	1.83165697	-1.75626524	1.49943721
H	-1.19793094	0.71789554	-0.35336430

$[U^{II}L^{2}]$

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C	1.31094641	-0.19909363	-0.68350182
N	-1.04710737	-0.02532737	0.10604571
H	1.14055972	-1.69135653	2.00864426
C	-1.06809421	-1.26844655	2.03201146
C	0.97014833	-1.34516331	-1.64740551
C	1.15216182	1.18888369	-1.32688777
C	2.72570539	-0.30124289	-0.09079581
C	-1.82766178	-0.47700870	1.14045660
H	-1.40082537	-1.73420304	2.95841694
C	-0.03476481	-1.20662524	-2.62993421
C	1.43051583	-2.64693591	-1.33858679
H	1.82391358	1.28932516	-2.19534300
H	1.41135107	1.96632767	-0.59032000
H	0.11621716	1.37347535	-1.64038365
H	3.48161428	-0.24877026	-0.89133586
H	2.89504257	-1.22783935	0.47708001
H	2.89156939	0.53878612	0.60211528
C	-3.33870507	-0.27754305	1.05414177
C	-3.67981473	-1.42393640	0.09075980
C	-3.78556515	-2.73513809	0.61181267
C	0.89754369	-3.80465972	-1.95303536
N	-1.20547300	-5.39327804	-0.56018155
C	-0.55226780	-2.34806767	-3.27283504
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H	2.19365129	-2.76468182	-0.57230655
C	-3.68179587	1.10713512	0.47912763
C	-4.01442394	-0.41443774	2.42818334
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C	-3.75224256	-3.88353016	-0.21400288
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C -0.10661578 -3.64014470 -2.93231011
C -1.96552581 -5.16356773 0.55913404
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H 1.06235128 -4.37373759 1.67564892
H -3.68925572 -7.37578785 0.06607111
H -3.34105202 -6.44302609 -1.39683869
H -4.98414321 -6.38295393 -0.67026093
H -3.83897416 -4.66125302 2.54654322
H -3.91046847 -6.40100176 2.22296800
H -5.25622500 -5.34168600 1.70768899
U -1.20599569 -2.68079369 -0.43899514

$[U^{II}L^{2N}]$
C 0.23146054 -0.48569519 0.37101510
C 0.25606146 -1.27749404 1.53905063
C 1.30813710 -0.28217645 -0.68847454
N -1.04649902 -0.05012284 0.10528301
H 1.12483246 -1.74250066 2.00084327
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C 0.89865942 -1.40212084 -1.65519386
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C 2.71860082 -0.50448205 -0.12555836
C -1.83031779 -0.48489140 1.14311455
H -1.41899715 -1.73999098 2.96567086
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H 1.86377240 1.18916512 -2.20076702
H 1.54523203 1.86860781 -0.57744294
H 0.18101455 1.36963315 -1.59197667
H 3.46775815 -0.37562654 -0.92419089
H 2.83283818 -1.51801328 0.28122061
H 2.92242367 0.23171941 0.66835186
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C 0.82958115 -3.74376533 -1.94589557
N -1.20313301 -5.36957681 -0.55469704
C -0.58814812 -2.34099946 -3.32364525
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C 1.16648108 -5.08776652 -1.28509169
C -0.12908956 -3.62579276 -2.96973455
C -1.96764812 -5.15672260 0.56364873
C 0.09604728 -5.08700133 -0.20005333
H -1.32633995 -2.22047732 -4.11901644
H -4.75298487 1.18549951 0.26039493
H -3.09910509 1.31444432 -0.43344395
H -3.40889646 1.88652348 1.21196105
H -5.11277987 -0.37064511 2.32642532
H -3.70145835 0.43423262 3.07391265
H -3.75491037 -1.33252995 2.96329281
C -3.59486157 -2.40005545 -2.13648618
H -3.49266880 -0.27419562 -1.73812910
C -3.66524360 -3.70061663 -1.60181740
C -3.48733888 -5.25043033 0.44176197
C 0.99508352 -6.28513639 -2.23209267
C 2.58349902 -5.09203009 -0.69541034
H -0.52434357 -4.51242901 -3.46593136
C -1.17789503 -4.64835888 1.62066002
C 0.15835446 -4.60717667 1.12575903
H -3.54388470 -2.26727973 -3.21939942
H -3.61991235 -4.56106544 -2.26974667
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H 1.27722965 -7.21055780 -1.70450194
H 1.64621002 -6.17490248 -3.11502169
H -0.04844557 -6.40043167 -2.55633023
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H 2.75359397 -4.21699636 -0.05420809
H 3.32948436 -5.06517306 -1.50685589
H -1.49702930 -4.41071028 2.63441423
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H -3.32790702 -6.44035370 -1.39496501
H -4.97633445 -6.38842503 -0.67846698
H -3.85246288 -4.66845215 2.54968576
H -3.90286201 -6.40881179 2.22543714
H -5.25954512 -5.36505042 1.70737162
U -1.21687398 -2.68021133 -0.44199347
N 1.29878795 -2.65152385 -1.27079179

