Supporting Information

Theoretical investigation of U(I) arene complexes: is the elusive monovalent oxidation state accessible?

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HOMO **H-1** **H-2**

H-3 **H-4** **H-5**
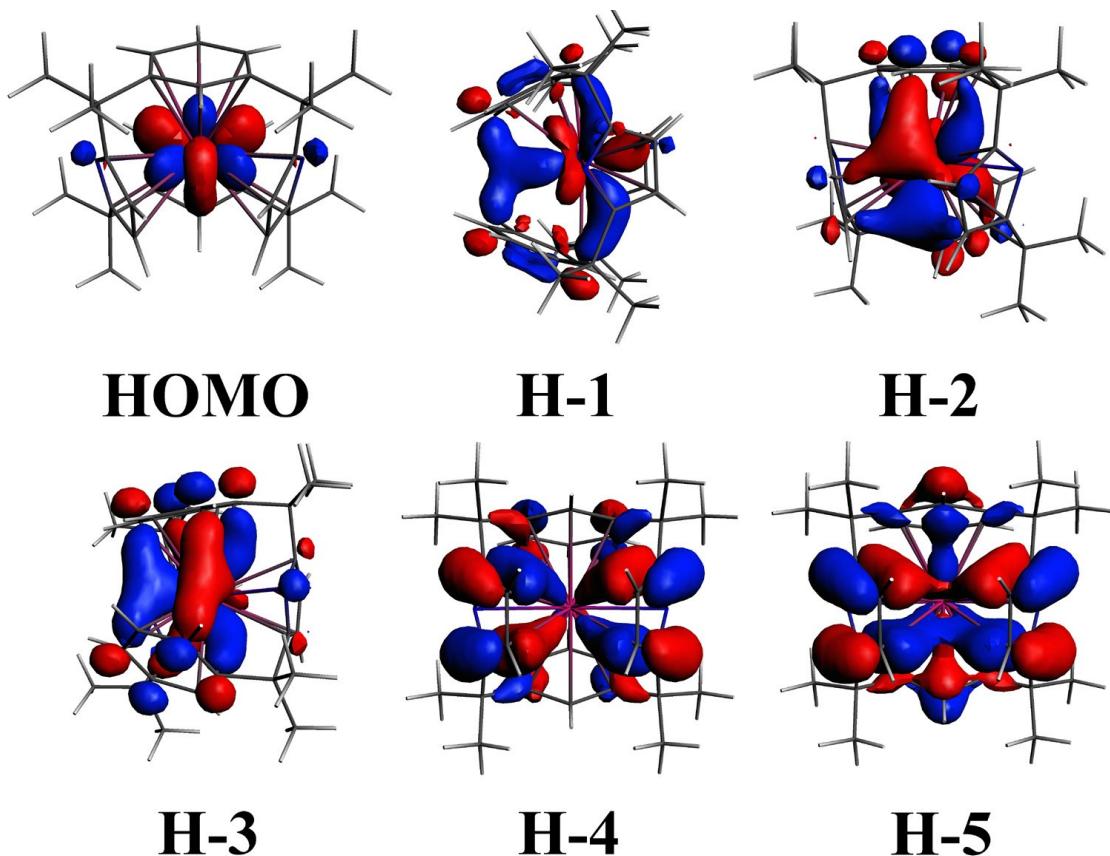
**Figure S1**. Characteristic α-spin orbitals of [U^{II}L] (quintet ground state).
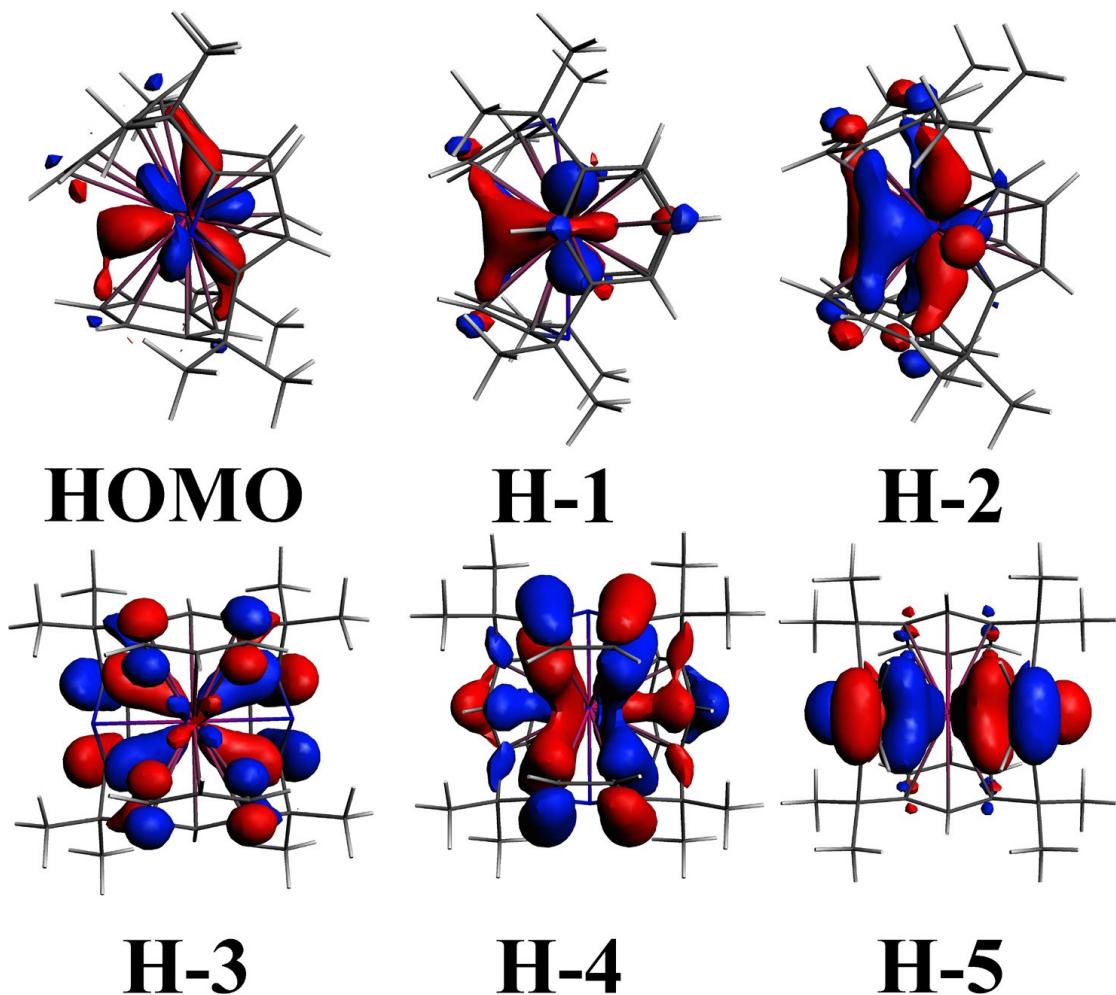
Figure S2. Characteristic α-spin orbitals of $[U^{III}L]^+$ (quartet ground state).
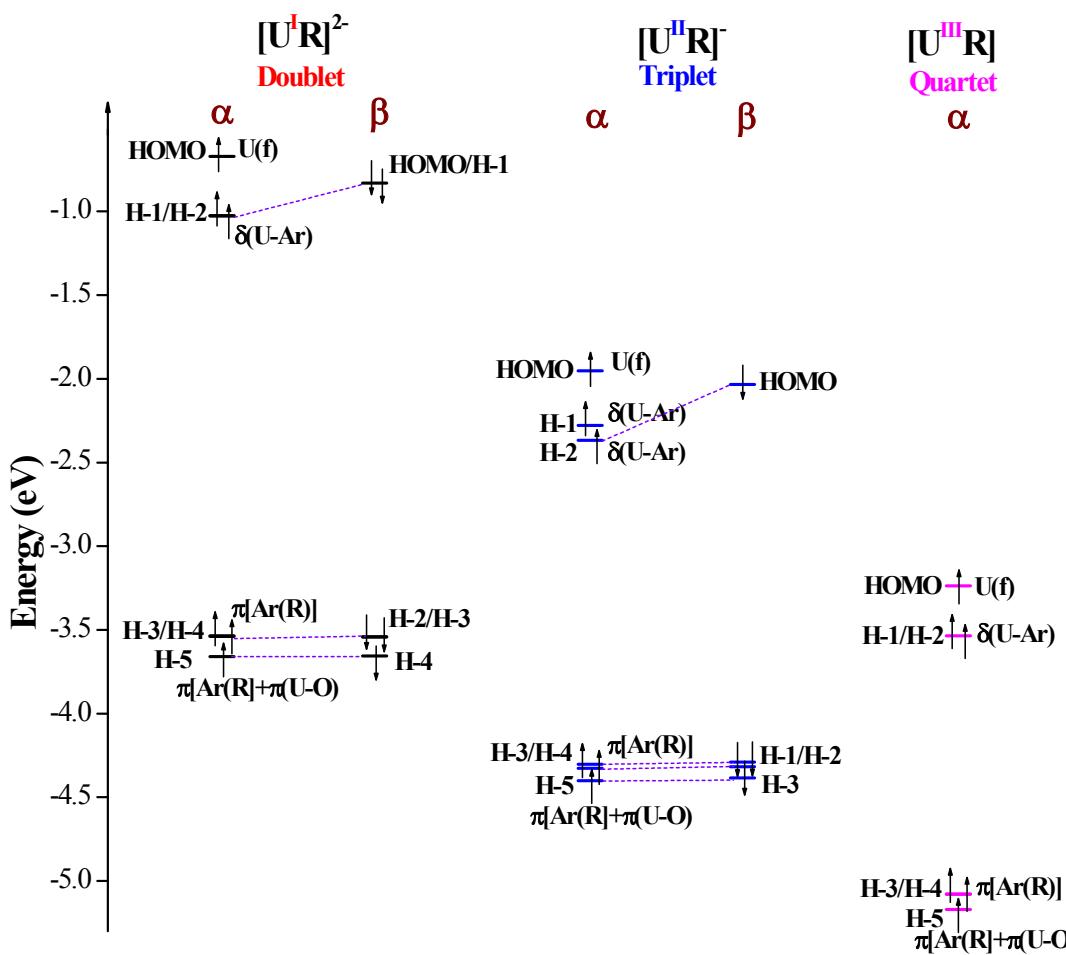
Figure S3. Energy levels of orbitals and character for [U^mR]^n complexes where the oxidation state (m) ranges from I to III. Noting that only spin-up orbitals (α) are illustrated for the U(III) complex. Ar mentioned in the diagram denotes the central arene group of H_3R and Ar(R) means others.
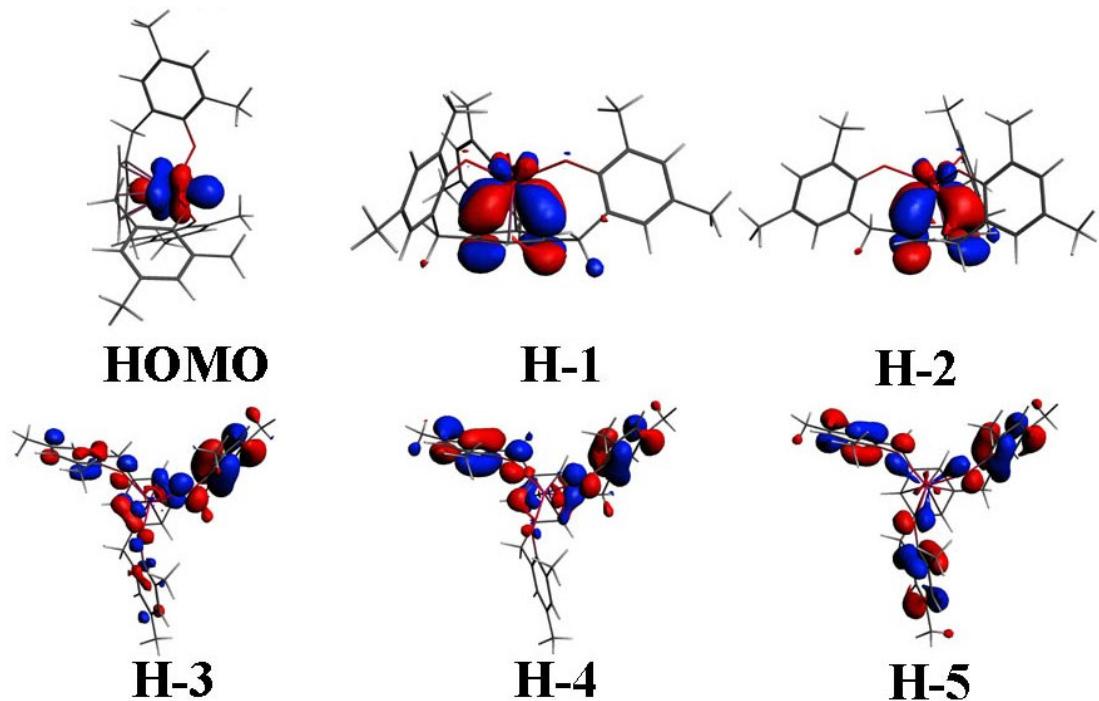
Figure S4. Characteristic α-spin orbitals of $[U^IR]^{2-}$ (doublet ground state).
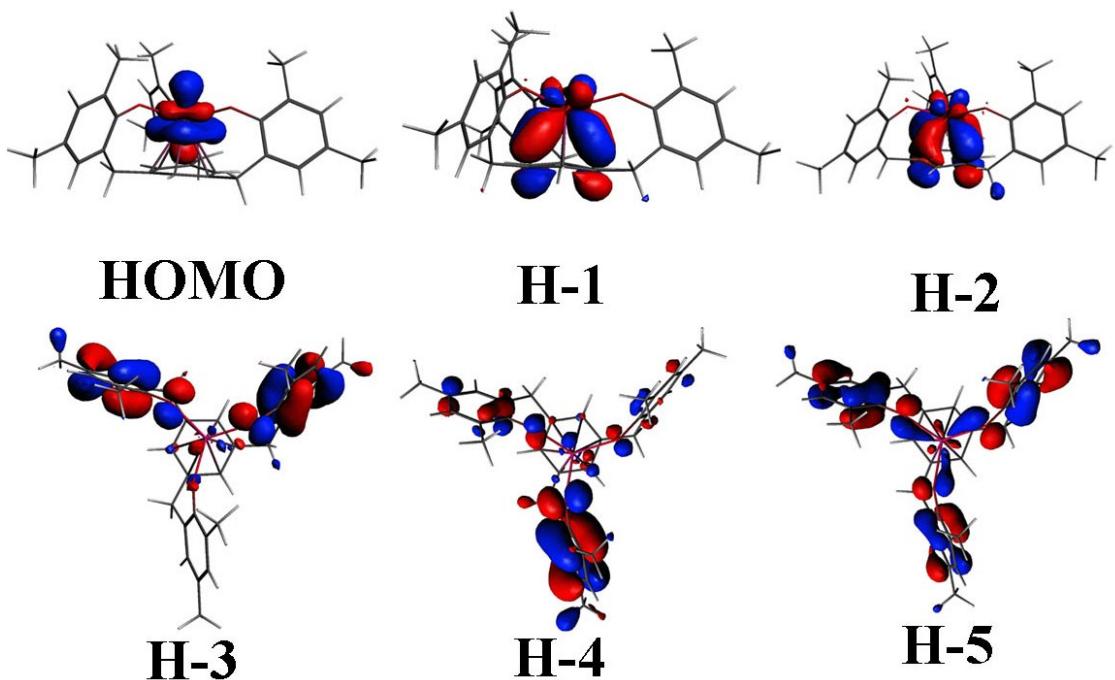
Figure S5. Characteristic α-spin orbitals of $[U^{II}R]^-$ (triplet ground state).

