Supporting information

Redox and Structural Properties of Accessible Actinide(II) Metallocalixarene (Ac to Pu): a Relativistic DFT Study

Shuai Niu,[§] Hong-Xue Cai,[§] Hong-Bo Zhao, Li Li and Qing-Jiang Pan*

Key Laboratory of Functional Inorganic Material Chemistry of Education Ministry, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, China

Corresponding author

*Email: panqjitc@163.com (QJP)

ORCID

Qing-Jiang Pan: 0000-0003-2763-6976

Author Contribution

[§] The two authors contributed to the work equally.

Discussion on isomers and effects of different levels of theory on structures

Regarding cases that valence electrons may be singly or doubly filled into frontier molecular orbitals, divalent and trivalent actinide complexes have different electron-spin state (ESS) for their ground state. Herein, we fully optimized U(II) and U(III) complexes of L^n at the level of theory Pri: PBE/B-I/gas. As seen in Table S1, the calculated relative energies show that the highest ESS is the energy-lowest among isomers for all the U(III) complexes, which is consistent with previous studies.[1-9]

Most divalent complexes give the same manner, for example L^2~L^4 ones. $[UL^1]^-$ is exceptional with the triplet ground state. So we further optimized structures of $[AnL^1]^-$ (An = Th~Pu) in all possible ESSs. Calculated energies (Table S2) show single, doublet, triplet, quartet and heptet ***ground*** state, respectively. Therefore, the highest ESS was centered on for all complexes with the exception of $[AnL^1]^-$ in the work.

Considering possible geometric isomers, we took $[UL^2]$ as an example. Three energetically stable isomers, labeled as $[UL^2]$, $[UL^2]'$ and $[UL^2]''$ (Figure 1), were found. Energetic comparison shows that $[UL^2]$ is the energy-lowest. Geometric parameters were presented in Table S4. Additionally, a larger basis set B-IV (see details in the footnote of Table S4) was used for optimization. Comparison indicates the smaller basis set B-I is sufficiently reliable for current calculations.

Unless otherwise noted, the level of theory, Pri: PBE/B-I/gas, was used for all structural optimizations. And thus, single-point calculations were conducted using ADF and Gaussian codes to obtain solvation/spin-orbit coupling energies and QTAIM-related parameters, respectively. To very this, we optimized structures of $[AnL^2]^z$ (An = Th, Pa, U and Np; z = 0 and +1) at the level of ADF: PBE/B-II/gas. Slight differences were found for geometric parameters, electron-spin density and atomic charges as seen in Tables S5~S8. Further considering the spin-orbit coupling effects using the ADF code, $[UL^2]$ was chosen and optimized, which shows close results to those at the scalar level (Table S4).

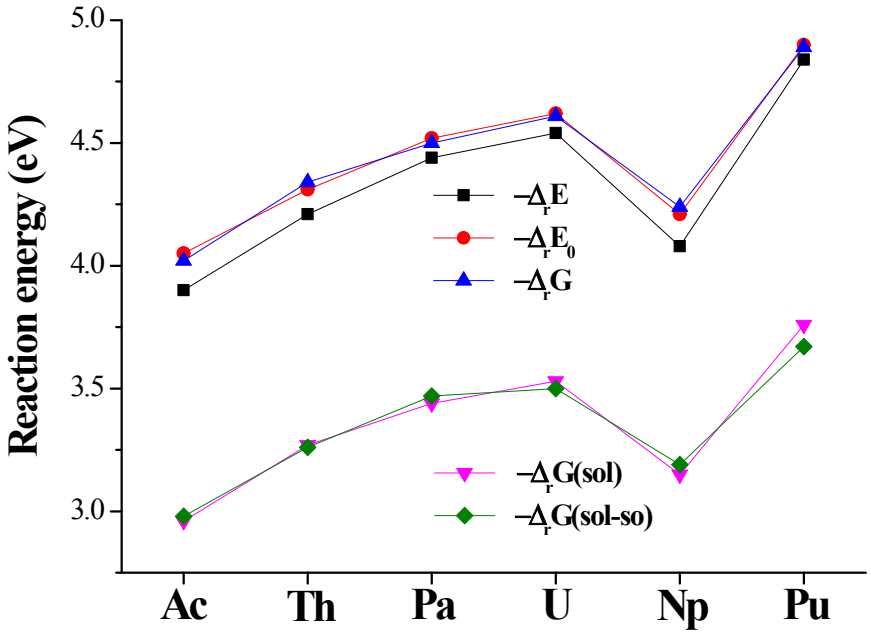

Figure S1. Plots of various energies of the single-electron reaction $[AnL^2]^+ + e = [AnL^2]$ (An = Ac~Pu). For convenient comparison, their minus values were used.

