Supporting Information

Theoretical investigation of low-valent uranium and transuranium complexes of a flexible small-cavity macrocycle: structural, formation reaction and redox properties

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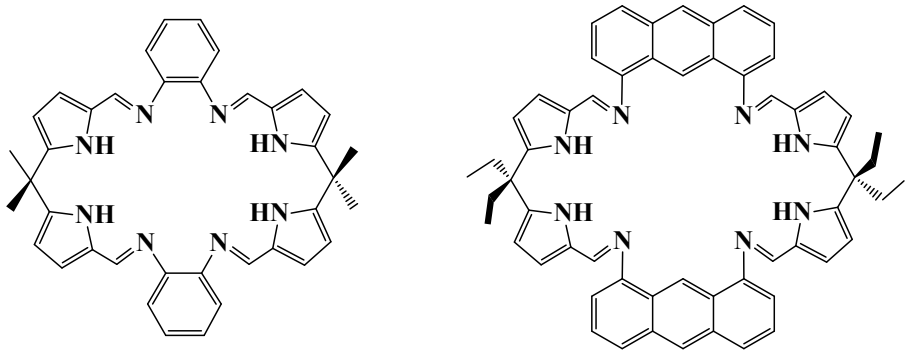

H_4L^1 H_4L^2

Chart S1. Polypyrrolic macrocycles H_4L^1 and H_4L^2.

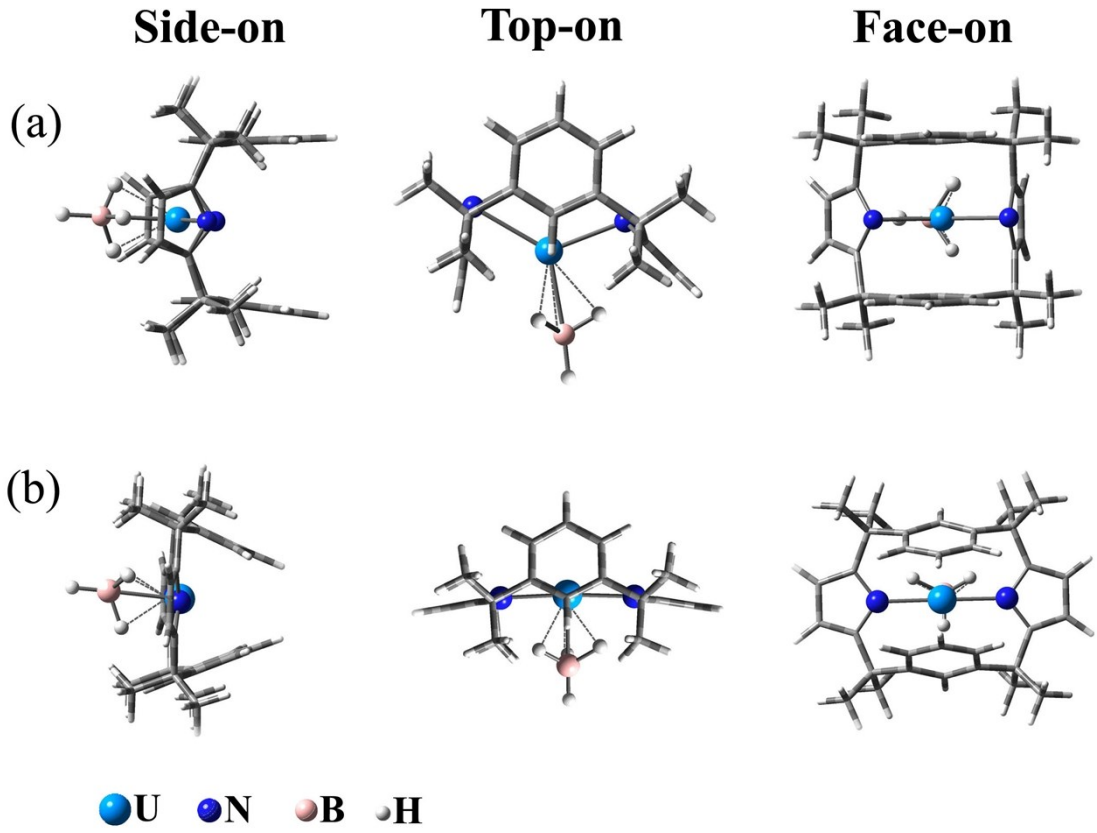

Figure S1. Structures of isomers where the BH_4 attacks the U^{III} (a) and U^{IV} (b) ions from the *bis*(pyrrolide) side. The bonds between U and *bis*(arene)/*bis*(pyrrolide) are omitted for clarity.

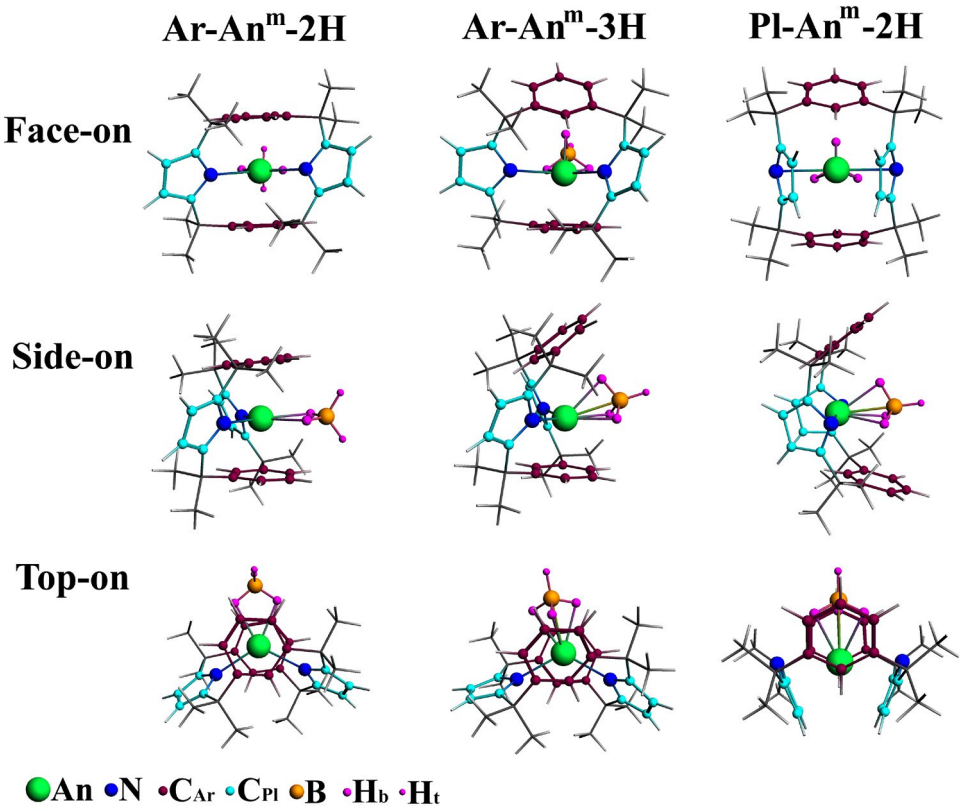

Figure S2. Optimized structures of low-valent uranium and transuranium complexes **BP-An^{m}-nH** (**BP** = **Ar** and **Pl**; An = U, Np and Pu; m = III and IV; n = 2 and 3), where the An-*bis*(arene)/*bis*(pyrrolide) bonds are omitted for clarity.

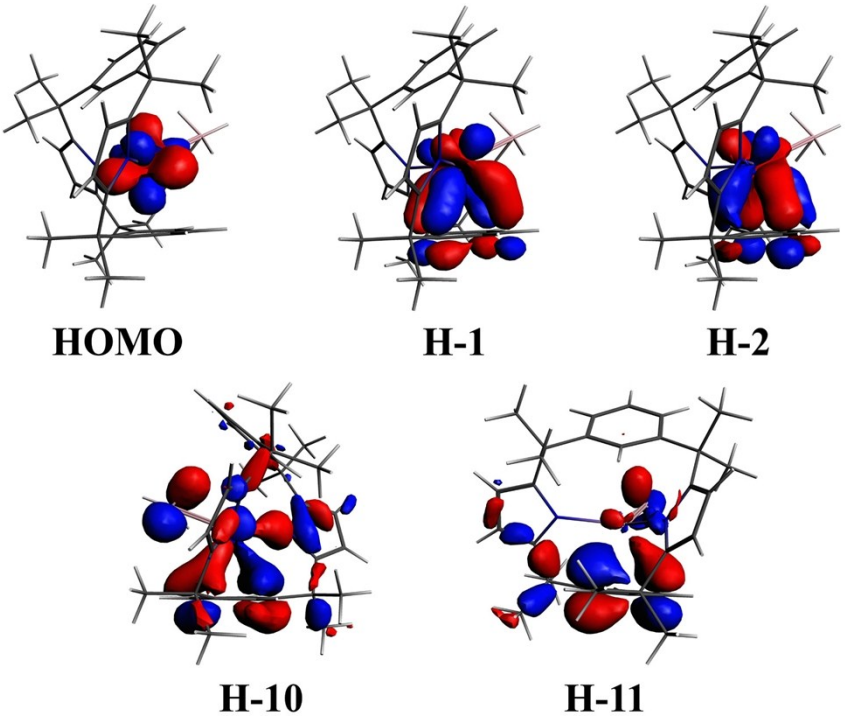

Figure S3. Characteristic α-spin orbitals of **Ar-U^{III}-3H**.

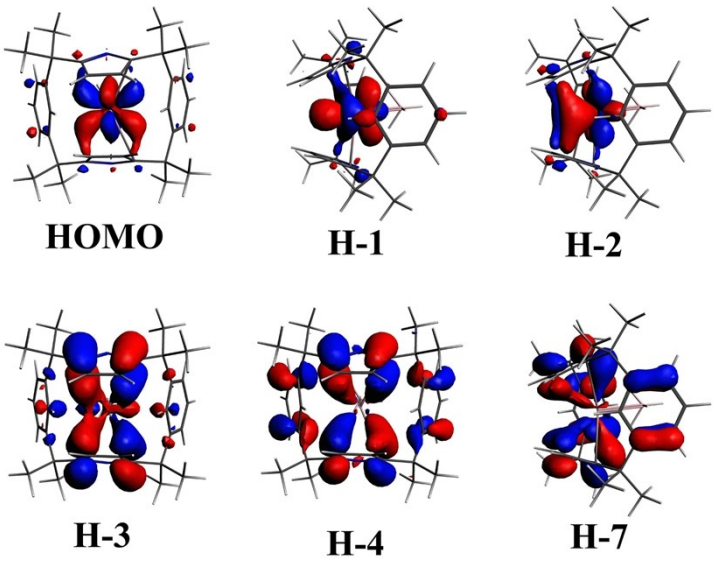

Figure S4. Characteristic α-spin orbitals of **Pl-U^{III}-3H**.

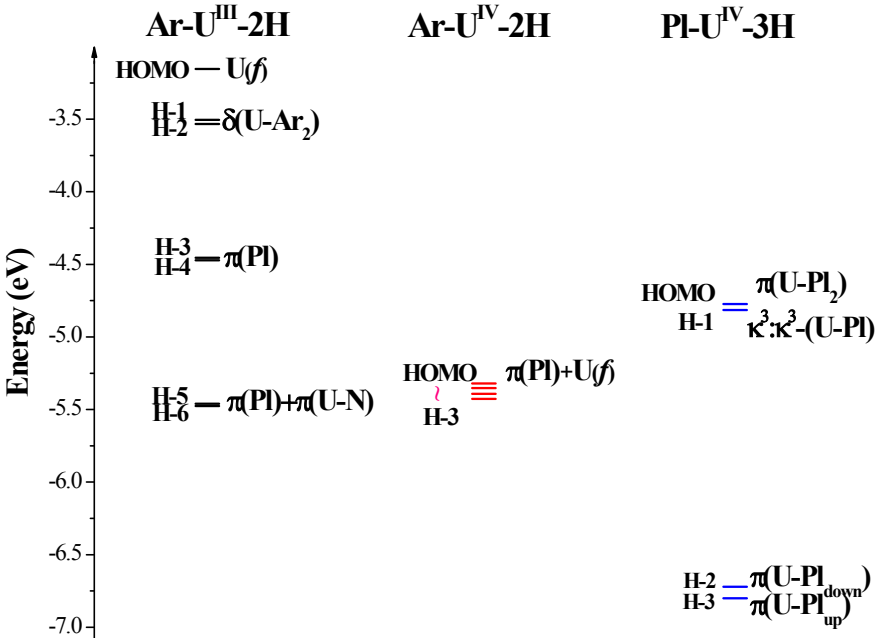

Figure S5. Diagrams of energy levels and character of orbitals of isomeric U^{IV} complexes calculated at the ADF: PBE/B-III/ZORA/COSMO level, compared with the U^{III} complex. The α-spin orbital energy levels are used.

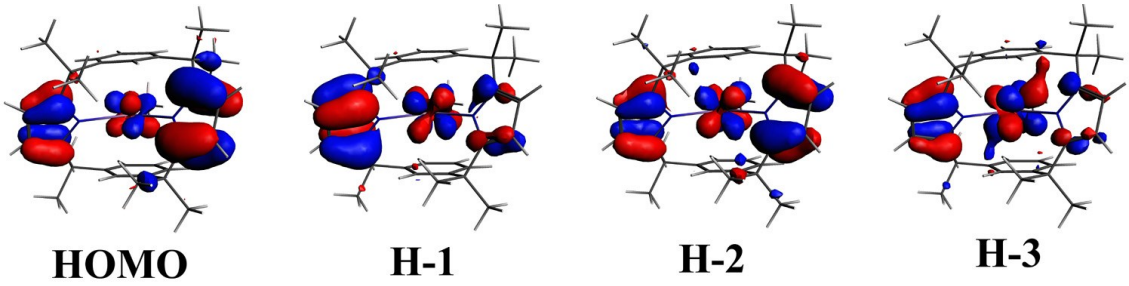

Figure S6. Characteristic α-spin orbitals of **Ar-U^{IV}-2H**.