HOMO H-1 H-2 H-3 H-4 H-5
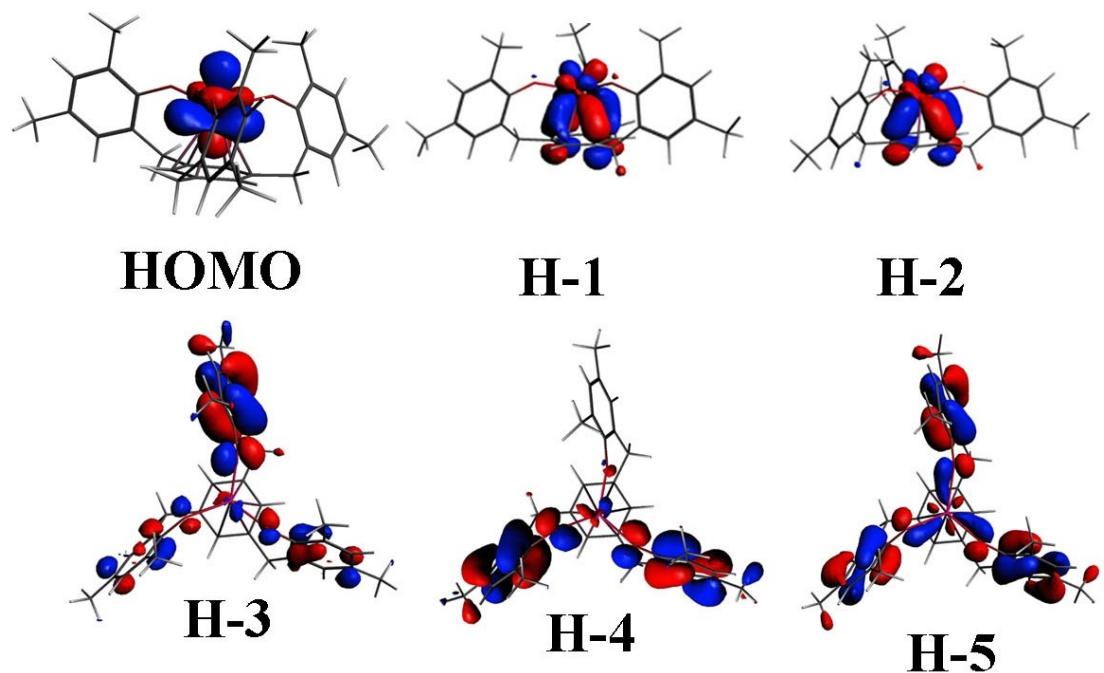
Figure S6. Characteristic α-spin orbitals of [U^{III}R] (quartet ground state).