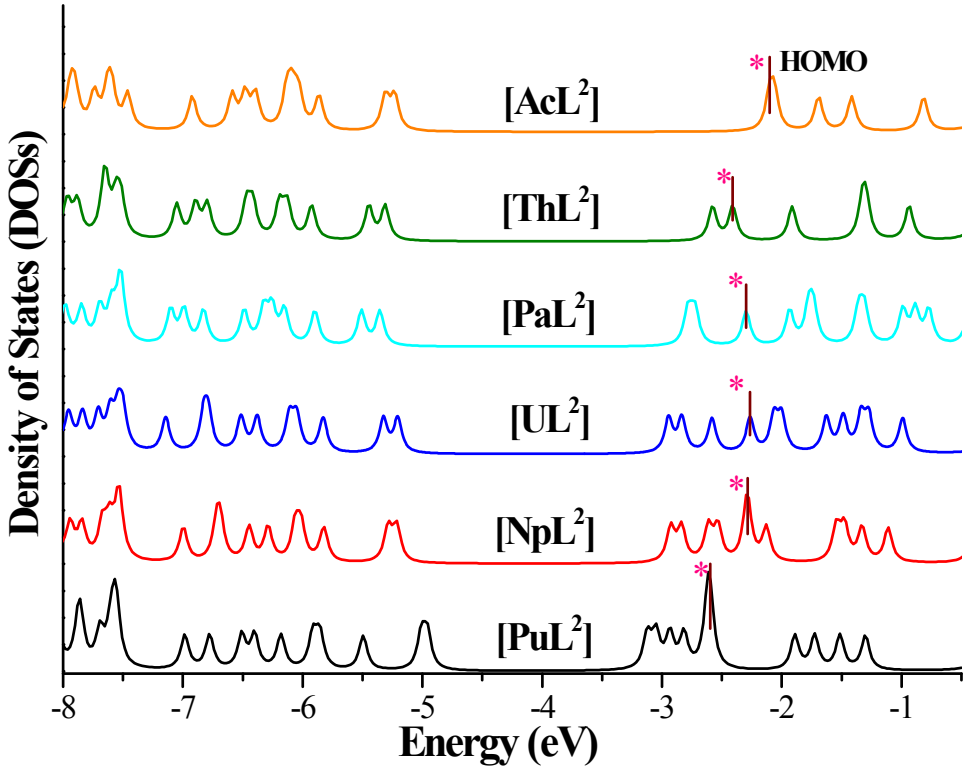

Figure S2. Total DOSs of [AnL^2] (An = Ac~Pu), where the α-spin orbitals are plotted and HOMO of each complex is marked with a star.