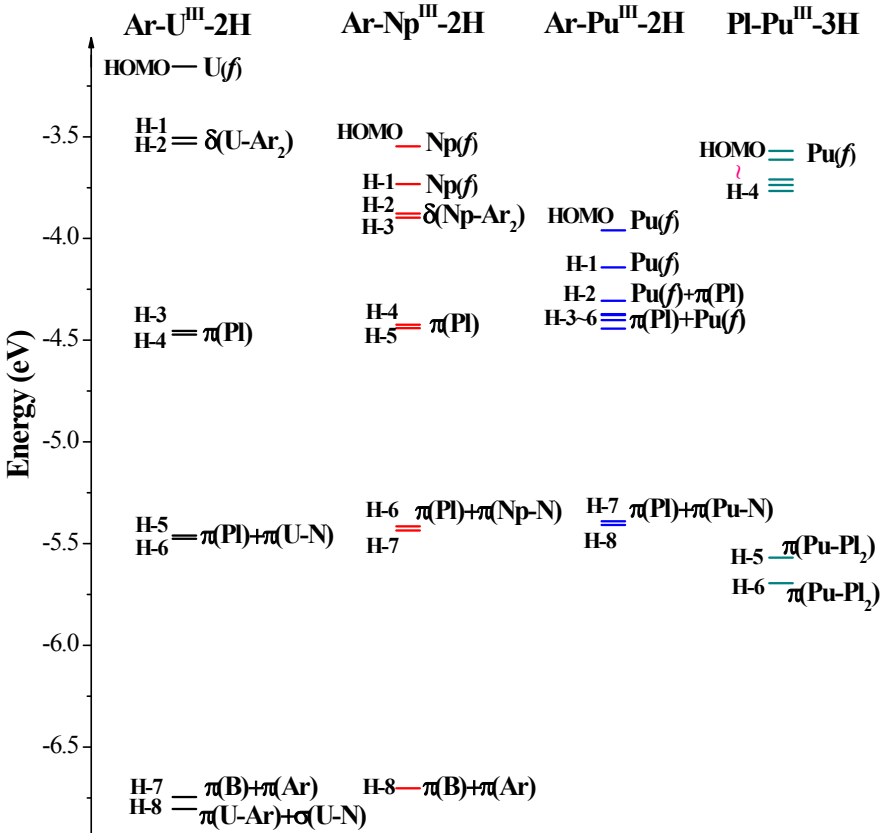

Figure S7. Diagrams of energy levels and character of orbitals of the An^{III} complexes (An = U, Np and Pu) calculated at the ADF: PBE/B-III/ZORA/COSMO level. The α-spin orbital energy levels are used.

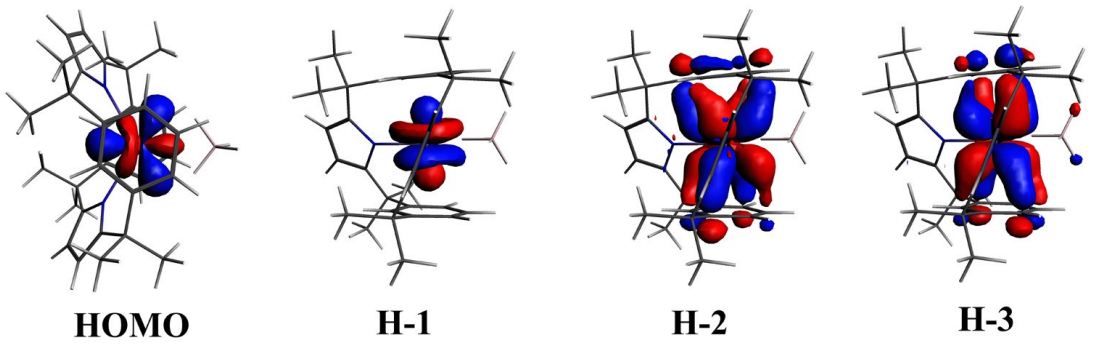

Figure S8. Characteristic α-spin orbitals of **Ar-Np^{III}-2H**.

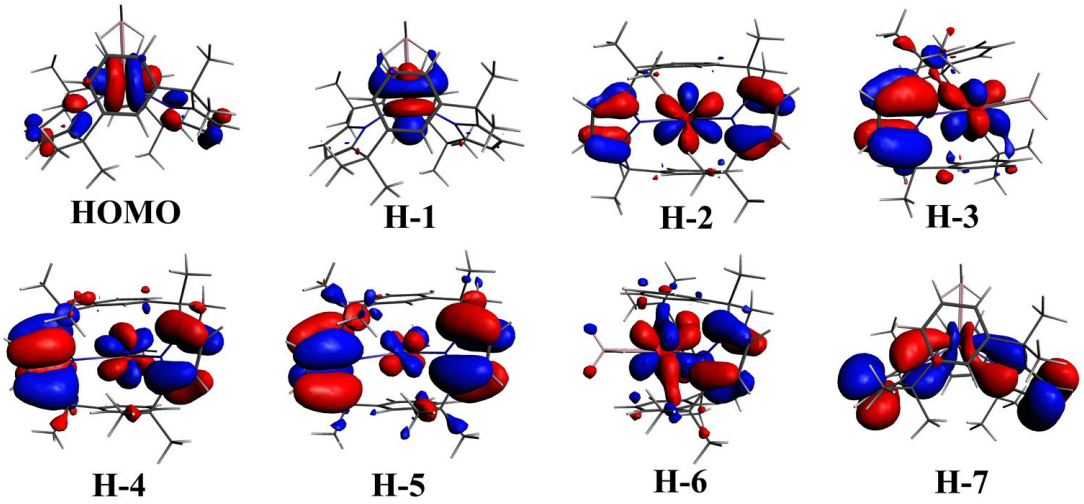

Figure S9. Characteristic α-spin orbitals of **Ar-Pu^{III}-2H**.

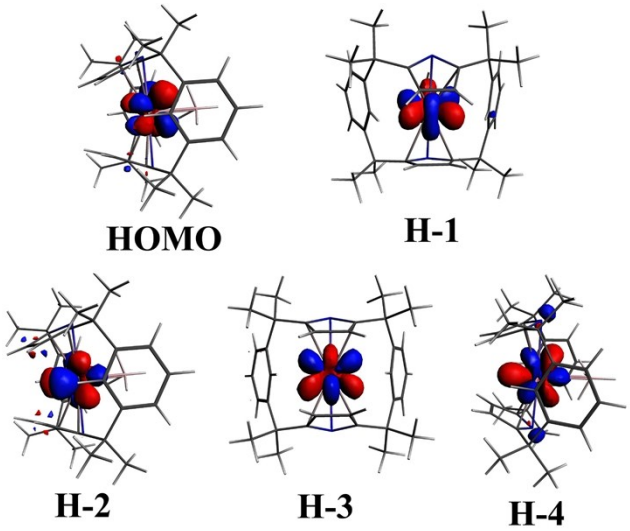

Figure S10. Characteristic α-spin orbitals of **Pl-Pu^{III}-3H**.

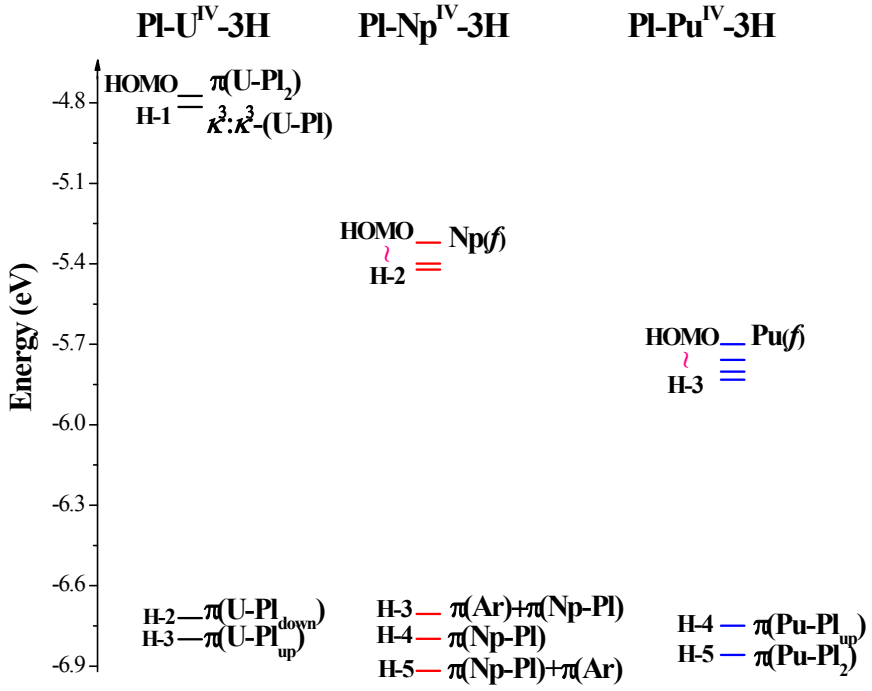

Figure S11. Diagrams of energy levels and character of orbitals of the An^{IV} complexes (An = U, Np and Pu) calculated at the ADF: PBE/B-III/ZORA/COSMO level. The α-spin orbital energy levels are used.

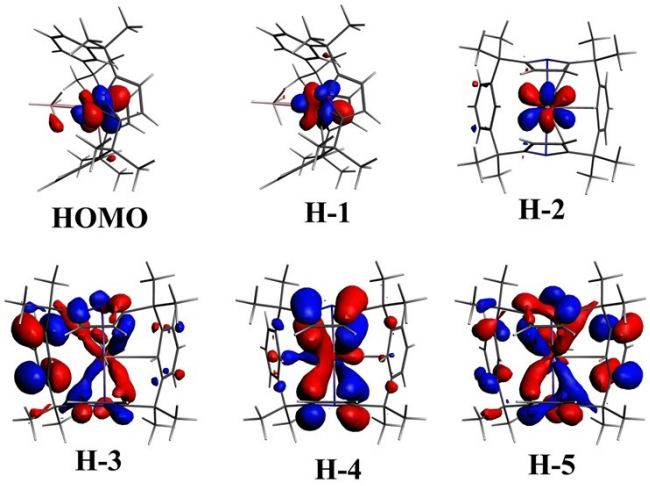

Figure S12. Characteristic α-spin orbitals of **Pl-Np^{IV}-3H**.

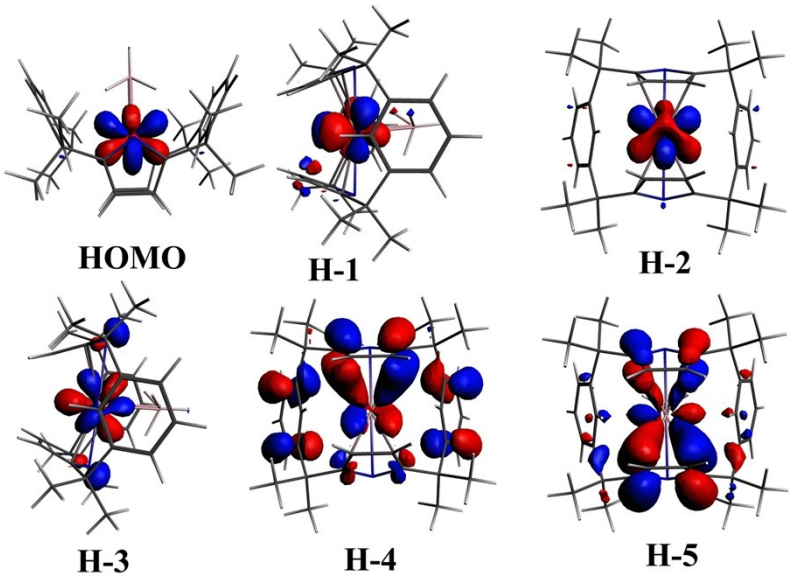

Figure S13. Characteristic α-spin orbitals of **Pl-Pu^{IV}-3H**.

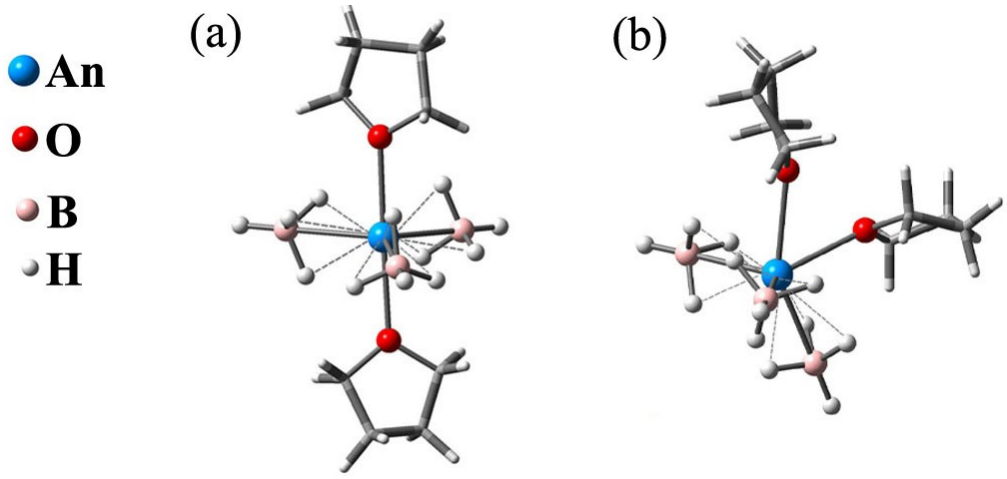

Figure S14. Optimized structures of precursors [{*trans*-$(THF)_2$}An^m{$(\eta\text{-}H)_3(BH)\}_3$]$^{z+}$ (a) and [{*cis*-$(THF)_2$}An^m{$(\eta\text{-}H)_3(BH)\}_3$]$^{z+}$ (b) (An = U, Np and Pu; m = III, z = 0 and m = IV, z = 1).

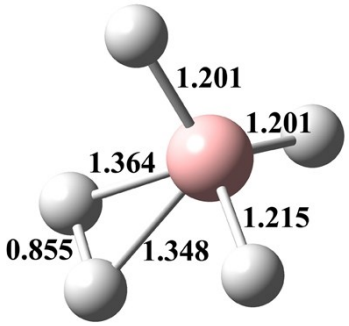

Figure S15. Optimized structure of the species BH_5; bond lengths labeled in Å.

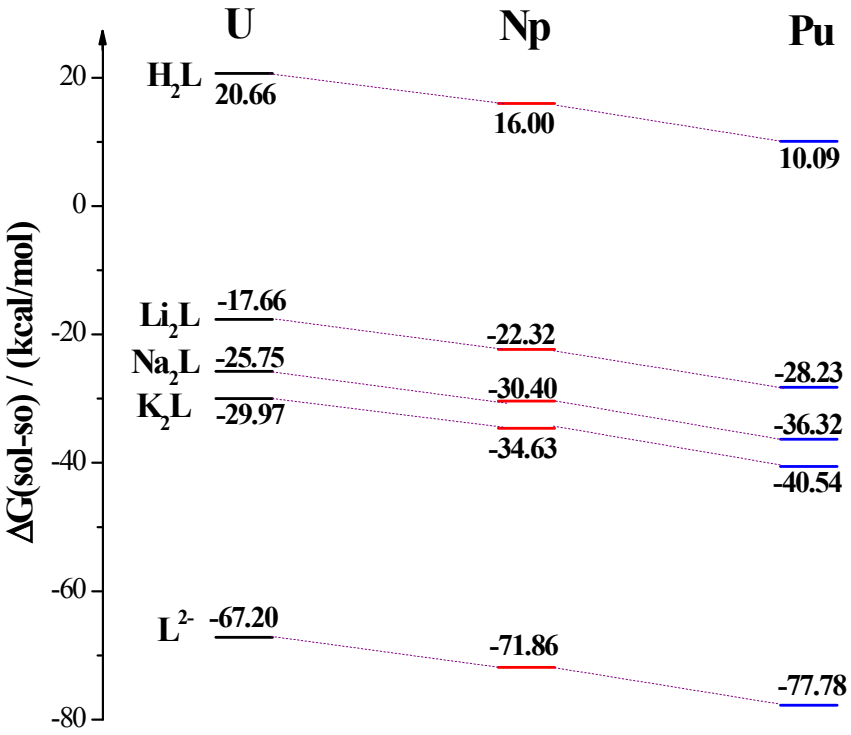

Figure S16. Free energies (Δ_rG(sol-so), kcal/mol) of formation reactions of **Pl-An^{IV}-3H** (An = U, Np and Pu) via various ligands A_2L (A = H, Li, Na, K and Vacant) in THF solution.