α-HOMO   **α-H-1**   **α-H-2**

α-H-3   **α-H-4**   **β-HOMO**
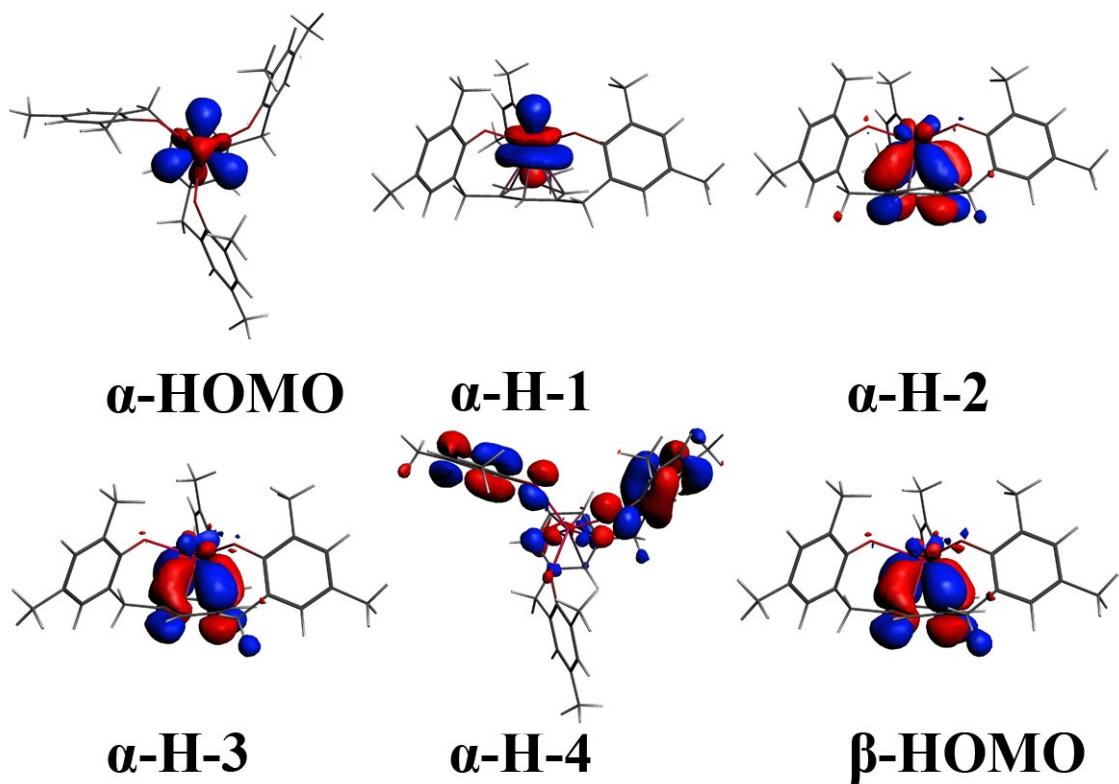
Figure S7. Characteristic orbitals of [U^{I}R]$^{2-}$ (quartet state)
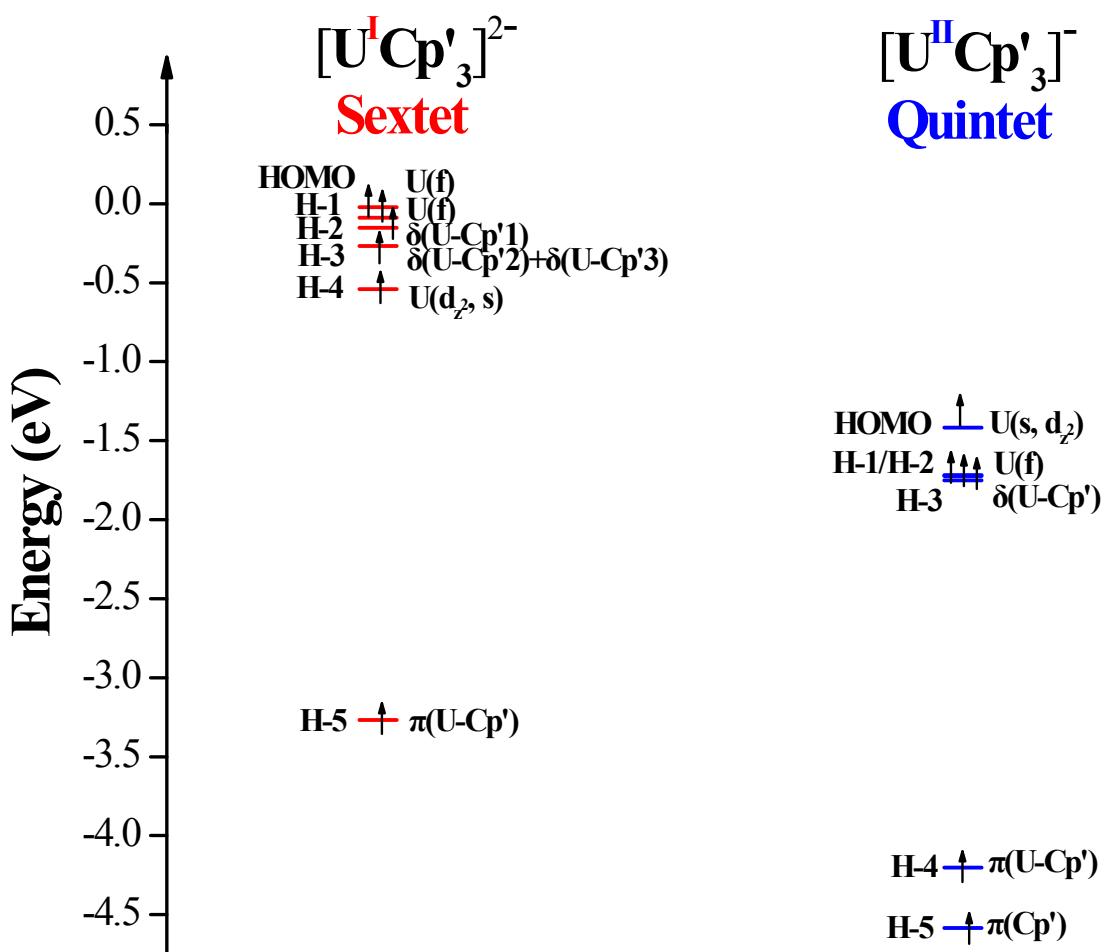
Figure S8. Energy levels of α-spin orbitals and character for $[U^mCp'_3]^n$ complexes (m = I and II).
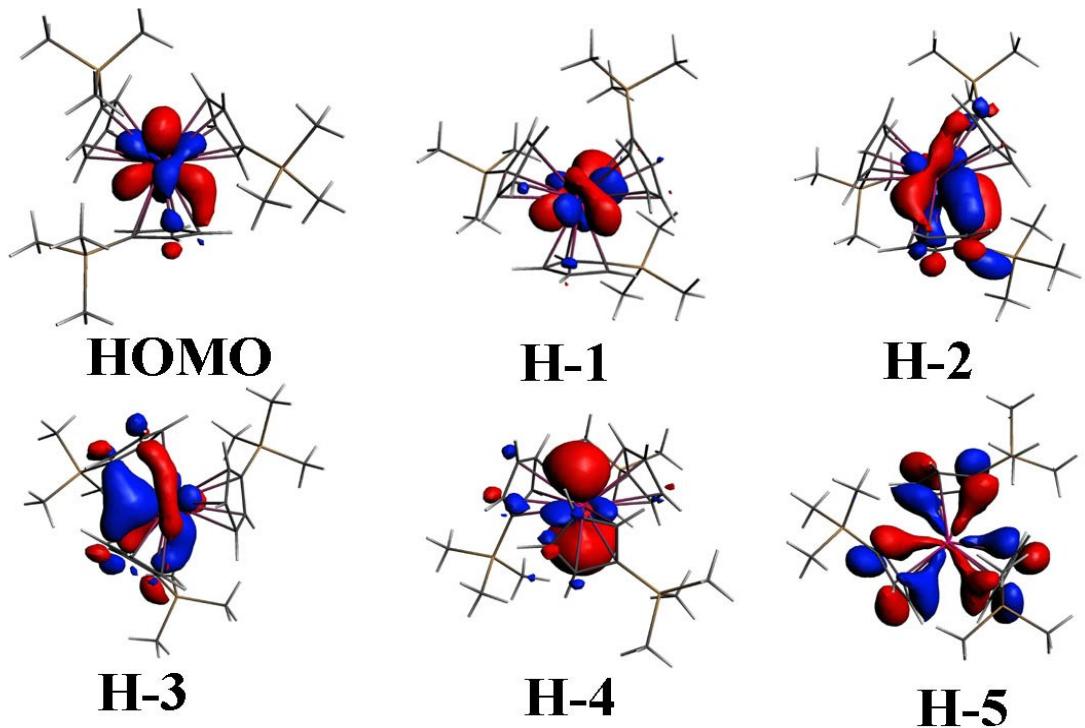
Figure S9. Characteristic α-spin orbitals of the sextet ground state [U$^{\text{I}}$Cp′$_3$]$^{2-}$.
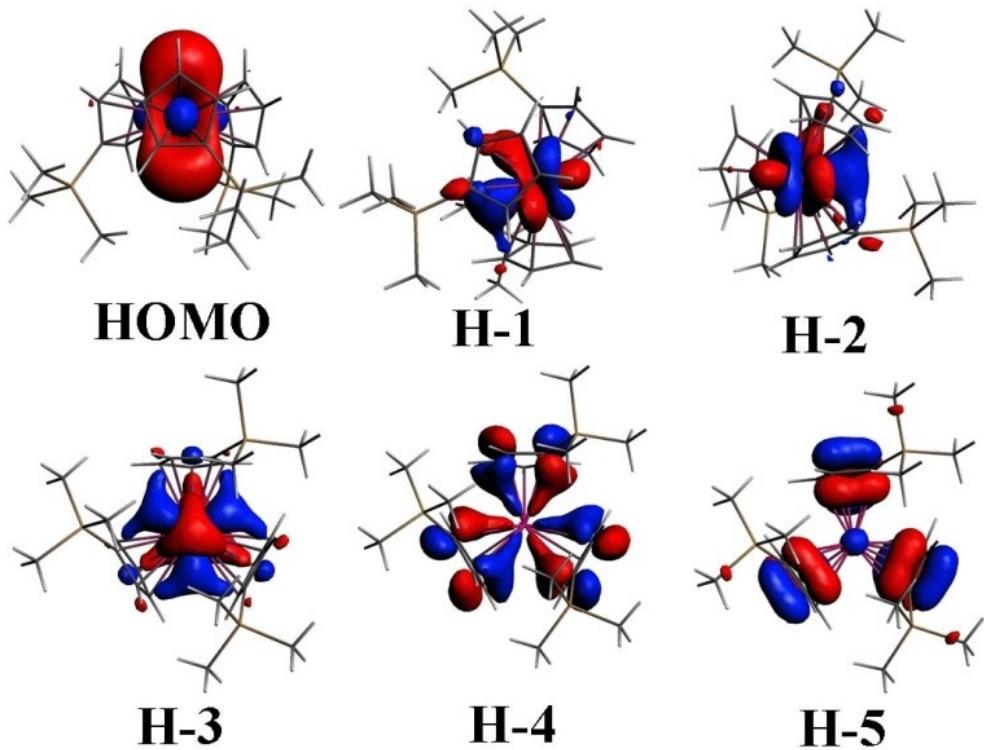
Figure S10. Characteristic α-spin orbitals of $[U^{II}Cp'_3]^-$ (quintet ground state).