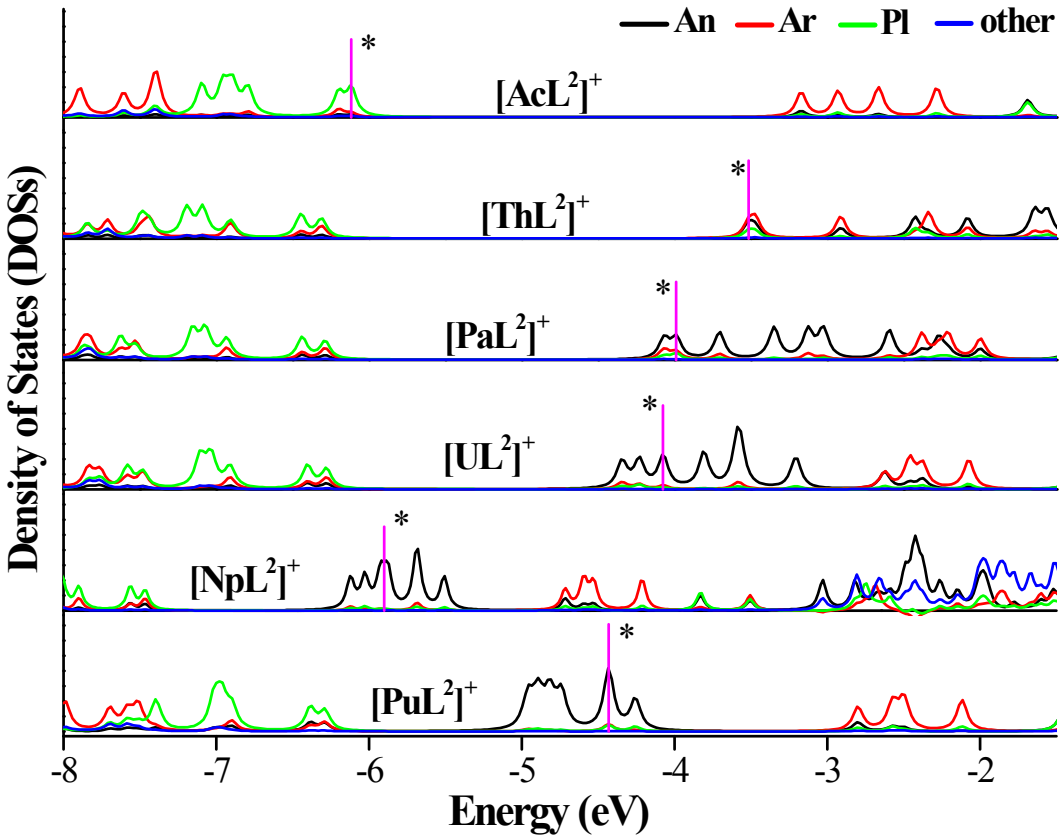

Figure S3. Density of states (DOSs) of each fragment of $[AnL^2]^+$ (An = Ac~Pu), where the α-spin orbitals are plotted except for close-shell $[AcL^2]^+$, and HOMO of each complex is marked with a star.

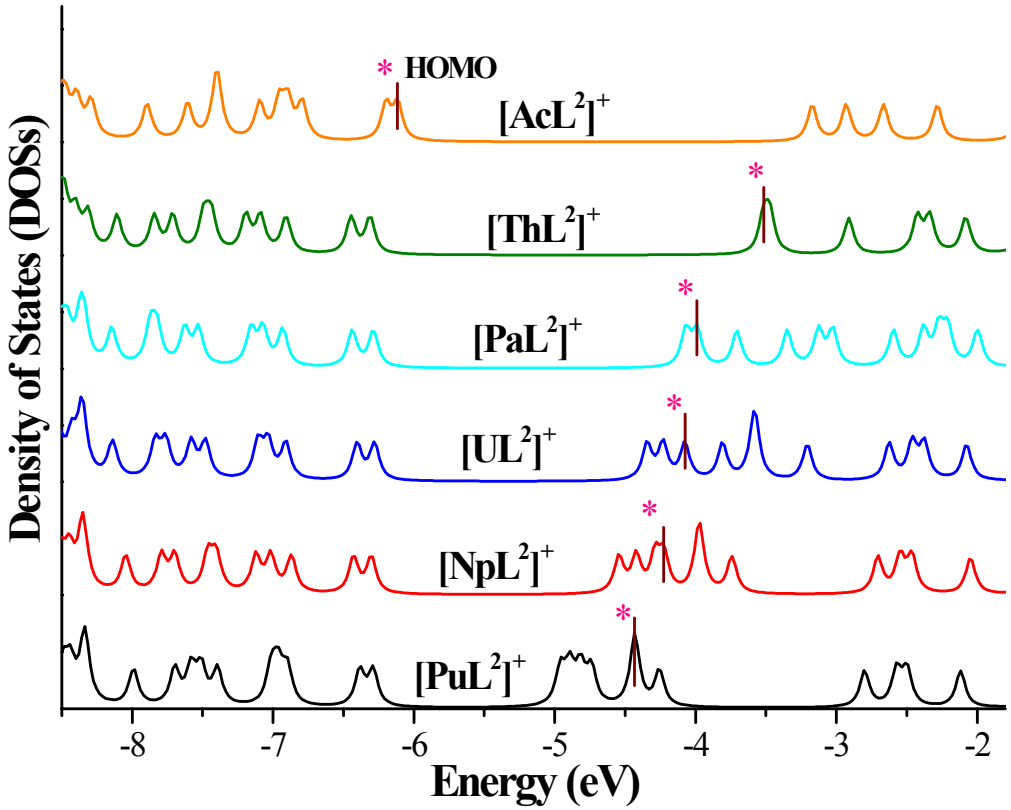

Figure S4. Total DOSs of $[AnL^2]^+$ (An = Ac~Pu), where the α-spin orbitals are plotted except for close-shell $[AcL^2]^+$, and HOMO of each complex is marked with a star.