Table S1. Complexes and their abbreviations.

Oxidation State	Binding Modes		Formula	Abbreviation
	L→An	$H_{4-n}B(\eta\text{-}H)_n$→An		
III	*bis*(arene) (**Ar**)	$(\eta\text{-}H)_2$	[(**Ar**-L)$An^{III}(\eta\text{-}H)_2(BH_2)$]	**Ar-An^{III}-2H** (An = U, Np and Pu)
	bis(arene)	$(\eta\text{-}H)_3$	[(**Ar**-L)$An^{III}(\eta\text{-}H)_3(BH)$]	**Ar-An^{III}-3H**
	bis(pyrrolide) (**Pl**)	$(\eta\text{-}H)_3$	[(**Pl**-L)$An^{III}(\eta\text{-}H)_3(BH)$]	**Pl-An^{III}-3H**
IV	*bis*(arene)	$(\eta\text{-}H)_2$	[(**Ar**-L)$An^{IV}(\eta\text{-}H)_2(BH_2)]^+$	**Ar-An^{IV}-2H**
	bis(arene)	$(\eta\text{-}H)_3$	[(**Ar**-L)$An^{IV}(\eta\text{-}H)_3(BH)]^+$	**Ar-An^{IV}-3H**
	bis(pyrrolide)	$(\eta\text{-}H)_3$	[(**Pl**-L)$An^{IV}(\eta\text{-}H)_3(BH)]^+$	**Pl-An^{IV}-3H**

Table S2. Calculated relative total energies (kcal/mol) of **BP-An^{m}-nH** (**BP** = **Ar** and **Pl**; An = U, Np and Pu; m = III and IV; n = 2 and 3) at various levels of theory.

Approach	Pri: ***PBE***/B-II	Pri: ***PBE***/B-I	Pri: ***B3LYP***/B-I	Gau: ***PBE***/B-IV [a]	Gau: ***B3LYP***/B-IV [a]
Geometry	Pri: PBE/B-II	Pri: PBE/B-I	Pri: PBE/B-I	Pri: PBE/B-II	Pri: PBE/B-II
Ar-U^{III}-2H	0.00	0.00	0.00	0.00	0.00
Ar-U^{III}-3H	3.68	3.96	4.46	3.93	5.12
Pl-U^{III}-3H	5.22	5.04	7.10	3.21	5.96
Ar-Np^{III}-2H	0.00	0.00	0.00	0.00	0.00
Ar-Np^{III}-3H	5.97	6.49	5.37	6.07	2.26
Pl-Np^{III}-3H	2.74	2.30	5.51	0.83	7.16
Ar-Pu^{III}-2H	2.25	2.65	0.00	3.84	0.00
Ar-Pu^{III}-3H	6.44	7.20	3.62	8.38	3.87
Pl-Pu^{III}-3H	0.00	0.00	2.81	0.00	2.36
Ar-U^{IV}-2H	9.99	10.05	2.53 [b]	11.89	8.99
Ar-U^{IV}-3H	11.43	12.01	5.49 [b]	12.82	11.00
Pl-U^{IV}-3H	0.00	0.00	0.00 [b]	0.00	0.00
Ar-Np^{IV}-2H	7.22	7.22	6.56	7.50	5.54
Ar-Np^{IV}-3H	10.72	10.58	9.87	11.58	14.67
Pl-Np^{IV}-3H	0.00	0.00	0.00	0.00	0.00
Ar-Pu^{IV}-2H	5.15	5.17	0.00 [b]	5.06	0.00
Ar-Pu^{IV}-3H	9.34	9.71	3.14 [b]	8.90	5.02
Pl-Pu^{IV}-3H	0.00	0.00	2.90 [b]	0.00	5.25

[a] Single-point energy calculations were performed using the approach of Gaussian: DFT/B-IV at the geometries optimized by Priroda: PBE/B-II. Two functionals of PBE and B3LYP were used in the Gaussian calculations. Stuttgart relativistic small-core effective core potentials (RSC-ECPs) and corresponding basis sets were used for U, Np and Pu, and 6-31G** was employed for other atoms. All together is labeled as B-IV. The Stuttgart RSC ECP basis sets were obtained from EMSL Basis Set Exchange Library (https://bse.pnl.gov/bse/portal). See the full reference of the Gaussion 09 code in SI.

[b] The geometries of isomers optimized by Priroda: PBE/B-II were used, for those from Priroda: PBE/B-I can not converge in the SCF calculations.

Table S3. Optimized bond angles (α in degree) and interplanar arene/pyrrolide angles (β) of uranium and transuranium complexes in the gas phase, compared with experimental values of the uranium complexes.

		α(N-An-N)	α[C(t)-An-C(t)] [b]	α(Ar_{cent}-An-Ar_{cent}) [b]	β(Ar-Ar)	β(Pl-Pl)
Ar-U^{III}-2H	Cal.	119.7	124.1	178.1	7.9	76.5
	Expt. [a]	118.9	122.0	174.7	14.2	81.5
Ar-U^{III}-3H	Cal.	120.8	124.3	174.2	41.4	68.8
Pl-U^{III}-3H	Cal.	178.7	172.8	144.6	52.8	44.7
Ar-Np^{III}-2H	Cal.	118.7	123.8	177.5	8.3	74.5
Ar-Np^{III}-3H	Cal.	120.5	127.0	177.4	41.2	70.8
Pl-Np^{III}-3H	Cal.	175.8	169.7	146.0	49.0	46.6
Ar-Pu^{III}-2H	Cal.	117.2	123.1	176.2	10.8	73.8
Ar-Pu^{III}-3H	Cal.	118.5	123.3	172.8	42.0	67.0
Pl-Pu^{III}-3H	Cal.	177.4	171.2	145.3	51.1	45.6
Ar-U^{IV}-2H	Cal.	120.5	126.4	179.6	7.8	76.7
Ar-U^{IV}-3H	Cal.	124.8	129.1	177.1	42.7	49.7
Pl-U^{IV}-3H	Cal.	179.2	173.9	143.4	53.5	40.9
	Expt. [a]	179.1	173.4	143.6	50.0	41.8
Ar-Np^{IV}-2H	Cal.	120.0	124.5	178.7	8.7	71.2
Ar-Np^{IV}-3H	Cal.	122.3	126.6	178.8	40.4	72.8
Pl-Np^{IV}-3H	Cal.	177.4	173.5	143.5	52.4	41.8
Ar-Pu^{IV}-2H	Cal.	118.3	123.2	177.0	10.4	70.6
Ar-Pu^{IV}-3H	Cal.	119.4	159.6	174.1	41.1	63.6
Pl-Pu^{IV}-3H	Cal.	177.6	172.1	144.1	51.0	43.1

[a.] The experimental values of **Ar-U^{III}-2H** and **Pl-U^{IV}-3H** from Refs. [39, 40].

[b.] See the C(t) atom in Chart 1(a), and the Ar_{cent} denotes the centroid of the arene (Ar) plane.

Table S4. Optimized bond lengths (Å) of uranium and transuranium complexes in the gas phase, compared with experimental values of the uranium complexes.

		An-N_{avg}	An-$C(t)_{avg}$ [b]	An-B	An-$H(b)_{avg}$ [b]	An-$Ar1_{cent}$ [c]	An-$Ar2_{cent}$ [c]	An-$Pl1_{cent}$ [c]	An-$Pl2_{cent}$ [c]
Ar-U^{III}-2H	Cal.	2.454	2.802	2.876	2.342	2.501	2.501	—	—
	Expt. [a]	2.464	2.845	2.927	—	2.601	2.580	—	—
Ar-U^{III}-3H	Cal.	2.415	2.805	2.538	2.348	3.418	2.361	—	—
Pl-U^{III}-3H	Cal.	2.608	2.764	2.560	2.369	3.563	3.436	2.440	2.440
Ar-Np^{III}-2H	Cal.	2.457	2.821	2.830	2.305	2.518	2.518	—	—
Ar-Np^{III}-3H	Cal.	2.427	2.803	2.516	2.327	3.281	2.424	—	—
Pl-Np^{III}-3H	Cal.	2.607	2.793	2.532	2.345	3.477	3.442	2.454	2.454
Ar-Pu^{III}-2H	Cal.	2.458	2.835	2.823	2.303	2.553	2.553	—	—
Ar-Pu^{III}-3H	Cal.	2.422	2.819	2.533	2.346	3.326	2.478	—	—
Pl-Pu^{III}-3H	Cal.	2.615	2.775	2.514	2.322	3.480	3.476	2.456	2.452
Ar-U^{IV}-2H	Cal.	2.373	2.814	2.822	2.272	2.530	2.524	—	—
Ar-U^{IV}-3H	Cal.	2.338	2.788	2.491	2.289	3.394	2.465	—	—
Pl-U^{IV}-3H	Cal.	2.544	2.711	2.485	2.278	3.475	3.474	2.433	2.427
	Expt. [a]	2.541	2.738	2.503	2.186	3.446	3.453	2.422	2.415
Ar-Np^{IV}-2H	Cal.	2.434	2.809	2.790	2.252	2.546	2.525	—	—
Ar-Np^{IV}-3H	Cal.	2.386	2.778	2.484	2.281	3.371	2.462	—	—
Pl-Np^{IV}-3H	Cal.	2.553	2.711	2.466	2.255	3.560	3.361	2.432	2.432
Ar-Pu^{IV}-2H	Cal.	2.455	2.821	2.776	2.243	2.544	2.544	—	—
Ar-Pu^{IV}-3H	Cal.	2.426	2.798	2.488	2.288	3.286	2.477	—	—
Pl-Pu^{IV}-3H	Cal.	2.552	2.719	2.460	2.251	3.442	3.442	2.433	2.429

[a] The experimental values of **Ar-U^{III}-2H** and **Pl-U^{IV}-3H** from Refs. [39, 40].

[b] The C(t) atom was marked in Chart 1(a). The H(b) denotes the hydrogen that bridges the actinide and boron.

[c] The distance was determined between the actinide and the centroid of planar arene (Ar) or pyrrolide (Pl).

Table S5. Calculated electron-spin density (S_{An}) and charge (Q_{An}) of the actinide atom of **Ar-An^{III}-2H**, **Pl-An^{IV}-3H** and **Pl-Pu^{III}-3H** (An = U, Np and Pu) at various levels of theory.

	Pri: PBE/B-I		Pri: B3LYP/B-I		Pri: PBE/B-II		ADF: PBE/B-III/THF [a]	
	PBE/B-I Geom. [b]		PBE/B-I Geom. [b]		PBE/B-II Geom. [c]		B-II Geom. [c]	
	S_{An}	Q_{An}	S_{An}	Q_{An}	S_{An}	Q_{An}	S_{An}	Q_{An}
Ar-U^{III}-2H	2.826	1.861	2.917	2.025	2.856	3.010	2.802	1.057
Ar-Np^{III}-2H	4.042	1.801	4.048	1.980	4.052	2.886	4.074	0.997
Ar-Pu^{III}-2H	5.153	1.802	5.099	1.974	5.146	2.763	5.167	1.092
Pl-Pu^{III}-3H	5.193	1.707	5.136	1.911	5.194	3.007	5.224	0.873
Pl-U^{IV}-3H	2.136	1.867	2.121	2.093	2.139	3.397	2.136	0.835
Pl-Np^{IV}-3H	3.314	1.838	3.258	2.059	3.309	3.300	3.378	0.777
Pl-Pu^{IV}-3H	4.573	1.804	4.500	2.017	4.566	3.220	4.673	0.813

[a.] Solvent effects of THF were considered using COSMO model.

[b.] Structures were optimized at the Pri: PBE/B-I level.

[c.] Structures were optimized at the Pri: PBE/B-II level.

Table S6. Calculated electron-spin density and charge of each fragment of **Ar-An^{III}-2H**, **Pl-An^{IV}-3H** and **Pl-Pu^{III}-3H** (An = U, Np and Pu) at the Pri: PBE/B-II level.[a]

	Electron-spin density				Charge			
	S_{An}	S_{Ar} [b]	S_{Pl} [b]	S_{BH4}	Q_{An}	Q_{Ar} [b]	Q_{Pl} [b]	Q_{BH4}
Ar-U^{III}-2H	2.856	0.251	-0.061	-0.042	3.010	-1.046	-0.814	-0.885
Ar-Np^{III}-2H	4.052	0.089	-0.081	-0.060	2.886	-0.826	-0.823	-0.891
Ar-Pu^{III}-2H	5.146	0.005	-0.089	-0.065	2.763	-0.721	-0.837	-0.842
Pl-Pu^{III}-3H	5.194	0.000	-0.125	-0.079	3.007	-0.387	-1.311	-1.039
Pl-U^{IV}-3H	2.139	-0.021	-0.077	-0.048	3.397	-0.272	-1.093	-0.945
Pl-Np^{IV}-3H	3.309	-0.051	-0.148	-0.075	3.300	-0.238	-1.275	-0.933
Pl-Pu^{IV}-3H	4.566	-0.122	-0.376	-0.102	3.220	-0.299	-1.002	-0.964

[a.] All structures were optimized at the Pri: PBE/B-II level.

[b.] S_{Ar} and Q_{Ar} denote electron-spin density and charge localizing on *bis*(arene), respectively, and S_{Pl} and Q_{Pl} stand for spin and charge of *bis*(pyrrolide).

Table S7. Contributions (%) to the α-spin orbitals of **Ar-U^{III}-3H**.[a,b]

Orbs.	Energy	Contribution (%)				Assignment
	eV	U	2Ar	2Pl	BH_4	
HOMO	-3.283	98.89(f_y,f_{z^2y})			-1.03(p_y)	U(f)
H-1	-3.580	76.14(f_{xyz},f_x)	16.21(p_z)			δ(U-Ar_{down})
H-2	-3.592	74.87(f_z,f_{z^2y})	17.31(p_z)			δ(U-Ar_{down})
H-3	-4.475			76.13(p_y,p_x,p_z)		π(Pl)
H-4	-4.518			85.74(p_x,p_y, p_z)		π(Pl)
H-5	-5.494	2.73(f_x,f_{z^2x})		85.14(p_x,p_y, p_z)		π(Pl)+π(U-N)
H-6	-5.537	2.7(f_x,$d_{x^2-y^2}$)		85.14(p_y,p_x)		π(Pl)+π(U-N)
H-7	-6.310		76.7(p_z,p_y)			π(Ar_{up})
H-8	-6.649	1.99(d_{z^2})	76.13(p_z,p_y)		1.35(s)	π(Ar_{up})
H-9	-6.966	3.24(d_{xy},p_x)	24.32(p_z)	34.51(p_x,p_y,s,p_z)	4.43(p_x, s)	σ(U-N)+π(Ar_{down})
H-10	-7.099	4.93(d_{xz} ,f_{z^2x})	33.68(p_z,p_y)	14.21(p_x,p_y)	13.30(s,p_z, p_x)	π(Ar_{down})+σ(U-N)+BH_4
H-11	-7.224	4.58(d_{xz},f_{z^2x})	56.45(p_z,p_y)	2.29(p_z,p_x)	5.7(s,p_y)	π(Ar_{down})
H-12	-7.443	4.09($d_{x^2-y^2}$,f_y)	1.68(p_y)	40.88(p_x,p_y,s)	7.5(s,p_y)	σ(U-N)

[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 Figure 1.