Table S1. Calculated relative energies (eV) of uranium complexes in various electron-spin states (ESSs).

| Complexes	ESSs	ΔE [a]	ΔE_0 [a]	ΔH [a]	ΔG [a]
$[U^{I}L]^-$	Doublet	0.192	0.180	0.185	0.170
	Quartet	0.000	0.000	0.000	0.000
	Sextet	0.614	0.595	0.597	0.571
$[U^{II}L]$	Singlet	0.508	0.485	0.489	0.483
	Triplet	0.116	0.101	0.104	0.095
	Quintet	0.000	0.000	0.000	0.000
	Septet	2.040	1.944	1.951	1.930
$[U^{III}L]^+$	Doublet	0.343	0.328	0.328	0.333
	Quartet	0.000	0.000	0.000	0.000
	Sextet	2.092	1.990	2.001	1.984
$[U^{I}R]^{2-}$	Doublet	0.000	0.000	0.000	0.000
	Quartet	0.000	0.010	0.006	0.024
	Sextet	0.673	0.624	0.634	0.593
$[U^{II}R]^-$	Singlet	0.164	0.176	0.165	0.255
	Triplet	0.000	0.000	0.000	0.000
	Quintet	0.059	0.086	0.082	0.086
$[U^{III}R]$	Doublet	0.294	0.248	0.261	0.199
	Quartet	0.000	0.000	0.000	0.000
$[U^{I}Cp'_3]^{2-}$	Doublet	0.353	0.309	0.314	0.314
	Quartet	0.165	0.180	0.177	0.177
	Sextet	0.000	0.000	0.000	0.000
$[U^{II}Cp'_3]^-$	Singlet	1.041	0.987	0.987	0.987
	Triplet	0.413	0.405	0.406	0.406
	Quintet	0.000	0.000	0.000	0.000

[a] The total energy (E), total energy including zero-point vibrational energy (E_0) and enthalpy (H) and free energy correction (G), where temperature is 298.15 K. And ΔE, ΔE_0, ΔH and ΔG (in eV) denote the relative energy with respect to the lowest-energy isomer.