$[U^{II}L^{3}]^{-}$
C 0.22544601 -0.39479164 0.42819726
C 0.28231880 -1.14503137 1.62408371
C 1.25930579 -0.24669073 -0.68298028
N -1.05789912 0.00662538 0.16697657

H	1.16104676	-1.60475775	2.07463955
C	-1.05216089	-1.16502037	2.13926898
C	1.00387864	-1.50400737	-1.50568834
C	1.01198084	1.02706192	-1.50383370
C	2.69198936	-0.24055839	-0.12526502
C	-1.82903778	-0.42148374	1.21879130
H	-1.37586397	-1.61267733	3.07886607
C	0.15156771	-1.73137764	-2.60665460
H	1.70224747	1.05976255	-2.36395276
H	1.17817222	1.92125790	-0.87895202
H	-0.02534258	1.06205598	-1.86590914
H	3.41987949	-0.15088452	-0.95027267
H	2.90254553	-1.17963874	0.40595418
H	2.82833323	0.60963245	0.56499381
C	-3.34133239	-0.27876209	1.08071750
C	-3.63066823	-1.42207076	0.09235833
C	-3.78634347	-2.73500256	0.61187164
C	0.93993076	-3.68927814	-1.77485632
N	-1.21839313	-5.43853151	-0.50805373
H	-0.35521469	-0.98483952	-3.21799133
C	-3.71388832	1.10147543	0.50947443
C	-4.05281538	-0.44653796	2.43305412
C	-3.37813039	-1.27028223	-1.29661328
H	-3.97371469	-2.86216925	1.67559669
C	-3.70389285	-3.88714145	-0.21507766
C	1.11684083	-5.12126900	-1.28390482
C	0.11011895	-3.15309628	-2.78191943
C	-1.97259404	-5.23609656	0.62083020
C	0.08375739	-5.18849086	-0.16402286
H	-4.78840022	1.13917454	0.25974555
H	-3.12075485	1.32885068	-0.38637980
H	-3.49367329	1.88421835	1.25545077
H	-5.14696891	-0.48170526	2.29455967
H	-3.80647502	0.40872355	3.08415713
H	-3.74502855	-1.35970290	2.96394290
C	-3.29782465	-2.40708703	-2.13469445
H	-3.20343505	-0.28049785	-1.71868262
C	-3.45031252	-3.70810424	-1.60057524
C	-3.48935536	-5.25277494	0.46062624
C	0.80340554	-6.14181493	-2.38750586
C	2.54207327	-5.34451356	-0.75241676
H	-0.43463186	-3.69871761	-3.55228387
C	-1.16212505	-4.78609187	1.69050388
C	0.17345166	-4.75737717	1.17846930
H	-3.10644557	-2.27946975	-3.20357487
H	-3.33073713	-4.57255159	-2.25386276
C	-3.93555191	-6.42660628	-0.43001657
C	-4.20222620	-5.38157009	1.81650239
H	0.91316335	-7.16857534	-1.99841251
H	1.49635133	-6.00590674	-3.23547441
H	-0.23164010	-6.02814762	-2.73976247
H	2.62403851	-6.34315881	-0.28998432
H	2.80114944	-4.57598913	-0.01035321
H	3.27059359	-5.27278243	-1.57860971
H	-1.46757123	-4.56336191	2.71281742
H	1.07333603	-4.47367692	1.72274261
H	-3.76756456	-7.37989860	0.09975963
H	-3.34836272	-6.46121481	-1.35740540
H	-5.00814616	-6.33940425	-0.67557074
H	-3.84841256	-4.64628112	2.55460653
H	-4.01095253	-6.38326525	2.23615085
H	-5.29129469	-5.25082716	1.69645612
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N	1.44431428	-2.69182222	-0.98037438