[c] Major orbital character of U, *bis*(arene) (2Ar), *bis*(pyrrolide) (2Pl) and BH_4 is listed in parentheses.

[d] Only the two most large composition of uranium is 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.

Table S8. Contributions (%) to the α-spin orbitals of **Pl-U^{III}-3H**.

Orb.s	Energy	Contribution (%)				Assignment
	eV	U	2Ar	2Pl	BH_4	
HOMO	-2.768	83.68(f_{z^2x},f_{xyz})	2.06(p_z)	1.15(p_x)		κ^3:κ^3-(U-Pl)
H-1	-2.771	82.49(f_y,f_z)		5.41(p_x)		U(*f*)
H-2	-2.812	83.25(f_z,f_{z^2y})		6.44(p_x)		π(U-Pl_2)
H-3	-5.585	9.76(f_{z^3},d_{yz})	1.2(p_z)	69.67(p_x,p_y)		π(Pl)
H-4	-5.760	9.58(d_{xz},f_{xyz})	29.14(p_z,p_y)	49.18(p_x,p_y)		π(Pl)
H-5	-5.934	2.31(p_x,f_x)	12.09(p_z)	47.51(p_y,p_x,*s*)	11.72(p_x,*s*)	π(Pl)+B
H-6	-6.154	2.32(*s*,f_y)		74.73(p_y,*s*,p_x)		π(Pl)+B
H-7	-6.173	3.99(f_x,d_{xy})	36.79(p_z,p_y)	39.70(p_y,p_x)		π(U-Pl)+π(Ar)
H-8	-6.291	5.43(f_x,p_x)	14.9(p_z)	56.3(p_x,p_y,*s*)		π(U-Pl)+π(Ar)

Table S9. Contributions (%) to the α-spin orbitals of **Ar-U^{IV}-2H**.

Orb.s	Energy	Contribution (%)			Assignment
	eV	U	2Ar	2Pl	
HOMO	-5.320	23.81(f_z,f_{xyz})		57.39(p_z,p_y,p_x)	π(Pl)+U(*f*)
H-1	-5.352	43.15(f_{xyz},f_y)		36.53(p_y,p_x,p_z)	π(Pl)+U(*f*)
H-2	-5.392	42.9(f_{xyz},f_z)	2.3(p_z)	39.96(p_y,p_z,p_x)	π(Pl)+U(*f*)
H-3	-5.427	63.97(f_z,f_{z^2y})	2.72(p_z)	12.4(p_y,p_x,p_z)	π(Pl)+U(*f*)
H-4	-6.472	8.13($d_{x^2-y^2}$,f_{z^2y})		79.44(p_y,p_x,p_z)	π(Pl)+π(U-N)
H-5	-6.497	9.67(f_x,f_{z^2x})		79.79(p_y,p_z,p_x)	π(Pl)+π(U-N)

Table S10. Contributions (%) to the α-spin orbitals of **Pl-U^{IV}-3H**.

Orb.s	Energy	Contribution (%)				Assignment
	eV	U	2Ar	2Pl	BH_4	
HOMO	-4.774	88.51(f_z,f_{xyz})		2.56(p_x)		π(U-Pl_2)
H-1	-4.815	88.81(f_{z^2x},f_y)		3.71(p_x)		κ^3:κ^3-(U-Pl)
H-2	-6.721	12.45(f_{z^3},d_{xz})	20.41(p_z,p_y)	30.55(p_x,p_y)		π(U-Pl_{down})
H-3	-6.800	13.16(f_{z^3},f_{xyz})	22.22(p_z,p_y)	31.78(p_x,p_y)		π(U-Pl_{up})
H-4	-6.909	2.17(p_x,f_{z^2x})	51.24(p_z,p_y)	22.35(p_y,*s*,p_x)	4.93(*s*,p_x)	L
H-5	-7.120		19.96(p_z)	50.50(p_y,*s*,p_x)		L

Table S11. Contributions (%) to the α-spin orbitals of **Ar-Np^{III}-2H**.

Orb.s	Energy	Contributions (%)				Assignment
	eV	Np	2Ar	2Pl	BH_4	
HOMO	-3.547	97.09(f_y,s)				Np(*f*)
H-1	-3.733	95.74(f_{z^3},f_{z^2x})				Np(*f*)
H-2	-3.877	84.98(f_{xyz},f_y)	6.68(p_z)			δ(Np-Ar_2)
H-3	-3.898	84.01(f_z,f_{z^2x})	7.01(p_z)			δ(Np-Ar_2)
H-4	-4.424			78.88(p_y,p_x,p_z)		π(Pl)
H-5	-4.441			81.92(p_y,p_x,p_z)		π(Pl)
H-6	-5.415	4.25(f_x)		86.73(p_y,p_x,p_z)		π(Pl)+π(Np-N)
H-7	-5.435	3.18(f_{z^2y},$d_{x^2-y^2}$)		69.88(p_y,p_x,p_z)		π(Pl)+π(Np-N)
H-8	-6.702	2.16(d_{yz})	21.39(p_z)		65.87(s,p_z,)	π(B)+π(Ar)

Table S12. Contributions (%) to the α-spin orbitals of **Ar-Pu^{III}-2H**.

Orb.s	Energy	Contributions (%)		Assignment
	eV	An	2Pl	
HOMO	-3.960	82.99(f_x,f_{z^2x})	2.31(p_y)	Pu(*f*)
H-1	-4.142	94.69(f_y,f_{z^2y})		Pu(*f*)
H-2	-4.306	79.18(f_z,f_{z^3})	9.82(p_y)	Pu(*f*)+π(Pl)
H-3	-4.372	61.95(f_{xyz},f_{z^3})	23.81(p_y,p_x,p_z)	π(Pl)+Pu(*f*)
H-4	-4.376	44.67(f_{z^3},f_{xyz})	36.25(p_y,p_x,p_z)	π(Pl)+Pu(*f*)
H-5	-4.401	20.38(f_{xyz},f_y)	60.97(p_y,p_x,p_z)	π(Pl)+Pu(*f*)
H-6	-4.443	72.84(f_z,f_{z^3})	8.47(p_y)	π(Pl)+Pu(*f*)
H-7	-5.390	6.97(f_x)	84.74(p_y,p_x,p_z)	π(Pl)+π(Pu-N)
H-8	-5.408	6.3(f_{z^2y},$d_{x^2-y^2}$)	84.73(p_y,p_x,p_z)	π(Pl)+π(Pu-N)

Table S13. Contributions (%) to the α-spin orbitals of **Pl-Pu^{III}-3H**.

Orb.s	Energy	Contributions (%)				Assignment
	eV	An	2Ar	2Pl	BH_4	
HOMO	-3.570	88.74(f_{xyz},d_{xz})				Pu(*f*)
H-1	-3.613	93.94(f_{z^2y},f_{z^2x})				Pu(*f*)
H-2	-3.710	91.42(f_z,f_y)				Pu(*f*)
H-3	-3.737	92.44(f_{z^2x},f_{z^2y})				Pu(*f*)
H-4	-3.766	93.16(f_y,f_z)		2.15(p_x)		Pu(*f*)
H-5	-5.569	15.98(f_{z^3},d_{yz})	2.3(p_z)	66(p_x,p_y)		π(Pu-Pl_2)
H-6	-5.694	11.97(f_{xyz},d_{xz})	21.05(p_z,p_y)	54.11(p_x,p_y)		π(Pu-Pl_2)
H-7	-5.897	2.72(f_x,p_x)	8.34(p_z)	53.45(s,p_x,p_y)	10.64(s,p_x)	L
H-8	-6.098	3.16(f_y, s)		75.18(p_y,s,p_x)		Pl

Table S14. Contributions (%) to the α-spin orbitals of **Pl-Np^{IV}-3H**.

Orb.s	Energy	Contributions (%)				Assignment
	eV	An	2Ar	2Pl	BH_4	
HOMO	-5.321	88.79(f_z,f_y,)				Np(*f*)
H-1	-5.399	89.95(f_y,f_{z^2y})				Np(*f*)
H-2	-5.421	89.81(f_{z^2x},f_{xyz})				Np(*f*)
H-3	-6.705	6.93(f_{xyz},d_{xz})	53.33(p_z,p_y)	17.56(p_x,p_y)	1.12(p_x)	π(Ar)+π(Np-Pl)
H-4	-6.798	24.35(f_{z^3},f_z)	1.10(p_z)	57.74(p_x,p_y)		π(Np-Pl)
H-5	-6.917	10.81(f_{xyz},f_{z^2x})	36.55(p_z,p_y)	31.48(p_x,p_y,s)	3.53(s,p_x)	π(Np-Pl)+π(Ar)
H-6	-7.170	2.31(f_{z^3})	72.72(p_z,p_y)	1.28(p_y)		π(Ar)

Table S15. Contributions (%) to the α-spin orbitals of **Pl-Pu^{IV}-3H**.

Orb.s	Energy	Contributions (%)				Assignment
	eV	Pu	2Ar	2Pl	BH_4	
HOMO	-5.700	93.36(f_{z^2y},f_{z^2x})				Pu(*f*)
H-1	-5.758	88.7(f_z,f_{xyz})		2.31(p_x)		Pu(*f*)
H-2	-5.802	89.99(f_{z^2x},f_{z^2y})				Pu(*f*)
H-3	-5.832	88.89(f_y,f_{z^2x})		6.23(p_y,p_x,)	1.07(s)	Pu(*f*)
H-4	-6.749	20.46(f_{xyz},f_{z^3})	37.08(p_z,p_y)	25.71(p_x,p_y)		π(Pu-Pl_{up})
H-5	-6.858	32.47(f_{z^3},f_z)		49.52(p_x,p_y)		π(Pu-Pl_2)
H-6	-6.896	4.9(f_{z^2x},p_x)	52.07(p_z,p_y)	21.66(p_y,p_x,s)	5.24(s,p_x)	L

Table S16. Calculated total energies E (Hartree) of thorium isomers and their relative energies ΔE (kcal/mol) at the Pri: PBE/B-I level.

			Ar-An^m-2H	**Ar-An^m-3H**	**Pl-An^m-3H**
An = Th	m = III	E (Hartree)	-27848.437441	-27848.432763	-27848.432115
		ΔE (kal/mol)	0.00	2.94	3.34
	m = IV	E (Hartree)	-27848.266352	-27848.264399	-27848.282048
		ΔE (kal/mol)	9.85	11.07	0.00
An = Pa	m = III	E (Hartree)	-28608.054552	-28608.047954	-28608.041006
		ΔE (kal/mol)	0.00	4.14	8.50
	m = IV	E (Hartree)	-28607.865347	-28607.858719	-28607.877777
		ΔE (kal/mol)	7.80	11.96	0.00

Table S17. Calculated energies (kcal/mol) of formation reactions (Eqs. 1-3 in the text) of low-valent uranium and transuranium complexes.

Complexes	Ligands	$\Delta_rE(gas)$ [a]	$\Delta_rE_0(gas)$ [a]	$\Delta_rH(gas)$ [a]	$\Delta_rG(gas)$ [a]	$\Delta_rG(sol)$ [b]	$\Delta_rG(sol\text{-}so)$ [b]	$\Delta_rE(gas)_{B3}$ [c]
Ar-U^{III}-2H	H_2L	71.15	61.44	61.83	33.76	27.97	26.63	86.95
	Li_2L	41.48	37.78	37.15	9.60	-10.36	-11.70	55.95
	Na_2L	47.41	43.78	42.69	13.52	-18.45	-19.78	61.59
	K_2L	45.22	41.48	40.45	9.81	-22.65	-24.00	57.15
	L^{2-}	-27.25	-30.66	-30.93	-56.53	-59.90	-61.24	-20.82
Ar-Np^{III}-2H	H_2L	75.21	65.61	66.11	37.38	30.98	30.02	88.67
	Li_2L	45.55	41.95	41.43	13.22	-7.35	-8.31	57.68
	Na_2L	51.48	47.95	46.98	17.14	-15.44	-16.39	63.32
	K_2L	49.28	45.65	44.73	13.43	-19.64	-20.61	58.88
	L^{2-}	-23.18	-26.49	-26.64	-52.91	-56.89	-57.85	-19.09
Ar-Pu^{III}-2H	H_2L	79.91	70.00	70.61	41.28	34.63	30.27	89.58
	Li_2L	50.24	46.35	45.93	17.13	-3.69	-8.05	58.59
	Na_2L	56.17	52.35	51.48	21.05	-11.78	-16.13	64.23
	K_2L	53.98	50.05	49.23	17.33	-15.99	-20.36	59.79
	L^{2-}	-18.49	-22.09	-22.14	-49.00	-53.23	-57.59	-18.18
Pl-Pu^{III}-3H	H_2L	77.66	67.80	68.29	39.08	32.14	29.04	92.39
	Li_2L	47.99	44.14	43.61	14.93	-6.18	-9.28	61.40
	Na_2L	53.92	50.14	49.16	18.84	-14.28	-17.37	67.04
	K_2L	51.73	47.84	46.91	15.13	-18.48	-21.59	62.60
	L^{2-}	-20.74	-24.29	-24.46	-51.21	-55.73	-58.83	-15.37
Pl-U^{IV}-3H	H_2L	64.74	54.68	55.44	26.14	23.92	20.66	81.20
	Li_2L	35.07	31.02	30.76	1.99	-14.40	-17.66	50.21
	Na_2L	41.00	37.02	36.31	5.90	-22.50	-25.75	55.85
	K_2L	38.81	34.72	34.06	2.19	-26.70	-29.97	51.40
	L^{2-}	-33.66	-37.42	-37.31	-64.14	-63.94	-67.20	-26.57
Pl-Np^{IV}-3H	H_2L	61.91	51.63	52.66	21.95	18.78	16.00	75.59
	Li_2L	32.24	27.97	27.98	-2.20	-19.54	-22.32	44.60
	Na_2L	38.17	33.97	33.52	1.72	-27.63	-30.40	50.24
	K_2L	35.98	31.67	31.28	-2.00	-31.84	-34.63	45.80
	L^{2-}	-36.49	-40.47	-40.10	-68.33	-69.08	-71.86	-32.17
Pl-Pu^{IV}-3H	H_2L	57.91	47.89	49.00	18.08	14.46	10.09	73.77
	Li_2L	28.25	24.23	24.32	-6.07	-23.86	-28.23	42.78
	Na_2L	34.18	30.23	29.86	-2.16	-31.96	-36.32	48.42
	K_2L	31.98	27.93	27.62	-5.87	-36.16	-40.54	43.98
	L^{2-}	-40.48	-44.21	-43.76	-72.21	-73.41	-77.78	-33.99

[a] $\Delta_rE(gas)$, $\Delta_rE_0(gas)$, $\Delta_rH(gas)$ and $\Delta_rG(gas)$ denote the total energy, total energy including zero-point vibration energy, enthalpy and free energy of the reaction in the gas phase, respectively.