Table S2. Optimized geometry parameters for the uranium complexes ligated by H_3R, compared with experimental values. (Distance in Å and angle in °)

Complexes	$[U^I R]^{2-}$	$[U^{II} R]^-$	$[U^{II} R^E]^-$		$[U^{III} R]$	$[U^{III} R^E]$		$[U^{III} R^{E2}]$	H_3R
Appr.s	Calc.	Calc.	Calc.	Expt.[b]	Calc.	Calc.	Expt.[b]	Expt.[c]	Calc.
$(U\text{-}C_{Ar})_{av}$	2.509	2.576	2.580	2.615	2.692	2.691	2.749	2.731	
$U\text{-}C_{Ar}$	2.498~2.520	2.492~2.612	2.476~2.649	2.597~2.633	2.689~2.694	2.669~2.712	2.729~2.774	2.719~2.745	
$U\text{-}Ar_{cent}$	2.055	2.143	2.144	2.180	2.288	2.280	2.350	2.335	
$U\text{-}O$	2.270	2.213	2.221	2.236	2.154	2.160	2.168	2.164	
U_{o3} [a]	0.867	0.685	0.674	0.668	0.479	0.508	0.475	0.465	
$(C_{Ar}\text{-}C_{Ar})_{av}$	1.440	1.431	1.442	1.432	1.418	1.429	1.423	1.419	1.400
$C_{Ar}\text{-}C_{Ar}$	1.439~1.441	1.398~1.448	1.402~1.464	1.432	1.417~1.418	1.428~1.431	1.417~1.428	1.414~1.424	1.398~1.401
$O\text{-}U\text{-}O$	106.3	110.9	111.2	111.5	115.2	114.6	115.3	115.5	
$\theta1$ [d]	4.3	2.4~13.7	4.6~21.4	5.7~5.8	0.8~0.9	6.5~6.6	4.1~6.8	0.7~2.8	0.1~0.8
$\theta2$ [d]	4.3	8.3	11.9	5.8	0.8	6.5	5.4	1.6	0.4

[a.] U_{o3} denotes the normal distance of the U ion to the plane defined by three oxygen donors, and a positive value refers to U being below the O3 plane.

[b.] Experimental values of $[U^{II} R^E]^-$ and $[U^{III} R^E]$ from Refs. [5, 8].

[c.] H_3R^{E2} is ($^{t\text{-}Bu, t\text{-}Bu}$ArOH)$_3$*mesitylene*; experimental values of its U^{III} complex taken from Ref. [9].

[d] $\theta1$ is the dihedral angle of the central arene and $\theta2$ is the average value.

Table S3. Optimized geometry parameters for the uranium complexes ligated by Cp' ligands, compared with experimental values. (Distance in Å and angle in °)

Complexes	$[U^{I}Cp'_3]^{2-}$	$[U^{II}Cp'_3]^{-}$	
Approaches	Calc.	Calc.	Expt.[c]
$(U-C)_{av}$	2.802	2.786	2.794
U-C	2.739~2.841	2.757~2.819	2.762~2.822
$(U-Cp'_{cent})_{av}$	2.524	2.508	2.521
$U-Cp'_{cent}$	2.516~2.531	2.508	2.514~2.530
β1 [a]	117.6	119.9	123.1
β2 [a]	120.1	119.9	118.8
β3 [a]	118	119.9	118.1
γ1 [b]	59.4	60.3	57.1
γ2 [b]	61.8	60.3	60.8
γ3 [b]	64.3	60.3	62.2

[a] β1, β2 and β3 denote the Cp'1$_{cent}$-U-Cp'2$_{cent}$, Cp'2$_{cent}$-U-Cp'3$_{cent}$, and Cp'1$_{cent}$-U-Cp'3$_{cent}$ angles, respectively.
[b] γ1 is the interplanar angle between Cp'1 and Cp'2, γ2 between Cp'2 and Cp'3, and γ3 is between Cp'1 and Cp'3.
[c] Experimental values for $[U^{II}Cp'_3]^{-}$ from Ref. [1].

Table S4. Electron-spin density (S) and Mulliken charge (Q) of uranium complexes calculated by the Priroda code.

Complexes	ESSs	S_U	S_{Ligand}	Q_U	Q_{Ligand}
$[U^IL]^-$	Quartet	2.679	0.321	1.905	-2.905
$[U^{II}L]$	Quintet	3.170	0.830	1.939	-1.939
$[U^{III}L]^+$	Quartet	2.742	0.258	2.006	-1.006
$[U^IR]^{2-}$	Doublet	1.250	-0.250	1.252	-3.252
$[U^{II}R]^-$	Triplet	1.987	0.013	1.368	-2.368
$[U^{III}R]$	Quartet	2.649	0.351	1.437	-1.437
$[U^ICp'_3]^{2-}$	Sextet	4.379	0.621	0.967	-2.967
$[U^{II}Cp'_3]^-$	Quintet	3.784	0.216	1.335	-2.335

Table S5. Electron-spin density (S) and Mulliken charge (Q) of uranium complexes in the gas phase calculated by the ADF code.

Complexes	ESSs	S_U	S_{Ligand}	Q_U	Q_{Ligand}
[U^{I}L]$^-$	Quartet	2.696	0.305	0.681	-1.681
[U^{II}L]	Quintet	3.205	0.795	0.532	-0.532
[U^{III}L]$^+$	Quartet	2.735	0.265	0.448	0.552
[U^{I}R]$^{2-}$	Doublet	1.250	-0.250	1.375	-3.375
[U^{II}R]$^-$	Triplet	2.000	0.000	1.467	-2.467
[U^{III}R]	Quartet	2.672	0.328	1.512	-1.512
[U^{I}Cp'$_3$]$^{2-}$	Sextet	4.156	0.844	0.555	-2.555
[U^{II}Cp'$_3$]$^-$	Quintet	3.829	0.171	0.561	-1.561

Table S6. Electron-spin density (S) and Mulliken charge (Q) of uranium complexes in solution calculated by the ADF code.

Complexes	ESSs	S_U	S_{Ligand}	Q_U	Q_{Ligand}
[U^{I}L]$^-$	Quartet	2.704	0.296	0.733	-1.733
[U^{II}L]	Quintet	3.205	0.795	0.548	-0.548
[U^{III}L]$^+$	Quartet	2.745	0.255	0.454	0.546
[U^{I}R]$^{2-}$	Doublet	1.310	-0.310	1.470	-3.470
[U^{II}R]$^-$	Triplet	2.000	0.000	1.480	-2.480
[U^{III}R]	Quartet	2.682	0.318	1.515	-1.515
[U^{I}Cp'$_3$]$^{2-}$	Sextet	4.311	0.689	0.557	-2.557
[U^{II}Cp'$_3$]$^-$	Quintet	3.846	0.154	0.566	-1.566

Table S7. Averaged QTAIM data[a] (au.) at U-X BCPs in uranium complexes.

Complexes	Ring	X [b]	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$ [c]	$V(r)$	$G(r)$
[U^{I}L]$^-$	Pl1	N	0.0306	0.1103	0.0006	-0.0263	0.0269
		C	0.0329	0.0892	-0.0023	-0.0269	0.0246
	Pl2	N	0.0306	0.1103	0.0006	-0.0263	0.0269
		C	0.0329	0.0893	-0.0023	-0.0269	0.0246
[U^{II}L]	Pl1	N	0.0521	0.3760	0.0092	-0.0756	0.0848
		C	0.0365	0.0977	-0.0032	-0.0309	0.0277
	Pl2	N	0.0360	0.1274	-0.0001	-0.0321	0.0320
		C	0.0365	0.0977	-0.0032	-0.0309	0.0277
[U^{I}R]$^{2-}$	—	O	0.0865	0.3006	-0.0118	-0.0987	0.0869
[U^{II}R]$^-$	—	O	0.0953	0.3623	-0.0154	-0.1214	0.1060

[a] QTAIM data include electron density $\rho(r)$, Laplacian $\nabla^2\rho(r)$ and energy density $H(r)$.
[b] X denotes N or C atoms of pyrrolic (Pl) rings, and O atom in R complexes.
[c] $H(r)$ is the sum of potential $V(r)$ and kinetic $G(r)$ energy density.

Table S8. Electron-spin density (S) of uranium complexes calculated by the Priroda code.