Discussion about the density-functional and geometry effects on electronic configuration of the U(II) center

The electronic configuration of the U(II) center in complex uranium could be density functional-dependent and geometry dependent. To consider the former, different functionals (GGA-PBE, hybrid PBE0, and hybrid B3LYP) implemented in the ADF code were used to calculate the complex [UL^2] at the Priroda-optimized geometry. Regarding the latter issue, we used Priroda and ADF codes to optimize the structure of [UL^2]. At these two geometries, the level of theory, ADF: PBE/B-II/ZORA/THF, was exploited to calculate electronic structures of [UL^2].

The inspection of high-lying uranium-based orbitals (Figures S5 and S6) and orbital compositions finds two pure 5f-character orbitals and two δ(U-Ar) bonding ones, regardless of what density functionals (GGA and Hybrid) and geometries (Priroda and ADF) are used. One can note that geometry change has almost no effect. Regarding different density functionals, the order of orbitals with different character is affected (Figure S5). However, the $5f^4$ electronic configuration for U(II) was obtained by all density functionals, but a little more 6d participation was found in the hybrid results.

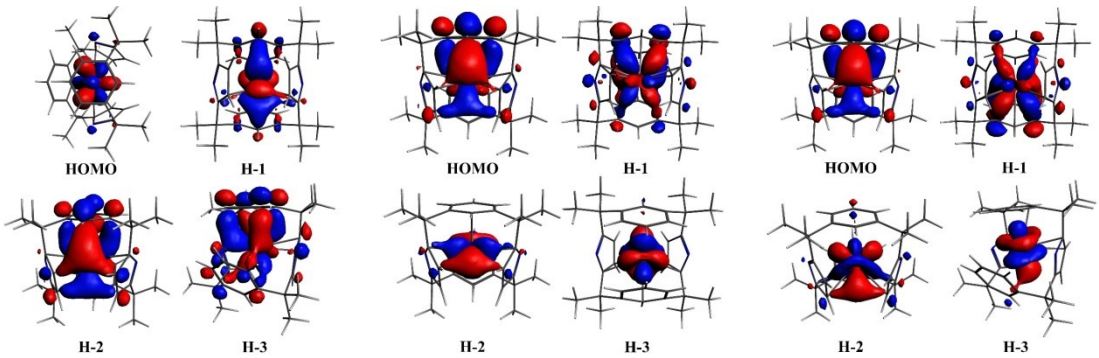

Figure S5. Four high-lying metal-based α-spin orbitals of [UL^2] calculated by ADF: DFT/TZP/ZORA/COSMO level, where density functionals are PBE (left), PBE0 (middle) and B3LYP (right).

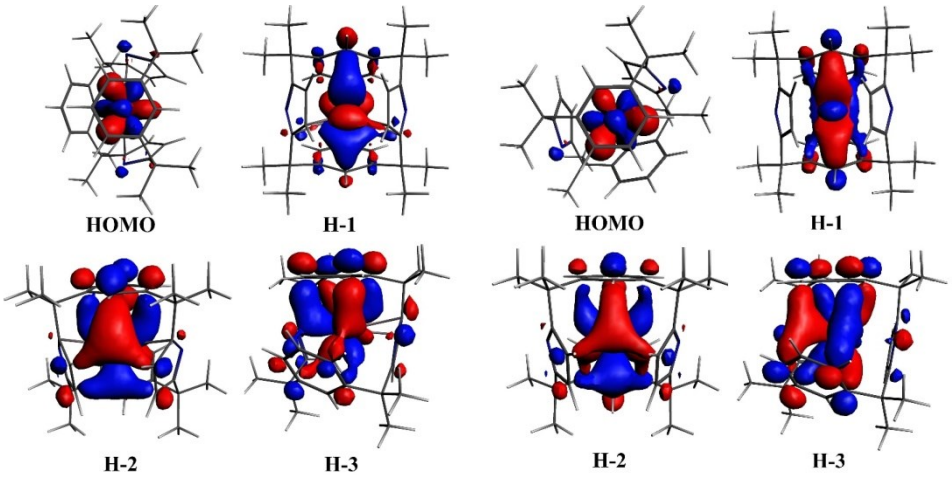

Figure S6. Four high-lying metal-based α-spin orbitals of [UL^2] calculated by ADF: PBE/TZP/ZORA/COSMO at Priroda-optimized (left) and ADF-optimized (right) geometries.