[b] $\Delta_rG(sol)$ stands for the reaction free energy in THF solution, which includes scalar relativistic corrections and is calculated by $\Delta_rG(sol) = \Delta_rG(gas) + \Delta G_{sol}$. $\Delta_rG(sol\text{-}so)$ is the reaction free energy, containing both solvation effect as well as scalar and spin-orbit relativistic effects, i.e. $\Delta_rG(sol\text{-}so) = \Delta_rG(gas) + \Delta G_{sol} + \Delta G_{so}$. [c] $\Delta G_{sol} = \sum \nu_B G_{sol}(B)$ and $\Delta G_{so} = \sum \nu_B G_{so}(B)$, where $G_{sol}(B)$ and $G_{so}(B)$ are the calculated solvation and spin-orbit coupling free energies of each molecule (B) in the formation reaction, respectively.

[a] $\Delta_rE(gas)_{B3}$ was the reaction change of the total energy, which was calculated using the B3LYP functional at the geometry of each reactant and product optimized by the Priroda: PBE/B-I approach.

Table S18. Total energies ($\Delta_r E$ in eV) of single-electron oxidation reactions of actinide complexes calculated with different functionals (GGA-PBE and hybrid B3LYP) and codes (Priroda and Gaussian).

Approach	Pri: ***PBE***/B-II	Pri: ***PBE***/B-I	Pri: ***B3LYP***/B-I	Gau: ***PBE***/B-IV	Gau: ***B3LYP***/B-IV
Geometry	Pri: PBE/B-II	Pri: PBE/B-I	Pri: PBE/B-I	Pri: PBE/B-II	Pri: PBE/B-II
Ar-U^{III}-2H - *e* = **Pl-U^{IV}-3H**	5.21	5.16	5.51	4.95	5.32
Ar-Np^{III}-2H - *e* = **Pl-Np^{IV}-3H**	5.63	5.58	6.02	5.36	5.75
Ar-Pu^{III}-2H - *e* = **Pl-Pu^{IV}-3H**	5.74	5.70	6.39	5.54	6.30
Pl-Pu^{III}-3H - *e* = **Pl-Pu^{IV}-3H**	5.84	5.81	6.27	5.70	6.20

The full reference of the ADF code:

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 Kessel, 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, A.L. Yakovlev. ADF2014, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

The full reference of the Gaussian code:

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.

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Cartesian coordiantes of complexes optimized at the Priroda: PBE/B-II level.

Ar-U^{III}-2H

C 13.60688052 5.29325040 5.45778233
C 14.37288979 5.90951644 6.43117986
C 13.16308630 5.84551123 4.11509265
N 13.35437236 3.96492092 5.81249669
H 14.72940037 6.93637722 6.42297567
C 14.61963466 4.93809840 7.44039757
C 11.96787406 5.00508892 3.68058039
C 12.73043816 7.32496212 4.24231714
C 14.32925288 5.77809317 3.10610660
C 13.99281215 3.77183340 7.03896665
U 12.08376877 2.29721787 4.53756081
H 15.18459016 5.08946967 8.35666264
C 10.85443470 4.91886443 4.55373955
C 11.95051813 4.23038582 2.51352693
H 12.39677080 7.71280893 3.26905642
H 13.57782503 7.93685765 4.57915635
H 11.91671750 7.45193640 4.96722693
H 14.04246388 6.17618381 2.12039065
H 14.69804859 4.75148058 2.97423188
H 15.16387521 6.38004203 3.48729009
C 13.87526270 2.45439025 7.78292591
C 13.60937520 1.38012550 6.73295528
C 14.47698469 1.31103354 5.61035163
C 10.87947537 3.34917887 2.20683897
N 12.93149380 1.51710799 2.37106064
C 9.76933313 4.10104320 4.24507119
H 10.86423461 5.48405048 5.48520796
H 12.80036519 4.25469011 1.83381337
C 12.74490782 2.54142560 8.83054748
C 15.19298809 2.12157004 8.52140007
C 12.51118108 0.50839552 6.77699348
H 15.32175549 1.99664695 5.57680974
C 14.23896974 0.44381702 4.53620598
C 11.01878570 2.44439619 0.98648940
C 9.78639078 3.30280941 3.08484689
C 14.09592491 0.78242249 2.12940423
C 12.35431152 1.73604294 1.11883099
H 8.92416180 4.02892024 4.92630727
H 12.65390348 1.61277741 9.41485738
H 11.77424750 2.75839860 8.36353283

H 12.96845993 3.35957535 9.52694712
H 15.10689154 1.15796950 9.04384742
H 15.41289084 2.89507973 9.26941150
H 16.04358415 2.07046446 7.82969637
C 12.27553474 -0.39583008 5.72324900
H 11.80860713 0.53937823 7.60605554
C 13.10941119 -0.40979251 4.60702939
C 15.06119065 0.44864173 3.25261136
C 9.88020087 1.40611643 0.89464008
C 10.98298525 3.31417973 -0.29203891
H 8.95346235 2.62852200 2.90194845
C 14.23864299 0.54706722 0.77357476
C 13.12702270 1.15624295 0.12838925
H 11.40236375 -1.04344986 5.76518442
H 12.88467669 -1.06514959 3.76610200
C 16.20530271 1.48410233 3.28932188
C 15.69144071 -0.94801659 3.04222733
H 10.06063411 0.75697960 0.02839849
H 8.89755858 1.88460914 0.76220215
H 9.84114840 0.76627032 1.78707333
H 11.10188426 2.68242718 -1.18251445
H 11.78852942 4.05959849 -0.29790919
H 10.01952508 3.83774897 -0.37272094
H 15.05046086 0.00970730 0.29004105
H 12.92100056 1.15530988 -0.93893675
H 16.74046266 1.45607170 2.33168776
H 16.92801923 1.26867422 4.09158500
H 15.82782128 2.50707903 3.42480280
H 16.26629909 -0.96406429 2.10669688
H 14.92956932 -1.73511023 2.98057735
H 16.37773242 -1.18811991 3.86706052
B 9.61111114 1.26148888 5.57803012
H 10.32770300 2.17052431 6.08165734
H 8.52720699 1.72099229 5.28700272
H 10.20392255 0.90065824 4.52357203
H 9.55748796 0.32570752 6.34751561

Ar-U^{III}-3H

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C 13.78264589 5.84544573 6.73765698
C 13.05277998 5.79798131 4.24606141
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H 13.90548208 6.91865241 6.85024962
C 14.11415545 4.85926302 7.70264025
C 11.79974809 5.17450182 3.61671985
C 12.86252989 7.32423442 4.37670194
C 14.30418041 5.57842429 3.35973468
C 13.83129475 3.63014075 7.13704604
U 12.23413182 2.02109627 4.63561030
H 14.51623217 5.03847658 8.69671264
C 10.50753977 5.60598747 3.95776311
C 11.91084981 4.14175697 2.66769183
H 12.60384821 7.75796235 3.40081946
H 13.79510102 7.79138814 4.71892045
H 12.07764925 7.58691802 5.09639803
H 14.15341935 5.96687315 2.34096360
H 14.58868764 4.52019308 3.28905334
H 15.15236713 6.10695492 3.81389186
C 13.98331199 2.26334194 7.79289880
C 13.75917962 1.19974243 6.72076309
C 14.61481288 1.17381434 5.58107926
C 10.78903289 3.50210514 2.09841244
N 12.96340307 1.41668282 2.40801361
C 9.39035680 5.05857829 3.32919218
H 10.37112748 6.38617249 4.70553720
H 12.89442678 3.84925889 2.30255297
C 12.97847565 2.13632859 8.95760888
C 15.40829415 2.10365177 8.37972561
C 12.68341255 0.29258853 6.76199387
H 15.44197094 1.87879498 5.54399628
C 14.37497204 0.32544603 4.48340952
C 10.96966121 2.34019488 1.10884544
C 9.52195758 4.00989106 2.41905933
C 14.18265806 0.81055929 2.09266361
C 12.36603147 1.75180748 1.19021023
H 8.39622194 5.43043195 3.58108412
H 13.06559009 1.16366707 9.46657432
H 11.94272842 2.27191557 8.61831585
H 13.18543727 2.92324455 9.69369162
H 15.52152147 1.11693540 8.85275603
H 15.58790911 2.87262816 9.14250177
H 16.18281546 2.21353988 7.61039201
C 12.43770519 -0.58048240 5.68110378
H 12.00900216 0.28086611 7.61411867
C 13.26019460 -0.55212115 4.54803720
C 15.16473588 0.39511977 3.17853395

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H 13.03356365 -1.19134649 3.69615495
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H 10.10271084 0.39040878 0.69450030
H 8.90163825 1.56620717 1.27898840
H 10.04222054 0.81958842 2.41630296
H 10.76846634 2.07139622 -1.05150733
H 11.43979787 3.65501765 -0.58317897
H 9.70183987 3.32182393 -0.37356478
H 15.20389750 0.36809419 0.18125939
H 12.99958266 1.49577712 -0.91364181
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H 17.05376292 1.14286209 4.03017814
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H 16.31860064 -0.95756992 1.91321902
H 15.00140324 -1.76787522 2.77772266
H 16.47995791 -1.29061996 3.65373948
B 9.87188300 1.89441416 5.55600359
H 10.71893130 2.06715453 6.45371271
H 8.74763947 1.80223142 5.97154644
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H 10.03463369 2.82719116 4.75587450

Pl-U^{III}-3H

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C 1.53239725 -1.35226939 -1.70151247
C 1.13487917 1.15498622 -1.42592137
C 2.71163040 -0.06330281 0.09427694
C -1.86614966 -0.53210326 0.96530821
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C 1.65544318 -1.21028334 -3.08955257

C 1.49444860 -2.66479640 -1.19364035
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H 1.01187500 1.95287069 -0.68166513
H 0.21633448 1.11318253 -2.02297992
H 3.54626033 0.16623982 -0.58297490
H 2.95765617 -0.99644872 0.61879498
H 2.63416070 0.74015218 0.84031818
C -3.37660940 -0.27130358 0.99475081
C -4.10689556 -1.47877222 0.36480785
C -3.68577304 -2.77771570 0.70044180
C 1.47801845 -3.81927192 -1.99926417
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H 1.67904375 -0.22097548 -3.54398177
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C -3.67116265 1.03393533 0.23917021
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C -5.15682969 -1.36427575 -0.55522670
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C 1.28566393 -5.18968799 -1.31289096
C 1.60256634 -3.63245196 -3.38180691
C -1.96934030 -5.09896352 0.41088843
C 0.12482183 -5.06956719 -0.31892811
H 1.80459651 -2.21393311 -4.98668816
H -4.73709862 1.29319738 0.30429465
H -3.37931120 0.95995408 -0.81517627
H -3.09594775 1.85438179 0.68823174
H -4.93915808 0.08316708 2.47142808
H -3.33588000 0.70589644 2.95105881
H -3.68931140 -1.03810378 3.03828377
C -5.71403997 -2.51086101 -1.12415399
H -5.52393776 -0.38540120 -0.85936360
C -5.21383368 -3.78407233 -0.84548674
C -3.49007557 -5.29343905 0.38536367
C 0.96983748 -6.30043343 -2.32566175
C 2.58877079 -5.54873060 -0.56640547
H 1.58588412 -4.48545462 -4.05849226
C -1.16383352 -4.72410262 1.51626805
C 0.17334531 -4.70540495 1.04941796
H -6.52865368 -2.40551189 -1.84275055
H -5.62433014 -4.64498260 -1.37060775
C -3.83764596 -6.36299057 -0.66189538
C -3.98319204 -5.77045864 1.76958412

H 0.80872505 -7.24626903 -1.79169649
H 1.80645663 -6.44438076 -3.02404842
H 0.05695462 -6.07826220 -2.89066684
H 2.47148243 -6.50224259 -0.03238672
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H -1.48462989 -4.55560716 2.54087892
H 1.05669716 -4.50977643 1.65206798
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H -3.53858031 -6.04839770 -1.66880395
H -4.91404103 -6.58424943 -0.65447184
H -3.77625626 -5.03209933 2.55590413
H -3.49532209 -6.71591504 2.04639322
H -5.07026619 -5.93061793 1.74419899
B -2.21910970 -2.39893038 -2.71368380
H -2.47894209 -1.47189134 -1.92929261
H -0.97476783 -2.42871438 -2.76580300
H -2.53558414 -3.46606854 -2.16311299
H -2.72673236 -2.25754178 -3.79666764
U -1.11598265 -2.69909886 -0.42335105

Ar-Np^{III}-2H

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N -1.85413642 -0.99242259 -0.30841977
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C -3.92232156 -1.36803208 -1.19265554
C 0.42095700 -2.54521292 -0.21943288
C -0.68956185 -4.34827919 -1.55500148
C 0.11251469 -2.29884453 -2.73842520
C -3.17429160 -0.54490502 -0.36791763
H -4.98128973 -1.27212542 -1.41869230
C -0.03782384 -2.90458598 1.07097511
C 1.63807932 -1.86110249 -0.31657857
H 0.27010141 -4.84998958 -1.74571380
H -1.35715387 -4.56057745 -2.40054691
H -1.14034289 -4.78470585 -0.65488755
H 1.06699561 -2.79087232 -2.98229719
H 0.27500941 -1.21256719 -2.71155321
H -0.59479969 -2.50538838 -3.55156834
C -3.65304355 0.62520193 0.47400384

C -2.43357204 1.49642005 0.75612509
C -1.62855868 1.89375313 -0.34151641
C 2.39268425 -1.49273866 0.82605442
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C 0.71418626 -2.59951461 2.20283908
H -1.00205129 -3.40158546 1.17314779
H 2.00250699 -1.54186387 -1.29111042
C -4.31254169 0.10509932 1.76898608
C -4.69899729 1.46417941 -0.29765912
C -2.01675468 1.85075232 2.04519490
H -1.94864337 1.60007728 -1.33938306
C -0.41743370 2.57436860 -0.17205679
C 3.62314851 -0.61528232 0.62172611
C 1.91850662 -1.88003882 2.08547726
C 1.84258944 2.17368567 -0.98914145
C 3.18213066 0.57670680 -0.21005419
H 0.34692138 -2.86166843 3.19271744
H -4.70203089 0.92585914 2.39108954
H -3.61073526 -0.48964318 2.36965973
H -5.15452606 -0.54559345 1.50087955
H -5.03003964 2.31873051 0.30999431
H -5.57953415 0.84974549 -0.52779217
H -4.29600147 1.84298850 -1.24568527
C -0.81938906 2.56632572 2.23516790
H -2.58879317 1.54648097 2.91809765
C -0.01740621 2.90006645 1.14654136
C 0.54037979 2.88130665 -1.31760821
C 4.22368650 -0.12959430 1.95810541
C 4.70308061 -1.43460208 -0.12383176
H 2.45053829 -1.59880014 2.99080361
C 3.11068194 2.44106878 -1.47589686
C 3.96614064 1.42073927 -0.97832369
H -0.49719218 2.80261061 3.24700743
H 0.94096197 3.39371189 1.30476379
C 0.00456965 2.39263893 -2.68004922
C 0.75059760 4.41076145 -1.40935275
H 5.07611264 0.52781712 1.74502546
H 4.58587453 -0.96655518 2.57509114
H 3.49522025 0.44923765 2.54236244
H 5.59277851 -0.81500007 -0.29808314
H 4.34323350 -1.78826221 -1.09855514
H 5.00689774 -2.30494923 0.47556759
H 3.39705436 3.26267271 -2.12747293
H 5.03431217 1.33021510 -1.15866932