Complexes	ESSs	S_U	S_{Ligand}	ΔS_U [a]	ΔS_{Ligand} [a]
$[U^IL]^-$	Doublet	0.903	0.097	0.903	0.097
	Quartet	2.679	0.321	0.691	0.309
	Sextet	3.478	1.522	0.308	0.692
	Average			*0.634*	*0.366*
$[U^{II}L]$	Singlet	0.000	0.000		
	Triplet	1.988	0.012	0.940	0.060
	Quintet	3.170	0.830	0.428	0.572
	Average			*0.684*	*0.316*
$[U^{III}L]^+$	Doublet	1.048	-0.048		
	Quartet	2.742	0.258		
$[U^IR]^{2-}$	Doublet	1.250	-0.250	1.250	-0.250
	Quartet	2.679	0.321	0.692	0.308
	Sextet	3.447	1.553	0.274	0.726
	Average			*0.739*	*0.261*
$[U^{II}R]^-$	Singlet	0.000	0.000		
	Triplet	1.987	0.013	1.079	-0.079
	Quintet	3.173	0.827	0.524	0.476
	Average			*0.802*	*0.199*
$[U^{III}R]$	Doublet	0.908	0.092		
	Quartet	2.649	0.351		
$[U^ICp_3']^{2-}$	Doublet	1.146	-0.146	1.146	-0.146
	Quartet	2.724	0.276	0.709	0.291
	Sextet	4.379	0.621	0.595	0.405
	Average			*0.817*	*0.183*
$[U^{II}Cp3']^-$	Singlet	0.000	0.000		
	Triplet	2.015	-0.015		
	Quintet	3.784	0.216		

[a] ΔS_U and ΔS_{Ligand} correspond to one-electron reduction, for instance the doublet state of $[U^IL]^-$ comes from the reduction of the singlet state of $[U^{II}L]$.

The full reference of ADF

E. J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F. M. Bickelhaupt, C. Bo, P. M. Boerrigter, L. Cavallo, D. P. Chong, L. Deng, R. M. Dickson, D. E. Ellis, M. van Faassen, L. Fan, T. H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S. J. A. van Gisbergen, A. W. Götz, J. A. Groeneveld, O. V. Gritsenko, M. Grüning, S. Gusarov, F. E. Harris, P. van den Hoek, C. R. Jacob, H. Jacobsen, L. Jensen, J. W. Kaminski, G. van Kesse, F. Kootstra, A. Kovalenko, M. V. Krykunov, E. van Lenthe, D. A. McCormack, A. Michalak, M. Mitoraj, S. M. Morton, J. Neugebauer, V. P. Nicu, L. Noodleman, V. P. Osinga, S. Patchkovskii, M. Pavanello, P. H. T. Philipsen, D. Post, C. C. Pye, W. Ravenek, J. I. Rodríguez, P. Ros, P. R. T. Schipper, H. van Schoot, G. Schreckenbach, J. S. Seldenthuis, M. Seth, J. G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T. A. Wesolowski, E. M. van Wezenbeek, G. Wiesenekker, S. K. Wolff, T. K. Woo and A. L. Yakovlev, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, ADF2014.06 edn., 2014.

The full reference of Gaussian

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. P. Cammi, C., J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, Gaussian 09, Revision D.01 edn., 2009.

Cartesian coordinates of optimized complexes

*Only the geometry of each complex in the energy-lowest electron-spin state is listed, as well as energy-degenerate doublet and quartet states for [U^{I}R]$^{2-}$.