$[U^{III}L^{1}]^{2+}$

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C	0.99112309	-1.33742692	-1.65923251
C	1.13530801	1.22130671	-1.38660711
C	2.87856044	-0.19243707	-0.33997828
C	-0.03833083	-1.20774602	-2.61490216
C	1.47059086	-2.63504838	-1.37170075
H	1.79172685	1.35169719	-2.26043032
H	1.37674978	2.01353591	-0.66167593
H	0.10300826	1.39012655	-1.72401027
H	3.50488913	-0.01507053	-1.22741288
H	3.21249656	-1.13835235	0.10795931
H	3.08370208	0.60864720	0.38657419
C	-3.38561958	-0.22104473	1.04573871
C	-3.65469383	-1.40315247	0.08647014
C	-3.79357766	-2.70848562	0.60922227
C	0.92932563	-3.79510854	-1.96674551
N	-1.22068765	-5.23511676	-0.63407065
C	-0.52662592	-2.34380909	-3.28031125
H	-0.42533106	-0.22390017	-2.88548446
H	2.26711991	-2.75566455	-0.63841755
C	-3.64526997	1.15417085	0.40536324
C	-4.23409930	-0.28833826	2.33036604
C	-3.51374492	-1.25979223	-1.30971979
H	-3.90631437	-2.83971830	1.68472755
C	-3.74967125	-3.86191245	-0.20326950
C	1.19682543	-5.17417305	-1.34339865
C	-0.07445381	-3.62601012	-2.94603464
C	-1.97731532	-5.18520888	0.52291299
C	0.11007697	-5.15597163	-0.26485557
H	-1.27064541	-2.22531761	-4.07190792
H	-4.71751343	1.26037880	0.18070022
H	-3.09478461	1.34301644	-0.52700385
H	-3.36884008	1.94818067	1.11569800
H	-5.29377239	-0.13470426	2.07584753
H	-3.92962870	0.51530805	3.01821925
H	-4.16767992	-1.23699283	2.88041827
C	-3.55739196	-2.39137384	-2.14024437
H	-3.42537358	-0.27016884	-1.76114577
C	-3.64499518	-3.68009408	-1.60017225
C	-3.50484526	-5.23974384	0.43168896
C	0.97179588	-6.33695995	-2.32741309
C	2.59992711	-5.30350378	-0.73029299
H	-0.50430842	-4.49598948	-3.44473148
C	-1.13824418	-4.92088381	1.61960835
C	0.19848451	-4.90206007	1.11516176
H	-3.52293243	-2.26415019	-3.22507509
H	-3.62883615	-4.54518379	-2.26477425
C	-3.95918227	-6.40785032	-0.46335303
C	-4.14838500	-5.39466074	1.81844779
H	1.16650159	-7.29058496	-1.81375098
H	1.66761116	-6.25650518	-3.17728959

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H 2.81479224 -4.56637376 0.05840318
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H -1.20218327 0.70463662 -0.36696024

$[U^{III}L^{2}]^{+}$

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C 0.27262681 -1.24823171 1.53689087
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H 1.38059417 1.95533584 -0.56121769
H 0.11213294 1.36845800 -1.64494691
H 3.48631518 -0.23515632 -0.88455087
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H 2.88402286 0.52469772 0.61296804
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C 0.90844021 -3.79970627 -1.96477856
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H -3.89748931 -6.38916634 2.22905642
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$[U^{III}L^{2N}]^{+}$

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H 2.84665717 -1.52132596 0.27747765
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C -3.62530075 -2.39787822 -2.13759526
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C -1.17911253 -4.64573329 1.63154925
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[$U^{III}L^{3}$]
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H -3.34836272 -6.46121481 -1.35740540
H -5.00814616 -6.33940425 -0.67557074

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H	-4.01095253	-6.38326525	2.23615085
H	-5.29129469	-5.25082716	1.69645612
U	-1.18808674	-2.70300054	-0.26329840
N	1.44431428	-2.69182222	-0.98037438