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H -0.15836750 1.30612768 -2.68831362
H 1.45577449 4.64454554 -2.21792828
H 1.15940326 4.82386274 -0.47875107
H -0.19992674 4.91731335 -1.63061139
B -0.08851017 -0.03729061 3.82761296
H -0.94985783 -0.52869923 3.04355173
H 0.40308468 -0.92434764 4.49296058
H 0.80683984 0.47348342 3.09576953
H -0.60987394 0.83284374 4.49263907
Np -0.02510362 -0.00082856 0.99864011

Ar-Np^{III}-3H

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C 14.53914340 5.92674335 6.08770779
C 12.88565413 6.11875154 4.09485522
N 13.20470759 4.12161430 5.67217338
H 15.00216380 6.90753081 6.01295159
C 14.85896591 4.91077189 7.02499833
C 11.74694937 5.22935742 3.61118285
C 12.32714394 7.50313045 4.50879847
C 13.94411973 6.35354553 2.99518939
C 14.03137106 3.83035169 6.76148085
H 15.60190245 4.98012939 7.81429566
C 10.60622875 5.03022560 4.43241266
C 11.83399309 4.48743948 2.42727211
H 11.84845760 8.00235751 3.65310309
H 13.14771033 8.14053040 4.86266223
H 11.59784170 7.42799011 5.32465237
H 13.50541149 6.82585862 2.10244261
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C 14.18741960 1.24661928 5.44752476
C 10.84006091 3.55379701 2.03377502
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C 15.08043508 2.41331804 8.54382693
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C 14.12418218 1.04858178 2.31504727
C 12.53313178 2.07729026 1.13462011
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H 11.68664166 2.85412268 7.90193522
H 12.70909732 3.73207289 9.06135111
H 14.96592975 1.50697446 9.15383230
H 15.17229626 3.27072907 9.22426438
H 16.00875552 2.32688504 7.96367471
C 13.19565151 -1.05287105 6.62951818
H 12.92442033 0.12240348 8.40210864
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C 14.73350194 0.03009573 3.27494922
C 10.13491734 1.51745275 0.66812387
C 11.17681941 3.49975696 -0.44845261
H 8.91149394 2.72107124 2.56875553
C 14.66443834 1.36979560 1.07432924
C 13.65373928 2.02109236 0.32414867
H 12.80807644 -1.96101303 7.09356807
H 13.52157003 -2.01461597 4.73936711
C 16.25489787 0.28653591 3.43120973
C 14.56128347 -1.36337654 2.62257116
H 10.44423123 0.88552577 -0.17445493
H 9.12792951 1.90508324 0.44910811
H 10.08511939 0.87968771 1.56066230
H 11.44424038 2.86940038 -1.30751287
H 11.90210742 4.32183986 -0.39106422
H 10.18146613 3.92668752 -0.63493304
H 15.65746499 1.11012146 0.71689889
H 13.74163325 2.39568415 -0.69204184
H 16.75850111 0.20597482 2.45903068
H 16.69814109 -0.45902559 4.10679097
H 16.45759227 1.28631558 3.83554449
H 15.02528447 -1.35023331 1.62917585
H 13.49999782 -1.61464196 2.48992409
H 15.04445693 -2.15520491 3.21493355
B 10.15839814 1.07245512 5.47601522
H 11.30363769 0.60365630 5.55332629

H 9.31749135 0.39339273 6.00280204
H 9.96318912 1.23454750 4.25355816
H 10.22665218 2.22337165 5.96825069
Np 11.89011054 2.53535010 4.38384139

Pl-Np^{III}-3H

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C 0.25302811 -1.19610079 1.45737466
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N -1.07520774 -0.11977742 -0.06953163
H 1.12751997 -1.58080726 1.97557951
C -1.08025462 -1.22543860 1.93805722
C 1.52988398 -1.36071447 -1.70059510
C 1.10832327 1.14444859 -1.43532903
C 2.69618853 -0.04883174 0.09132887
C -1.86653157 -0.54321043 0.98089936
H -1.40633574 -1.63528594 2.89041452
C 1.63064551 -1.21809017 -3.09096427
C 1.52912606 -2.66944419 -1.18482000
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H 0.97336444 1.94302928 -0.69388058
H 0.19245858 1.09108595 -2.03556925
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C 1.27436060 -5.18875623 -1.30751349
C 1.57054878 -3.63614535 -3.37885960
C -1.97064721 -5.09525228 0.43281240
C 0.11585221 -5.05723372 -0.31264484

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H -3.37310019 0.99181926 -0.76416250
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H -4.93523356 0.04746737 2.50424692
H -3.32917518 0.65555761 2.99267126
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H -5.45155913 -0.37570324 -0.92300029
C -5.15338103 -3.77455867 -0.90555877
C -3.49121256 -5.28842699 0.40725190
C 0.94832485 -6.29809290 -2.31846538
C 2.57474428 -5.55965221 -0.56213943
H 1.53333072 -4.49019745 -4.05334933
C -1.16302299 -4.69640559 1.52297093
C 0.17171009 -4.67085927 1.04573623
H -6.42242629 -2.39037911 -1.95442942
H -5.53929006 -4.63373386 -1.45193370
C -3.84180844 -6.37964629 -0.61541358
C -3.99055789 -5.73061996 1.80038502
H 0.77880839 -7.24192761 -1.78353241
H 1.78392691 -6.44958454 -3.01641933
H 0.03769027 -6.06974004 -2.88463848
H 2.44888914 -6.50982746 -0.02417137
H 2.86883562 -4.79026277 0.16417201
H 3.39938968 -5.66992520 -1.28034989
H -1.47857900 -4.51045118 2.54626057
H 1.05808950 -4.45949097 1.63812388
H -3.31829536 -7.30866159 -0.35363595
H -3.52940040 -6.09539922 -1.62721986
H -4.92123119 -6.58670506 -0.61228471
H -3.78317392 -4.97599622 2.57085530
H -3.50709106 -6.67115147 2.10021093
H -5.07809447 -5.88764784 1.77489405
B -2.17109848 -2.38419842 -2.77269078
H -2.49636562 -1.48805361 -1.97517881
H -0.92507079 -2.37081080 -2.77724268
H -2.48149116 -3.46957504 -2.25203050
H -2.64984790 -2.23456248 -3.86786699
Np -1.16975269 -2.69559809 -0.46762558

Ar-Pu^{III}-2H

C 1.64247792 2.22932410 -1.20204116
C 2.88671230 2.52477480 -1.73905146
C 0.31415724 2.90973322 -1.48005917
N 1.72112037 1.09673358 -0.39632701
H 3.12876192 3.34988963 -2.40393008
C 3.78491619 1.53559029 -1.26104190
C -0.57621980 2.63106796 -0.27370251
C 0.49723532 4.43778708 -1.63276218
C -0.28916835 2.37145889 -2.79478956
C 3.05119059 0.68220953 -0.45097145
H 4.84760372 1.46955198 -1.48009436
C -0.12146215 3.01763941 1.00984475
C -1.77625468 1.91767897 -0.35709157
H -0.47145076 4.92529435 -1.81429068
H 1.15030674 4.65253942 -2.48885073
H 0.95461262 4.88672200 -0.74219038
H -1.25195443 2.85020590 -3.03275334
H -0.43771867 1.28358435 -2.76031722
H 0.40834013 2.58219437 -3.61530955
C 3.56181602 -0.48945901 0.37244741
C 2.37111371 -1.40193023 0.64502157
C 1.56067742 -1.78386181 -0.45401509
C -2.51529043 1.54115507 0.79294795
N -1.93209648 -0.96242077 -0.27578610
C -0.85992131 2.70549546 2.14762687
H 0.83209411 3.53702058 1.10196862
H -2.13859563 1.58063198 -1.32618419
C 4.21338160 0.02549926 1.67353141
C 4.62622863 -1.28835743 -0.41747509
C 1.98321082 -1.81100146 1.92557656
H 1.86092735 -1.45168323 -1.44575511
C 0.36852761 -2.49675400 -0.29132145
C -3.72073644 0.62758135 0.60089169
C -2.04707527 1.95631663 2.04435544
C -1.90459810 -2.09906510 -1.07910759
C -3.26314291 -0.54849766 -0.24706099
H -0.49297414 2.98519904 3.13342274
H 4.63467210 -0.79427378 2.27602115
H 3.49715472 0.58405370 2.29179464
H 5.03122159 0.70928240 1.41345351
H 4.98265025 -2.14375157 0.17450652
H 5.48866721 -0.64680285 -0.64144563
H 4.22812782 -1.66168406 -1.36975121

C 0.80523211 -2.55972421 2.10745681
H 2.55882723 -1.51842085 2.80048272
C -0.00388541 -2.87710835 1.02031843
C -0.59649649 -2.78097172 -1.43752038
C -4.28884973 0.11956259 1.94317245
C -4.83300974 1.42255968 -0.12442358
H -2.56595224 1.66791138 2.95538734
C -3.18051626 -2.39749966 -1.53382360
C -4.04675895 -1.40610101 -1.00423927
H 0.50156919 -2.83467607 3.11585477
H -0.94949476 -3.39609634 1.17518952
C -0.07764811 -2.24905571 -2.79031556
C -0.78867242 -4.30967490 -1.57097827
H -5.12178521 -0.56490978 1.73876622
H -4.67094538 0.94262101 2.56695061
H -3.53520262 -0.43642323 2.51770725
H -5.70817193 0.78025102 -0.28907582
H -4.49637445 1.78972098 -1.10247290
H -5.15072488 2.28182238 0.48377008
H -3.46423387 -3.22616930 -2.17746676
H -5.12130669 -1.34130631 -1.15525018
H -0.82582853 -2.46312251 -3.56399763
H 0.86799371 -2.72940485 -3.08664168
H 0.07310836 -1.16111116 -2.77031739
H -1.49394554 -4.52852396 -2.38349774
H -1.18940041 -4.75410385 -0.65132505
H 0.16682448 -4.79832297 -1.81020085
B 0.02402486 0.07662050 3.76603199
H 0.87186499 0.59093389 2.98221726
H -0.47472041 0.95145177 4.44159361
H -0.87125908 -0.44129300 3.03943442
H 0.56439438 -0.79518725 4.41290548
Pu -0.06490064 0.07018045 0.94405664

Ar-Pu^{III}-3H

C 13.64599168 5.33784206 5.41630086
C 14.48722883 5.87355062 6.37890129
C 13.23452966 5.95169214 4.08713251
N 13.28856564 4.03601607 5.76038499
H 14.92921238 6.86662377 6.37876265
C 14.67026221 4.86842553 7.36335113
C 11.99712846 5.19277203 3.61821304

C 12.88095182 7.44841843 4.25791888
C 14.39906494 5.85404904 3.07891372
C 13.93160321 3.76131172 6.96618984
H 15.26766826 4.95904466 8.26616602
C 10.85747326 5.17145454 4.45995186
C 11.96909767 4.41684068 2.45105868
H 12.57372910 7.88583349 3.29679969
H 13.76012435 7.99935792 4.61658470
H 12.07457855 7.59934488 4.98641237
H 14.13535949 6.28842466 2.10166219
H 14.72261645 4.81536909 2.92659448
H 15.25842973 6.40777182 3.47723951
C 13.70997673 2.47297282 7.74057910
C 13.70341364 1.24942001 6.81347641
C 14.30631357 1.31848389 5.53992127
C 10.86591936 3.58922261 2.11719340
N 12.85025106 1.61386620 2.40329928
C 9.73509915 4.41974542 4.11458839
H 10.87456742 5.73348482 5.39284736
H 12.84380329 4.38701737 1.80505634
C 12.37486319 2.58085477 8.52162845
C 14.85046292 2.27127605 8.76550709
C 13.18275850 0.01107921 7.21669783
H 14.82654221 2.23910118 5.28158864
C 14.31020756 0.24181679 4.63546791
C 10.99355408 2.63950838 0.93126774
C 9.74039452 3.62452203 2.95408797
C 13.86250891 0.66973007 2.20942525
C 12.20115732 1.73650925 1.16861468
H 8.86341513 4.40906103 4.76845017
H 12.20445046 1.71433334 9.17678625
H 11.51491991 2.66570148 7.84273818
H 12.40085529 3.48096867 9.14991843
H 14.70532829 1.33070801 9.31460828
H 14.86103342 3.09212573 9.49555795
H 15.82821686 2.23704240 8.26710578
C 13.20742686 -1.08089081 6.34861682
H 12.73987074 -0.10448196 8.20563942
C 13.72393353 -0.96268379 5.05934862
C 14.94191822 0.39029481 3.24448677
C 9.72929814 1.77446506 0.74141306
C 11.19491646 3.47593501 -0.35812563
H 8.87438634 3.00508588 2.73360446
C 13.82138827 0.19448431 0.90736323

C 12.76787319 0.87508360 0.24534899
H 12.78321405 -2.03279711 6.67135209
H 13.68335524 -1.81862348 4.38684746
C 15.97358687 1.54498445 3.20839743
C 15.70526807 -0.90096266 2.88022323
H 9.88248335 1.10610017 -0.11481877
H 8.83841959 2.38886931 0.53645810
H 9.53387767 1.14183672 1.61795308
H 11.30205451 2.80780313 -1.22229392
H 12.09813097 4.09680255 -0.30518362
H 10.32804901 4.12995384 -0.53454015
H 14.48385810 -0.54483190 0.46668406
H 12.46244654 0.73987109 -0.78935739
H 16.44834264 1.56026050 2.21863898
H 16.75667737 1.41366745 3.97071080
H 15.50640404 2.52740020 3.35556347
H 16.25102285 -0.76163939 1.93789714
H 15.03499296 -1.75935026 2.74991878
H 16.43725718 -1.14221767 3.66348619
B 10.04135609 1.07053270 5.34606107
H 11.15390228 0.56764712 5.55018689
H 9.12960186 0.41298574 5.77277587
H 9.97636750 1.24371134 4.11091018
H 10.08180550 2.21734063 5.85027189
Pu 11.93381194 2.49633570 4.45132833

Pl-Pu^{III}-3H

C 0.22704590 -0.48638676 0.24699437
C 0.26615117 -1.17388822 1.48192964
C 1.39767849 -0.17863780 -0.69413710
N -1.06791676 -0.11621715 -0.04932843
H 1.14232949 -1.55549329 2.00000901
C -1.06443879 -1.19770602 1.96943264
C 1.56265274 -1.36021549 -1.67524892
C 1.11667799 1.14178389 -1.42752556
C 2.70447198 -0.03236313 0.11607404
C -1.85414468 -0.52534925 1.00878257
H -1.38617798 -1.60044894 2.92649550
C 1.71535954 -1.21571300 -3.05920417
C 1.51485336 -2.67056356 -1.16599450
H 1.96583647 1.42560263 -2.06497335
H 0.96402765 1.94276279 -0.69208054