[U^{I}L]$^-$

```
C    0.24255659 -0.41070499 0.39573044
C    0.27098134 -1.23886706 1.54505335
C    1.30187643 -0.19884195 -0.67488606
N   -1.03128509 0.04223901 0.15139815
H    1.13702370 -1.72136776 1.99710047
C   -1.06251772 -1.26129020 2.04326492
C    0.93229546 -1.34406162 -1.62690817
C    1.15993313 1.18654315 -1.32975040
C    2.72482630 -0.31326409 -0.10404754
C   -1.81894299 -0.44534323 1.16594711
H   -1.40535657 -1.76398328 2.94712303
C   -0.13238728 -1.20503181 -2.57591301
C    1.41041215 -2.64514581 -1.34907336
H    1.81357264 1.26286811 -2.21593440
H    1.44569095 1.97052005 -0.60747434
H    0.11867873 1.37677160 -1.62231893
H    3.46933434 -0.28869126 -0.91834156
H    2.88206733 -1.23721623 0.47213739
H    2.91575254 0.53269576 0.57751256
C   -3.32642521 -0.27687902 1.05429082
C   -3.63769134 -1.42146883 0.08091553
C   -3.77754037 -2.73271183 0.59044754
C    0.85929460 -3.80857893 -1.93328539
N   -1.19388071 -5.47111748 -0.53251639
C   -0.63374957 -2.35159254 -3.22331508
H   -0.51956226 -0.22174619 -2.84133799
H    2.19745180 -2.76090605 -0.60544653
C   -3.68994086 1.10447193 0.48159098
C   -4.02248876 -0.42705925 2.41689059
C   -3.46086463 -1.26213649 -1.33218984
H   -3.88037063 -2.86292145 1.66667708
C   -3.71017548 -3.88613286 -0.22421133
C    1.15480232 -5.17138750 -1.29301921
C   -0.20485313 -3.64896797 -2.87965834
C   -1.95861980 -5.20096914 0.57639533
C    0.10247029 -5.16623350 -0.19491371
H   -1.39848151 -2.23310449 -3.99400817
H   -4.76628301 1.15087856 0.24130523
H   -3.10136325 1.32226772 -0.41960056
H   -3.45615608 1.88793596 1.22285512
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H   -3.74688201 0.42138886 3.06558490
H   -3.73394438 -1.34775076 2.94562763
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H   -3.37201057 -0.27103264 -1.77606836
C   -3.53300899 -3.70625579 -1.63481556
C   -3.47255335 -5.24948631 0.43856763
C    0.93655119 -6.34378382 -2.26571201
C    2.57809832 -5.28329815 -0.72255013
H   -0.64679553 -4.51317370 -3.37468535
C   -1.16187417 -4.66915500 1.62043994
C    0.17135906 -4.64667695 1.12150114
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C   -4.16778869 -5.39595513 1.80198742
H    1.17185495 -7.29588613 -1.75966929
H    1.59019934 -6.23848584 -3.14892220
H   -0.11216757 -6.39605053 -2.58735366
H    2.71450961 -6.27965778 -0.26954033
H    2.78535554 -4.53874483 0.06043993
H    3.32542868 -5.15184608 -1.52391601
H   -1.48093941 -4.38315289 2.62222657
H    1.06099103 -4.34029618 1.67092778
H   -3.72812804 -7.37887765 0.07534117
H   -3.33100586 -6.45113193 -1.38242032
H   -4.98737813 -6.35071749 -0.68650545
H   -3.83042497 -4.64981265 2.53675510
H   -3.94557107 -6.39124340 2.22228254
H   -5.26086427 -5.29352334 1.68982685
U   -1.21531270 -2.67754491 -0.46382269


[UᴵᴵL]
C    0.23341612 -0.44237158 0.37013194
C    0.26832886 -1.24607941 1.53245555
C    1.31092612 -0.19917848 -0.68360706
N   -1.04708470 -0.02536441 0.10605836
H    1.14052340 -1.69162446 2.00852108
C   -1.06807473 -1.26863582 2.03190876
C    0.97014185 -1.34526024 -1.64749080
C    1.15197823 1.18882592 -1.32692110
C    2.72568256 -0.30134944 -0.09086761
C   -1.82764080 -0.47712928 1.14041743
H   -1.40072298 -1.73443230 2.95832566
C   -0.03481554 -1.20675826 -2.63000097
C    1.43048838 -2.64700153 -1.33862102
H    1.82314607 1.28932218 -2.19580058
H    1.41166754 1.96614908 -0.59039126
H    0.11569913 1.37348426 -1.63941566
H    3.48167030 -0.24943749 -0.89135780
H    2.89474278 -1.22770862 0.47749605
H    2.89171869 0.53894764 0.60168750
C   -3.33868201 -0.27760570 1.05421794
C   -3.67976381 -1.42396647 0.09075437
C   -3.78556305 -2.73518069 0.61174754
C    0.89751227 -3.80478270 -1.95294205
N   -1.20534360 -5.39360225 -0.55991830
C   -0.55229799 -2.34824916 -3.27286714
H   -0.42891186 -0.22176208 -2.88125225
H    2.19374966 -2.76469874 -0.57245537
C   -3.68182520 1.10712138 0.47943807
C   -4.01421091 -0.41464422 2.42834095
C   -3.57033615 -1.26697831 -1.30845542
H   -3.85534662 -2.86664839 1.68937277
C   -3.75215195 -3.88356824 -0.21407131
C    1.16422030 -5.16944517 -1.30081323
C   -0.10669639 -3.64033184 -2.93219734
C   -1.96549416 -5.16362615 0.55927415
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C   0.09536521 -5.12880920 -0.21157051
H -1.30824953 -2.22916391 -4.05202152
H -4.76114423 1.17819372 0.26594502
H -3.11176789 1.31841264 -0.43485696
H -3.41687382 1.88484910 1.21365355
H -5.11098495 -0.39383603 2.32038414
H -3.71004801 0.42808463 3.06911924
H -3.74179244 -1.33919104 2.95819890
C -3.56769188 -2.39988644 -2.14546863
H -3.46730094 -0.27368430 -1.74594385
C -3.64198073 -3.70061243 -1.61006963
C -3.48494011 -5.24809347 0.43817014
C   0.92919193 -6.34652013 -2.26253985
C   2.57836756 -5.29766383 -0.71169204
H -0.55553619 -4.50942463 -3.41373512
C -1.16741270 -4.65928163 1.61134798
C   0.16885544 -4.63671346 1.11153353
H -3.51217683 -2.26734682 -3.22809349
H -3.59352602 -4.56147055 -2.27732453
C -3.90380196 -6.42843366 -0.45458730
C -4.16106910 -5.41132742 1.80912214
H   1.13786868 -7.29401024 -1.74017982
H   1.59952332 -6.27060709 -3.13455616
H -0.11383497 -6.38851436 -2.60306373
H   2.69039263 -6.28992900 -0.24676000
H   2.79712113 -4.54973646 0.06452228
H   3.33558098 -5.19623661 -1.50625883
H -1.47890715 -4.41530213 2.62589984
H   1.06214975 -4.37226923 1.67542413
H -3.69062340 -7.37578251 0.06620709
H -3.33928466 -6.44354543 -1.39624069
H -4.98361950 -6.38196956 -0.67220737
H -3.83895251 -4.66146760 2.54648807
H -3.91112206 -6.40116119 2.22270654
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U -1.20600384 -2.68085249 -0.43902616

[U^{III}L]$^+$
C   0.23349349 -0.48681756 0.35141885
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C   1.31708199 -0.20837002 -0.68925337
N -1.06202825 -0.12507192 0.06176010
H   1.14982093 -1.65303124 2.03971500
C -1.06811641 -1.27087220 2.03809458
C   0.98081214 -1.34798800 -1.66047216
C   1.14289903 1.18682328 -1.31282427
C   2.72836768 -0.30864757 -0.08893978
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C   1.44133478 -2.64474909 -1.35948969
H   1.82977553 1.31145720 -2.16505247
H   1.38059417 1.95533584 -0.56121769
H   0.11213294 1.36845800 -1.64494691
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H   2.90952865 -1.23885835 0.46947378

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N  -1.21418398 -5.28546834 -0.57837208
C  -0.51611704 -2.34519509 -3.30742890
H  -0.40120771 -0.22222372 -2.91068226
H   2.19698658 -2.76319667 -0.58489983
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C  -4.01457883 -0.42277431  2.43183551
C  -3.60124898 -1.26957344 -1.31262794
H  -3.86637781 -2.86552070  1.68182840
C  -3.76848604 -3.87883049 -0.21615158
C   1.17095983 -5.15956105 -1.30375965
C  -0.08572795 -3.63403628 -2.95453034
C  -1.97395079 -5.11612980  0.55617909
C   0.09805390 -5.08116214 -0.21866757
H  -1.25988995 -2.22499673 -4.09895389
H  -4.74625028  1.20112191  0.29430180
H  -3.11171612  1.31351318 -0.44031064
H  -3.37326280  1.87496559  1.21620224
H  -5.11032710 -0.38160190  2.32925365
H  -3.69703333  0.41374109  3.07274417
H  -3.75661194 -1.35137008  2.96202151
C  -3.61771264 -2.39784120 -2.14788221
H  -3.50725470 -0.27488425 -1.74981377
C  -3.67261160 -3.69485890 -1.61343247
C  -3.49264913 -5.23831029  0.44018156
C   0.92029773 -6.34767151 -2.24784651
C   2.58140692 -5.29114911 -0.70753735
H  -0.52761070 -4.50375584 -3.44208037
C  -1.16775024 -4.65839122  1.61785670
C   0.17292914 -4.63570702  1.11647485
H  -3.57938577 -2.26453668 -3.23181943
H  -3.63321496 -4.55646960 -2.28085535
C  -3.88735960 -6.42921093 -0.44953347
C  -4.16132233 -5.40454221  1.81401336
H   1.10755298 -7.28894294 -1.70843222
H   1.60476023 -6.30014507 -3.10974966
H  -0.11692096 -6.38244643 -2.60665364
H   2.68332387 -6.27824828 -0.23149553
H   2.81244805 -4.53758822  0.05973187
H   3.33940158 -5.21211961 -1.50257233
H  -1.46918080 -4.46038576  2.64551988
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H  -3.85368996 -4.65002209  2.55292881
H  -3.89748931 -6.38916634  2.22905642
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[U$^{I}$R]$^{2-}$
U   15.27970170 10.42006001 14.39715085
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O   17.40747662 10.21014264 15.15886765
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C   16.55576446 9.99432001 12.29199783
C   16.22437424 11.39469698 12.27440348
C   14.85175168 11.82188130 12.37393213
C   13.80383704 10.83578907 12.39795151
C   14.12318761 9.43071607 12.41570570
C   17.99428770 9.52816147 12.37919486
H   17.96914700 8.48571897 12.76328642
H   18.48391600 9.47275262 11.37886100
C   18.91818077 10.33366717 13.27730382
C   18.56061787 10.61225053 14.63311386
C   19.48572808 11.32467269 15.44974416
C   20.70719332 11.75122097 14.91981516
H   21.40040087 12.30356505 15.57022475
C   21.06498252 11.50313588 13.58871333
C   20.14733562 10.79197109 12.79750076
H   20.39697654 10.57814789 11.74842703
C   14.54801469 13.29594946 12.54474499
H   14.27562021 13.78754412 11.58161820
H   15.49180312 13.77977034 12.87647363
C   13.46276084 13.65674312 13.54527562
C   13.50375020 13.15345088 14.88253492
C   12.49285442 13.56670472 15.79798689
C   11.47831870 14.43317713 15.38056168
H   10.70818341 14.73208495 16.10596284
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C   13.31469300 7.26462279 13.56652192