H 0.20911984 1.07373002 -2.03881571
H 3.53784284 0.20701380 -0.55930611
H 2.96530047 -0.95681274 0.64855912
H 2.60892769 0.77556078 0.85531753
C -3.36472793 -0.26517592 1.05152547
C -4.08962867 -1.46410877 0.40046026
C -3.67998080 -2.76613976 0.74080945
C 1.46709708 -3.81858524 -1.97726749
N -1.19778712 -5.30642749 -0.66488767
C 1.75769731 -2.34555733 -3.87866841
H 1.76327551 -0.22622632 -3.51091038
H 1.50610893 -2.80295202 -0.07852269
C -3.66578113 1.05257505 0.32120836
C -3.84018044 -0.14516388 2.51620062
C -5.10830688 -1.34109792 -0.55159345
H -2.96408570 -2.88631732 1.56137625
C -4.13121903 -3.92122732 0.07647389
C 1.25956563 -5.19456690 -1.30564017
C 1.59803747 -3.63142701 -3.35954111
C -1.96965074 -5.11289500 0.46094479
C 0.11025028 -5.07541357 -0.29996793
H 1.86584719 -2.21700941 -4.95687494
H -4.73345176 1.30436103 0.38913546
H -3.37024386 1.00073350 -0.73331012
H -3.09623188 1.86724453 0.78773862
H -4.91929018 0.06163870 2.54256194
H -3.31321304 0.67453663 3.02484355
H -3.66678107 -1.06991851 3.08274380
C -5.63312561 -2.48082538 -1.16394052
H -5.46993490 -0.35913406 -0.85219456
C -5.13219700 -3.75443979 -0.88913456
C -3.49198821 -5.28205301 0.43373112
C 0.91982213 -6.28867825 -2.32898071
C 2.56400975 -5.58164381 -0.57500637
H 1.56091254 -4.48122000 -4.03920236
C -1.15409299 -4.72357933 1.54905056
C 0.17688704 -4.69841139 1.06189469
H -6.41784235 -2.36837602 -1.91384359
H -5.51511011 -4.61004251 -1.44298724
C -3.85723833 -6.37369258 -0.58347335
C -4.00124895 -5.70825773 1.82811714
H 0.74091482 -7.23675870 -1.80472681
H 1.75220821 -6.44157539 -3.03022303
H 0.01105442 -6.04270903 -2.89074791

H 2.43913991 -6.54007670 -0.05144609
H 2.86451112 -4.82402444 0.16110363
H 3.38360633 -5.68221576 -1.30030494
H -1.46237183 -4.53912942 2.57498271
H 1.06802565 -4.49077468 1.64873016
H -3.34884005 -7.30899542 -0.31433280
H -3.53735401 -6.10062802 -1.59595361
H -4.93965690 -6.56433747 -0.58205919
H -3.78066791 -4.95421921 2.59552060
H -3.53516190 -6.65614773 2.13236326
H -5.09139379 -5.84562762 1.80251842
B -2.05399907 -2.34902836 -2.73284615
H -2.69215964 -1.73909019 -1.85619292
H -0.88738246 -1.94321450 -2.58842307
H -2.04477064 -3.54455261 -2.38919822
H -2.48706871 -2.17303177 -3.84301455
Pu -1.15876496 -2.70408078 -0.41045807

Ar-U^{IV}-2H

C 13.62409250 5.25994377 5.40896776
C 14.33477594 5.87462419 6.41525074
C 13.20434479 5.82562917 4.06604920
N 13.35285748 3.92118250 5.76459174
H 14.68104698 6.90396888 6.42521390
C 14.53604084 4.90985575 7.44408757
C 11.98241629 5.01958047 3.64961028
C 12.81065855 7.31701216 4.19123048
C 14.36340677 5.71803197 3.05351312
C 13.93841929 3.73802582 7.03572828
U 12.12211675 2.31675858 4.53203864
H 15.06888498 5.07061083 8.37681885
C 10.88954613 4.94196542 4.55278726
C 11.92610721 4.25560218 2.48129076
H 12.47447692 7.70528356 3.22021211
H 13.68008134 7.90819721 4.50564931
H 12.01271275 7.47441410 4.92740282
H 14.08755109 6.13573515 2.07388667
H 14.69614461 4.68007260 2.91132533
H 15.22080156 6.28813565 3.43150487
C 13.83072101 2.42825912 7.79640866
C 13.60368338 1.34335247 6.75270996
C 14.48312858 1.29843034 5.63582873

C 10.84781378 3.37326640 2.21191151
N 12.91034795 1.55125715 2.42302654
C 9.78661983 4.14327647 4.26646510
H 10.92461475 5.51428124 5.47958138
H 12.75564548 4.28231249 1.77669843
C 12.68562901 2.50602692 8.82816001
C 15.14727775 2.12215554 8.55187338
C 12.52470033 0.45387251 6.78551779
H 15.32399868 1.98955193 5.61797637
C 14.26574520 0.43922943 4.55325349
C 10.97086085 2.44587684 1.01200069
C 9.77464785 3.33876414 3.11094072
C 14.09321507 0.82981606 2.16882644
C 12.31257010 1.75388655 1.15728283
H 8.94998981 4.09287324 4.96083125
H 12.61155726 1.58475515 9.42454830
H 11.71335533 2.69831467 8.35317167
H 12.88430298 3.33468123 9.51862112
H 15.07178220 1.15836770 9.07371132
H 15.33680570 2.89743403 9.30502273
H 16.01130796 2.08942384 7.87624332
C 12.30177138 -0.43240327 5.71442902
H 11.82353668 0.46288650 7.61673702
C 13.14445813 -0.42242640 4.60464646
C 15.08125120 0.48594931 3.26974079
C 9.83661624 1.40087583 0.95048653
C 10.92459270 3.29219709 -0.28301277
H 8.93233971 2.67228601 2.94204072
C 14.21775049 0.59488622 0.81618601
C 13.08665459 1.18017288 0.17598384
H 11.44040256 -1.09672929 5.74221171
H 12.93256271 -1.07144020 3.75518985
C 16.21016862 1.53681942 3.32023962
C 15.72465221 -0.89982265 3.02477190
H 10.01091950 0.73603244 0.09576449
H 8.85413761 1.87509297 0.81005822
H 9.80142421 0.77584836 1.85356720
H 11.02314739 2.64090172 -1.16077038
H 11.73294275 4.03342458 -0.32060368
H 9.96254431 3.81681018 -0.36082163
H 15.02841384 0.06426687 0.32504645
H 12.87606771 1.16715735 -0.88938890
H 16.73717983 1.53952618 2.35837822
H 16.94531511 1.30700373 4.10585203

H 15.82614644 2.55347936 3.48519830
H 16.30803954 -0.88255484 2.09551965
H 14.97465394 -1.69528939 2.93505729
H 16.40938740 -1.15354659 3.84557958
B 9.69763800 1.26854233 5.52423138
H 10.45739921 2.13387311 6.06331005
H 8.63093742 1.77332931 5.27703453
H 10.28441377 0.97886875 4.43348312
H 9.64618289 0.29368215 6.23128920

Ar-U^{IV}-3H

C 13.11807271 5.14175303 5.66325433
C 13.04763241 5.73192091 6.92184504
C 13.04002989 5.81042604 4.29856830
N 13.39307141 3.77662296 5.81142022
H 12.87392581 6.78363297 7.12707937
C 13.30196866 4.72937382 7.88312127
C 11.81062021 5.23614983 3.57592428
C 12.91017302 7.33678987 4.46053338
C 14.34991783 5.54507636 3.52265982
C 13.54349536 3.55007833 7.19229078
U 12.29255737 2.15592788 4.54789661
H 13.36297195 4.87075710 8.95799906
C 10.51880529 5.72970705 3.82022705
C 11.93995654 4.16228925 2.66716692
H 12.80785100 7.81024035 3.47515060
H 13.81139199 7.73898386 4.94123793
H 12.04915760 7.63160780 5.07173453
H 14.29804451 5.96495417 2.50818549
H 14.59763197 4.47743339 3.44421902
H 15.18343771 6.02440725 4.05195834
C 14.09155629 2.24692087 7.75910380
C 13.82918475 1.17965739 6.70049003
C 14.67543617 1.08662461 5.56882731
C 10.82156782 3.54362682 2.05826541
N 12.98398172 1.40555479 2.43675543
C 9.41859513 5.19839430 3.15048148
H 10.36800990 6.55014084 4.51965081
H 12.93342361 3.86091571 2.32564511
C 13.39267978 1.91584013 9.09377106
C 15.60779920 2.39521449 8.03934200
C 12.67373196 0.37722688 6.73225540

H 15.56499698 1.70882442 5.52945898
C 14.37430359 0.25850516 4.47626613
C 10.98564262 2.34034456 1.12085250
C 9.55934595 4.10713401 2.29411133
C 14.18999100 0.74919603 2.10756008
C 12.37336717 1.74123145 1.20934664
H 8.42962148 5.62550750 3.31976892
H 13.72230317 0.93914083 9.47448787
H 12.29859734 1.92111803 9.01100638
H 13.66052123 2.66925863 9.84427019
H 16.04269053 1.43674954 8.35851272
H 15.75422924 3.12436617 8.84572331
H 16.16497857 2.76544355 7.17008335
C 12.38308563 -0.50370493 5.67212835
H 11.99574448 0.42436909 7.58087908
C 13.21259226 -0.55017897 4.55112779
C 15.16454052 0.28072455 3.17540351
C 9.95054713 1.23983173 1.47850915
C 10.70767862 2.81614680 -0.32291956
H 8.67575817 3.69627166 1.80651800
C 14.33316786 0.69977083 0.74172704
C 13.18554196 1.32964816 0.17473939
H 11.49641937 -1.13502429 5.72441015
H 12.95865398 -1.19910089 3.71387911
C 16.37920443 1.23024489 3.23586282
C 15.68439180 -1.14373230 2.86055489
H 10.09315992 0.37828106 0.81357527
H 8.91673140 1.59212128 1.36479786
H 10.06720110 0.88532617 2.51464733
H 10.74821302 1.96885087 -1.02006755
H 11.43957235 3.56924862 -0.64248611
H 9.70541048 3.25807318 -0.39148608
H 15.16148493 0.26194991 0.19204484
H 12.98683618 1.45056493 -0.88555559
H 16.89227285 1.21378139 2.26680320
H 17.10266779 0.91872116 4.00421898
H 16.08340706 2.27155007 3.42719114
H 16.23343069 -1.13648484 1.91063456
H 14.86997176 -1.87246501 2.76625830
H 16.37268711 -1.48460367 3.64638695
B 9.99380377 2.16345785 5.50816358
H 10.88104958 2.39443041 6.35988712
H 8.88293894 2.14486583 5.95232300
H 10.33155711 1.07169592 4.98450846

H 10.18423034 3.00904075 4.61341131

Pl-U^{IV}-3H

C 0.20038389 -0.49552071 0.23540458
C 0.25127690 -1.11340468 1.50522940
C 1.34049467 -0.18126523 -0.73380880
N -1.11418864 -0.18738237 -0.07997708
H 1.13725946 -1.44578722 2.03995621
C -1.07701359 -1.13592839 2.00178221
C 1.43613040 -1.34778017 -1.73590493
C 1.05854757 1.16190106 -1.42587873
C 2.67716698 -0.08449423 0.03306158
C -1.88981196 -0.53100305 1.01677587
H -1.38480079 -1.48861435 2.98273092
C 1.57050960 -1.20111983 -3.12043865
C 1.38858284 -2.66123559 -1.22885480
H 1.89408686 1.44068153 -2.08161604
H 0.95159613 1.95116804 -0.67061810
H 0.13374884 1.13156566 -2.01405188
H 3.48961022 0.15094380 -0.66694862
H 2.93971392 -1.02423263 0.53751780
H 2.62844496 0.71312198 0.78715557
C -3.39489132 -0.26201551 1.03617509
C -4.08887592 -1.44224770 0.32940427
C -3.68169413 -2.74774063 0.66755803
C 1.41342996 -3.81510439 -2.03687690
N -1.26659431 -5.23319875 -0.71509345
C 1.68481641 -2.33408832 -3.93305657
H 1.59870807 -0.21161176 -3.57379332
H 1.41917380 -2.79369969 -0.13673942
C -3.67644229 1.08107712 0.34377974
C -3.90342090 -0.19669142 2.49264312
C -5.10154489 -1.31569958 -0.62716160
H -2.98516020 -2.86833092 1.51102011
C -4.19534784 -3.91111467 0.06130210
C 1.19832132 -5.18364037 -1.36323948
C 1.59248859 -3.62663819 -3.41202838
C -2.03112080 -5.06744756 0.42016616
C 0.05018822 -5.03168296 -0.35961725
H 1.81625572 -2.20368097 -5.00796807
H -4.74520350 1.32700250 0.39973013
H -3.36354753 1.07185519 -0.70699408

H -3.12434344 1.88168216 0.85270286
H -4.98254528 0.00570959 2.49943119
H -3.39671647 0.61097554 3.03866095
H -3.74196218 -1.13787206 3.03542906
C -5.68622952 -2.46090843 -1.17827709
H -5.44928937 -0.33276537 -0.94078672
C -5.23678011 -3.74405625 -0.85855026
C -3.55088414 -5.26457463 0.41569354
C 0.84001086 -6.27999888 -2.37864289
C 2.49590655 -5.58039400 -0.62512913
H 1.62695539 -4.47929975 -4.08801679
C -1.20055357 -4.69394643 1.50610628
C 0.12653682 -4.67118730 1.00892827
H -6.49332305 -2.34689326 -1.90305858
H -5.68002444 -4.60522259 -1.35564955
C -3.91469023 -6.36308388 -0.59538254
C -4.03282504 -5.68847489 1.82069047
H 0.64166402 -7.22108315 -1.84977068
H 1.67545746 -6.45675173 -3.06892048
H -0.05673813 -6.02340307 -2.95491448
H 2.35822920 -6.53209324 -0.09374125
H 2.81395075 -4.82019583 0.10121679
H 3.31171147 -5.70398201 -1.34972842
H -1.49685468 -4.53405098 2.53961169
H 1.02385256 -4.49086880 1.59527539
H -3.39061426 -7.29158556 -0.33476143
H -3.62391123 -6.08877119 -1.61630538
H -4.99244135 -6.57168777 -0.56976841
H -3.81751053 -4.92851634 2.58408306
H -3.55269064 -6.62948412 2.12237354
H -5.11988180 -5.84336841 1.80877104
B -2.06482420 -2.61076154 -2.73462489
H -1.89743484 -1.47797751 -2.23909618
H -2.48362462 -2.59811853 -3.85604692
H -0.97332041 -3.20283374 -2.60247365
H -2.78570311 -3.23126529 -1.92549943
U -1.19471374 -2.65884412 -0.40766452