C   13.83255253 7.49770620 14.87822044
C   14.04532805 6.37981318 15.73606173
C   13.76517234 5.08595199 15.28707966
H   13.94265513 4.24125514 15.96798793
C   13.27590522 4.83845116 13.99805717
C   13.06233410 5.95010916 13.16644517
H   12.67614676 5.79175970 12.14939442
C   19.10448414 11.60544846 16.87999119
C   22.36407518 12.01744697 13.01276624
H   22.22720553 12.94704250 12.42532451
H   22.83083945 11.27940559 12.33538800
H   23.09131043 12.24395236 13.81226388
C   12.55007589 13.03923880 17.20805833
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H   10.62578817 16.57616750 12.89839504
H   9.81644300 16.33531943 14.46871917
H   9.47201446 15.24236311 13.10837554
C   14.58096206 6.63637901 17.12064567
C   13.03209688 3.43097691 13.50460490
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[U^{II}R]$^-$
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C   15.45505458 8.99802706 12.35921408
C   16.50994057 9.98586128 12.44506559
C   16.12842932 11.37575270 12.31711692
C   14.78566966 11.76874402 12.39754530
C   13.75726319 10.76633707 12.55877049
C   14.10938227 9.36675913 12.44632920
C   17.96008826 9.55525585 12.46568881
H   17.98219962 8.50706362 12.83066274
H   18.39830074 9.52489155 11.44395813
C   18.89570915 10.37918419 13.33462635
C   18.55220061 10.71648677 14.67094449
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C   20.70681514 11.81775172 14.92195578
H   21.40650361 12.38468210 15.54919545
C   21.06507091 11.50182281 13.60559632
C   20.13739688 10.78801133 12.83766452
H   20.38614521 10.53282438 11.79944335
C   14.42752788 13.23983128 12.46923590
H   14.05574306 13.58341136 11.48275778
H   15.36345138 13.80233868 12.65919134
C   13.39279622 13.65092905 13.50585618
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C   12.38935054 14.56106836 13.15671306
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H   12.13658973 8.86446277 13.05422540
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C   14.09550259 6.26117122 15.68594481
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H    22.37605705 11.97547560 11.94486651
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H    10.18510945 15.98882983 12.58416792
C    14.64977372 6.50140100 17.06562077
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H    11.77575405 13.58468538 17.82165238
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H    19.90828263 12.34739911 17.37918748
H    18.18639091 12.43678099 16.89420094
H    18.84702002 10.90545213 17.46752664
H    15.63892414 6.99203944 17.02093508
H    14.00013099 7.17951173 17.64573626
H    14.75573364 5.55405098 17.61767356


[U^{III}R]
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O    17.41738899 10.40874660 15.12680107
O    14.28355226 12.24955106 15.28073940
O    14.26009359 8.61178617 15.29077111
C    15.51926334 9.05018508 12.45225416
C    16.54974775 10.02155153 12.40385286
C    16.19273701 11.39419646 12.41244876
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C    14.15399139 9.42732961 12.52648268
C    18.00221660 9.58851389 12.41423682
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C    18.62777423 10.73061601 14.61005936
C    19.56337621 11.40992568 15.42210106
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H    21.52089085 12.28678894 15.50981335
C    21.13885261 11.47150066 13.54675016
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H    14.21697348 13.64482853 11.57801245
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H   12.61877630 5.77081442 12.13859776
C   19.20931387 11.73782219 16.84820048
C   22.46608464 11.90243844 12.97107716
H   22.72552275 11.31192218 12.07873685
H   23.27879515 11.78492593 13.70569652
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C   12.37583394 13.06301712 17.18894942
C   10.31846224 15.95450777 13.57212577
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H   9.42000541 15.41211428 13.22811438
H   10.66719859 16.57862795 12.73450288
C   14.65229284 6.47830404 17.08941814
C   12.88601605 3.39779931 13.47573620
H   12.17082522 3.42719927 12.63905810
H   12.44592758 2.78560309 14.27910083
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H   15.77744636 7.98681905 12.49182141
H   16.98729098 12.14759031 12.42049545
H   13.33949467 13.25847016 17.68943437
H   11.57382446 13.52755753 17.78152404
H   12.22934842 11.96849503 17.20879768
H   20.05531662 12.21983126 17.36019676
H   18.34132106 12.41870445 16.90100747
H   18.92984342 10.83085262 17.41081205
H   15.67292947 6.89806117 17.04555301
H   14.04456617 7.19424311 17.66857499
H   14.69511720 5.52848582 17.64273054

$[U^{I}Cp'_{3}]^{2-}$
C   -5.36224495 0.80221835 2.90721858
H   -5.19352095 1.86727423 3.06119514
C   -4.36306049 -0.21245186 2.89830918
H   -3.29210586 -0.06249087 3.04544565
C   -5.01283740 -1.45971430 2.68440771
H   -4.51872269 -2.43297202 2.66303112
C   -6.43450831 -1.23699713 2.55959213
C   -6.61896434 0.19229240 2.68294546
C   -4.42989604 2.55220268 0.46627956
H   -4.39299151 3.01070065 1.45485297

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C   -5.56486161 2.57097138 -0.41823916
C   -5.13687951 1.88413354 -1.61573980
C   -3.78595559 1.47720388 -1.45722710
H   -3.18481206 0.94688091 -2.19533252
C   -3.34884754 1.88462541 -0.16311663
H   -2.35580196 1.72611283 0.26103736
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C   -3.88273320 -1.74426657 -1.55530783
H   -2.97724809 -1.31424240 -1.98794023
C   -3.93836307 -2.48920642 -0.34294041
H   -3.09686400 -2.70420796 0.31930871
C   -5.28694127 -2.92000906 -0.16191190
H   -5.66074477 -3.50615071 0.67792100
C   -6.05992068 -2.43274326 -1.24263454
U   -5.24996289 -0.15880781 0.24964290
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H   -7.58088481 0.70520720 2.65362860
H   -7.12969733 -2.58819093 -1.38411271
Si -7.10484699 3.57197403 -0.22679800
Si -7.78915810 -2.48862773 2.70482000
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H   -9.11964660 -1.99188502 0.64367505
H   -9.74996351 -3.48536727 1.44592585
H   -8.57642232 -1.66868704 4.97124853
H   -9.87339379 -2.62340424 4.17730426
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H   -6.57549241 -3.99040907 4.34153894
H   -6.36082927 -4.58497430 2.67643912
H   -7.89861317 -4.88914655 3.53036668
H   -6.79666975 4.29598258 2.17396806
H   -7.84122368 2.85574518 2.06895008
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[U^II Cp'_3]^−

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 H   -4.65497473 -2.15594294 2.84495696
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 H   -8.15039240 -2.16599497 4.90777074
 H   -9.66528236 -2.70161861 4.11880016
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[U^{I}R]$^{2-}$ (Doublet)

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O	14.09884779	8.71999682	15.32844437
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C	16.55576446	9.99432001	12.29199783
C	16.22437424	11.39469698	12.27440348
C	14.85175168	11.82188130	12.37393213
C	13.80383704	10.83578907	12.39795151
C	14.12318761	9.43071607	12.41570570
C	17.99428770	9.52816147	12.37919486
H	17.96914700	8.48571897	12.76328642
H	18.48391600	9.47275262	11.37886100
C	18.91818077	10.33366717	13.27730382
C	18.56061787	10.61225053	14.63311386
C	19.48572808	11.32467269	15.44974416
C	20.70719332	11.75122097	14.91981516
H	21.40040087	12.30356505	15.57022475
C	21.06498252	11.50313588	13.58871333
C	20.14733562	10.79197109	12.79750076
H	20.39697654	10.57814789	11.74842703
C	14.54801469	13.29594946	12.54474499
H	14.27562021	13.78754412	11.58161820
H	15.49180312	13.77977034	12.87647363
C	13.46276084	13.65674312	13.54527562
C	13.50375020	13.15345088	14.88253492
C	12.49285442	13.56670472	15.79798689
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H	10.70818341	14.73208495	16.10596284
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H	12.15067488	8.98536722	13.05302502
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C	13.83255253	7.49770620	14.87822044
C	14.04532805	6.37981318	15.73606173
C	13.76517234	5.08595199	15.28707966
H	13.94265513	4.24125514	15.96798793
C	13.27590522	4.83845116	13.99805717

C   13.06233410 5.95010916 13.16644517
H   12.67614676 5.79175970 12.14939442
C   19.10448414 11.60544846 16.87999119
C   22.36407518 12.01744697 13.01276624
H   22.22720553 12.94704250 12.42532451
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H   9.81644300 16.33531943 14.46871917
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[U^I R]^{2-} (Quartet)
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C   16.62319730 9.98528513 12.23896273
C   16.28508723 11.34974421 12.23154719
C   14.91345508 11.78378623 12.44598199
C   13.87232411 10.77216329 12.34251662
C   14.19110877 9.40179908 12.34269107
C   18.07035542 9.52912214 12.33391107
H   18.04616931 8.49326734 12.73039352
H   18.54851059 9.46754572 11.33243809
C   18.97165309 10.35566302 13.23153282
C   18.61355709 10.57274976 14.60153268
C   19.51546678 11.31076228 15.42506211
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C   20.16616921 10.89115981 12.74657742
H   20.41469097 10.71965402 11.68947313
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H   15.53317944 13.75277898 12.90433506
C   13.51236555 13.60775871 13.59429756

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[U^{II}R^E]⁻

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