Ar-Np^{IV}-2H

C -1.79848921 -2.15641708 -1.06548154
C -3.06133220 -2.44607132 -1.56476292
C -0.48756795 -2.84290051 -1.38385565

N -1.84229506 -0.98486686 -0.28709729
H -3.32622728 -3.27933672 -2.20866606
C -3.92793204 -1.43162711 -1.10530566
C 0.43500110 -2.55694005 -0.20588404
C -0.67890173 -4.37152808 -1.52598913
C 0.06847272 -2.30105483 -2.71928706
C -3.16350999 -0.55500749 -0.33516578
H -4.99324050 -1.35436646 -1.30309937
C -0.00111275 -2.92735255 1.08852270
C 1.64382561 -1.86146381 -0.31952269
H 0.28600831 -4.85792062 -1.72336116
H -1.34384996 -4.59049360 -2.37104717
H -1.11854846 -4.81990726 -0.62653909
H 1.02055893 -2.78486340 -2.98323442
H 0.22076393 -1.21293432 -2.69367658
H -0.64996286 -2.51414899 -3.52003820
C -3.65005389 0.64005463 0.46058555
C -2.42673171 1.50267205 0.74695146
C -1.61242315 1.89700973 -0.34547695
C 2.40401712 -1.48324849 0.81706503
N 1.86125315 1.02703250 -0.19571376
C 0.75380419 -2.60713896 2.21273922
H -0.94885451 -3.45320234 1.20255356
H 2.00019370 -1.55659819 -1.30215477
C -4.34314076 0.14934236 1.75049878
C -4.67013798 1.46927559 -0.35731993
C -2.02220272 1.85925383 2.03829665
H -1.92731868 1.61791511 -1.34921327
C -0.40540985 2.58064968 -0.16386601
C 3.63595143 -0.61281842 0.60147908
C 1.94346317 -1.86533020 2.08268304
C 1.84347822 2.17826250 -0.98564668
C 3.18550623 0.59324346 -0.19455964
H 0.40583747 -2.88763446 3.20441420
H -4.73358944 0.99088957 2.34146398
H -3.66749143 -0.44349888 2.38209738
H -5.19249943 -0.49005228 1.48088753
H -4.99570548 2.34574951 0.21955229
H -5.55845748 0.86397112 -0.57819034
H -4.25173409 1.81427774 -1.31138313
C -0.82440736 2.56994019 2.23996065
H -2.60939982 1.56466816 2.90441479
C -0.01528560 2.90574611 1.15754362
C 0.55468952 2.90502254 -1.30204234

C 4.26899894 -0.14068090 1.92981657
C 4.69655489 -1.42749729 -0.17951633
H 2.48628310 -1.58127290 2.98120181
C 3.12601027 2.45688404 -1.46174600
C 3.97646204 1.45749450 -0.95657396
H -0.51599307 2.81786533 3.25362463
H 0.93299488 3.41582974 1.32592377
C 0.02743099 2.44135415 -2.67832289
C 0.77773108 4.43544833 -1.36514431
H 5.12016759 0.51521451 1.70986179
H 4.64499501 -0.99040239 2.51806428
H 3.55968053 0.43108249 2.54382732
H 5.59577713 -0.82004087 -0.34277544
H 4.32665823 -1.75438285 -1.15951654
H 4.99083985 -2.31495079 0.39708301
H 3.41146702 3.28868520 -2.09885519
H 5.04515951 1.36982467 -1.12896360
H 0.77362671 2.67591413 -3.44727360
H -0.90482153 2.96066513 -2.94482559
H -0.14859865 1.35720536 -2.71070416
H 1.46586163 4.68284594 -2.18337289
H 1.20401979 4.83200301 -0.43552150
H -0.17352149 4.94902636 -1.56017432
B -0.20200676 -0.08739607 3.75687927
H -1.02026726 -0.57248416 2.91428222
H 0.27934210 -0.97558629 4.41687601
H 0.71343316 0.44388709 3.05106746
H -0.75522453 0.76798401 4.40389484
Np -0.01486353 -0.00092158 0.97441346

Ar-Np^{IV}-3H

C 13.56508155 5.40442051 5.26430743
C 14.59644904 5.88713678 6.06000206
C 12.91354902 6.11721146 4.09235367
N 13.19982422 4.11884875 5.67851043
H 15.07914574 6.85649799 5.97439253
C 14.87902653 4.88988830 7.01941589
C 11.76704344 5.23247248 3.62113376
C 12.36673252 7.50012529 4.53057610
C 13.96492513 6.35460863 2.98587496
C 14.01793375 3.82568155 6.78207842
H 15.62484021 4.95142236 7.80546383

C 10.63368065 5.04206396 4.45334535
C 11.83776122 4.48822575 2.43897286
H 11.86945660 8.00128425 3.68814890
H 13.19594346 8.13687742 4.86276660
H 11.65796331 7.42648546 5.36410567
H 13.51553461 6.83480256 2.10397842
H 14.46315694 5.42654448 2.67481448
H 14.74468044 7.02338952 3.36970667
C 13.82972333 2.59263593 7.63472421
C 13.71532009 1.31821404 6.79155898
C 14.18395060 1.26193335 5.46080170
C 10.83870168 3.55225363 2.06683480
N 12.80585842 1.53867566 2.41545127
C 9.60741390 4.17555749 4.07252145
H 10.56171029 5.57654424 5.39908798
H 12.71288898 4.57808068 1.79617966
C 12.55623852 2.80125353 8.50015494
C 15.03674929 2.41253209 8.58554923
C 13.23119873 0.12897839 7.36465272
H 14.71223121 2.13510919 5.06167198
C 14.11654218 0.08319548 4.68263094
C 11.13090201 2.65889856 0.86565489
C 9.70809925 3.42355726 2.88488537
C 14.08722090 1.01719043 2.30677120
C 12.49498138 2.06634157 1.14252506
H 8.73487034 4.05242918 4.71331696
H 12.42584702 1.99802889 9.23743349
H 11.64826320 2.85048396 7.88286436
H 12.64435736 3.74750099 9.04928805
H 14.90693671 1.50766364 9.19303132
H 15.11663342 3.26658946 9.27096508
H 15.97716580 2.32062114 8.02671305
C 13.17629500 -1.04424150 6.62195770
H 12.89674165 0.11972000 8.40120498
C 13.58411944 -1.06420172 5.28672306
C 14.74344849 0.05427026 3.28558433
C 10.09465354 1.52777817 0.69420190
C 11.14138175 3.51494906 -0.41938923
H 8.91521219 2.72517145 2.62560328
C 14.58730090 1.27363660 1.01711738
C 13.58007834 1.92888684 0.28811720
H 12.79349242 -1.95665269 7.08017122
H 13.51171352 -1.99511080 4.72902363
C 16.25186419 0.39039994 3.43605872

C 14.64141570 -1.35568782 2.65171593
H 10.38988574 0.89666430 -0.15319336
H 9.09531239 1.93224355 0.47697231
H 10.03630146 0.88502752 1.58238249
H 11.36814489 2.88485388 -1.28927229
H 11.88590779 4.32031791 -0.37718017
H 10.15270771 3.96511333 -0.57896297
H 15.55716614 0.96686934 0.63615049
H 13.63373424 2.25010038 -0.74731817
H 16.76321179 0.30427246 2.46910946
H 16.72512219 -0.31640219 4.13101332
H 16.41337505 1.40807546 3.81319657
H 15.12679089 -1.35095949 1.66876942
H 13.59719905 -1.66274568 2.50531310
H 15.15198609 -2.10509579 3.27330515
B 10.20665832 1.02226795 5.34281528
H 11.37016135 0.65015369 5.57290840
H 9.35109538 0.32129823 5.79994221
H 10.16190005 1.13262530 4.09779748
H 10.15766015 2.20450543 5.76823491
Np 11.95529328 2.52410820 4.41596877

Pl-Np^{IV}-3H

C 0.23309247 -0.50172218 0.23112432
C 0.25670133 -1.15989763 1.48508469
C 1.39826376 -0.18703701 -0.71051578
N -1.06476363 -0.16800662 -0.10160156
H 1.12875918 -1.51481528 2.02845699
C -1.07987711 -1.18841560 1.94707236
C 1.49179920 -1.35391037 -1.71244693
C 1.14231440 1.15883193 -1.40566186
C 2.72002649 -0.10500319 0.08240633
C -1.86619194 -0.55058289 0.95677179
H -1.41464443 -1.56761566 2.90901696
C 1.58758324 -1.21150331 -3.10281069
C 1.45716444 -2.66735371 -1.20363749
H 1.98812916 1.42542089 -2.05361351
H 1.03949677 1.94912757 -0.65102649
H 0.22139564 1.14202338 -2.00020908
H 3.54895053 0.12818706 -0.59894857
H 2.96617333 -1.04759374 0.58986324
H 2.66074226 0.68959820 0.83873728

C -3.37075641 -0.27322143 0.97638629
C -4.08051449 -1.46777406 0.31298014
C -3.63593089 -2.76634283 0.62916176
C 1.43241969 -3.82274936 -2.00961166
N -1.18581148 -5.23559494 -0.71182780
C 1.63828160 -2.34480804 -3.91975403
H 1.61717621 -0.22205403 -3.55619227
H 1.51539629 -2.80023819 -0.11205436
C -3.64791053 1.04917589 0.24287795
C -3.86654911 -0.15579918 2.43489150
C -5.13188402 -1.35213375 -0.60051199
H -2.94075156 -2.88420771 1.46909458
C -4.13919413 -3.93015274 0.01581431
C 1.27874478 -5.18825707 -1.31252146
C 1.52863387 -3.63574469 -3.39461550
C -1.97457771 -5.07761412 0.41139485
C 0.12430684 -5.05167762 -0.31655845
H 1.72553374 -2.21697638 -4.99926529
H -4.71183452 1.31178237 0.30989817
H -3.35595147 0.99822769 -0.81272927
H -3.07571410 1.85969539 0.71239079
H -4.94255963 0.06272254 2.44280847
H -3.34424756 0.65955925 2.95437852
H -3.71609914 -1.08365863 3.00311090
C -5.68978598 -2.50036051 -1.16906966
H -5.51476471 -0.37396696 -0.88658265
C -5.18938964 -3.77569651 -0.89329755
C -3.49062989 -5.28027300 0.37278045
C 0.96388260 -6.31741628 -2.30553324
C 2.59081695 -5.51794672 -0.56940033
H 1.51358182 -4.48974834 -4.06981254
C -1.16502235 -4.73045655 1.52041276
C 0.17145075 -4.71154086 1.05757542
H -6.51691557 -2.39576373 -1.87247192
H -5.61586542 -4.63864657 -1.40189494
C -3.82559522 -6.37630797 -0.65192554
C -4.00015548 -5.71685035 1.76441516
H 0.81994674 -7.25835624 -1.75917244
H 1.79985576 -6.46212097 -3.00305443
H 0.04810416 -6.11703901 -2.87390009
H 2.49040720 -6.46599509 -0.02344584
H 2.87777617 -4.73563811 0.14634063
H 3.41178810 -5.62068166 -1.29133388
H -1.48726782 -4.57480112 2.54663306

H 1.05614676 -4.53706839 1.66478090
H -3.29722848 -7.30191298 -0.38937885
H -3.52251144 -6.09191940 -1.66649942
H -4.90146489 -6.59497713 -0.64525751
H -3.80975951 -4.95841417 2.53574035
H -3.51984690 -6.65582179 2.07282430
H -5.08526107 -5.88020517 1.72594091
B -2.18795777 -2.40704655 -2.63869509
H -2.42756810 -1.49800252 -1.81855575
H -0.93677060 -2.42994989 -2.67816120
H -2.47177546 -3.47446487 -2.05860799
H -2.70453198 -2.26552060 -3.70899245
Np -1.08894261 -2.69729512 -0.45045576

Ar-Pu^{IV}-2H

C 1.65407774 2.26364120 -1.17080114
C 2.90957131 2.58046502 -1.68545592
C 0.33131279 2.94237284 -1.44489943
N 1.72993091 1.10049260 -0.38465360
H 3.15511666 3.42720547 -2.31896541
C 3.79620402 1.59311210 -1.22452407
C -0.56670599 2.63378595 -0.25187536
C 0.50714316 4.47485980 -1.57153168
C -0.24592191 2.41502335 -2.77784855
C 3.04836519 0.70021415 -0.43687827
H 4.86056816 1.53112264 -1.43281266
C -0.12949526 3.01167354 1.03936583
C -1.76210403 1.91466931 -0.35783722
H -0.46669786 4.95468941 -1.73822491
H 1.14856475 4.71058989 -2.43009965
H 0.96490809 4.91563486 -0.67742842
H -1.20766145 2.89438546 -3.01318459
H -0.38684878 1.32545417 -2.76577664
H 0.45360137 2.64824924 -3.58975107
C 3.56691968 -0.49298224 0.34053262
C 2.37061101 -1.39092683 0.63139261
C 1.54669796 -1.78134029 -0.45423728
C -2.51546280 1.52954458 0.77968648
N -1.94044736 -0.96680136 -0.26263148
C -0.87734386 2.68085393 2.16659723
H 0.80919232 3.55418034 1.15098782
H -2.11389818 1.59907303 -1.33830516

C 4.26369097 0.00244121 1.62693334
C 4.59860735 -1.29051499 -0.49634505
C 1.99628874 -1.78429371 1.92165716
H 1.83560581 -1.47050859 -1.45653890
C 0.36052143 -2.49976269 -0.26925959
C -3.72790040 0.63079038 0.56943941
C -2.06009399 1.92882973 2.04174997
C -1.91435851 -2.13363308 -1.04659201
C -3.25963026 -0.56682323 -0.23275364
H -0.52835582 2.96400435 3.15769588
H 4.68471719 -0.83602166 2.20093768
H 3.57976602 0.56749266 2.27494228
H 5.09179424 0.66868090 1.35590655
H 4.94835073 -2.16477950 0.06918788
H 5.47117153 -0.66351999 -0.71919865
H 4.17821461 -1.63629184 -1.44925393
C 0.82405686 -2.53569122 2.12478939
H 2.58796628 -1.49110919 2.78567225
C 0.00621423 -2.87160860 1.04885844
C -0.61153842 -2.81361236 -1.40130796
C -4.34323772 0.14325178 1.89962738
C -4.80980699 1.42457577 -0.20535553
H -2.59575702 1.63973499 2.94290462
C -3.19994860 -2.45288845 -1.47882124
C -4.05574469 -1.46338389 -0.96702034
H 0.53874042 -2.81421032 3.13734398
H -0.92337983 -3.41352065 1.22233043
C -0.12050706 -2.29216427 -2.77063750
C -0.79472116 -4.34662663 -1.50975979
H -5.18808856 -0.52232287 1.68443962
H -4.72569880 0.98569409 2.49437402
H -3.62155770 -0.42029230 2.50671203
H -5.69487511 0.79700311 -0.36954005
H -4.44999540 1.76488646 -1.18466278
H -5.12299876 2.30213206 0.37627945
H -3.48552872 -3.30271593 -2.09108009
H -5.13122022 -1.40237124 -1.10750725
H -0.87027657 -2.52894706 -3.53528911
H 0.82439976 -2.77259500 -3.06466470
H 0.02063395 -1.20255765 -2.77233617
H -1.48948799 -4.58608628 -2.32467553
H -1.19447652 -4.78344176 -0.58637443
H 0.16663265 -4.82721403 -1.73607973
B 0.02347994 0.07651416 3.70979731

H 0.86929299 0.58644873 2.90788516
H -0.47406787 0.95146209 4.37604166
H -0.87163073 -0.43710111 2.96584005
H 0.56265714 -0.79532539 4.34710345
Pu -0.06511504 0.06985190 0.93544754

Ar-Pu^{IV}-3H

C 13.60268014 5.35886720 5.43597705
C 14.41704870 5.92415340 6.41920045
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Pl-Pu^{IV}-3H

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Pu -1.16100224 -2.71838741 -0.42250631