Table S1. Calculated relative energies (eV) of uranium complexes of various ligands (L^n, n = 1~4) in all possible electron-spin states (ESSs).

Complexes	ESS	ΔE [a]	ΔE_0 [a]	ΔH [a]	ΔG [a]
$[UL^1]^-$	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
$[UL^2]$	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
$[UL^3]^-$	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
$[UL^4]^{2-}$	Singlet	0.713	0.697	0.696	0.707
	Triplet	0.036	0.035	0.033	0.044
	Quintet	0.000	0.000	0.000	0.000
$[UL^1]$	Doublet	0.294	0.248	0.261	0.199
	Quartet	0.000	0.000	0.000	0.000
$[UL^2]^+$	Doublet	0.343	0.328	0.328	0.333
	Quartet	0.000	0.000	0.000	0.000
$[UL^3]$	Doublet	0.520	—	—	—
	Quartet	0.000	0.000	0.000	0.000
$[UL^4]^-$	Doublet	0.424	0.420	0.417	0.425
	Quartet	0.000	0.000	0.000	0.000

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

Table S2. Calculated relative energies (eV) of $[AnL^1]^-$ (An = Ac~Pu) in various ESSs.

Complexes	ESS	ΔE	ΔE_0	ΔH	ΔG
$[ThL^1]^-$	Singlet	0.000	0.000	0.000	0.000
	Triplet	0.154	0.149	0.177	0.096
$[PaL^1]^-$	Doublet	0.000	0.000	0.031	0.000
	Quartet	0.376	0.405	0.407	0.344
$[UL^1]^-$	Singlet	0.164	0.176	0.165	0.254
	Triplet	0.000	0.000	0.000	0.000
	Quintet	0.059	0.086	0.082	0.086
$[NpL^1]^-$	Doublet	0.462	0.447	0.452	0.418
	Quartet	0.000	0.000	0.000	0.000
	Sextet	0.081	0.109	0.105	0.137
$[PuL^1]^-$	Singlet	2.157	2.157	2.127	2.217
	Triplet	1.062	1.035	1.034	1.024
	Quintet	0.413	0.370	0.376	0.367
	Heptet	0.000	0.000	0.000	0.000

Table S3. Calculated relative energies (eV) of geometric isomers of [UL^2] in the quintet state.

Isomers	ΔE	ΔE_0	ΔH	ΔG
[UL^2]	0.000	0.000	0.000	0.000
[UL^2]'	0.160	0.138	0.160	0.160
[UL^2]''	0.259	0.221	0.226	0.137

Table S4. Optimized bond lengths, angles (α and β in degree) and interplanar arene/pyrrolide angles (γ) for [UL^2] in various electron-spin states and geometric isomers, compared with those calculated at larger basis sets.

Compls.	[UL^2]						[UL^2]'	[UL^2]"
ESS	Quintet	Quintet	Quintet	Quintet	Triplet	Singlet	Quintet	Quintet
Approach [a]	Pri	Pri-2	ADF	ADF-so	Pri	Pri	Pri	Pri
An-C(t)	2.786	2.784	2.768	2.794	2.775	2.797	2.721	2.659
An-N	2.715	2.716	2.710	2.720	2.698	2.717	2.432	2.381
An-Ar$_{cent}$	2.484	2.478	2.465	2.486	2.421	2.442	2.321	2.316
An-Pl$_{cent}$	2.530	2.526	2.549	2.525	2.522	2.457	3.595	3.574
α1 [b]	176.7	176.6	174.8	176.9	177.7	177.5	155.4	147.8
α2 [b]	170.4	170.3	168.8	170.6	169.5	170.6	146.7	136.0
β1 [c]	123.6	123.6	124.8	123.5	122.3	122.8	142.5	150.9
β2 [c]	118.1	118.0	116.6	118.3	117.0	118.1	158.7	134.3
γ1 [d]	49.9	50.1	49.4	50.2	53.7	52.3	36.5	24.2
γ2 [d]	55.3	55.8	54.8	55.9	55.5	62.8	2.9	56.4

[a] Levels of theory Pri, Pri-2, ADF and ADF-so correspond to Pri: PBE/B-I/AE, Pri: PBE/B-IV/AE, ADF: PBE/B-II/ZORA and ADF: PBE/B-II/SOC-ZORA, respectively. Noting that B-IV, larger than B-I, is all-electron Gaussian correlation-consistent basis sets of triple-zeta quality. AE and ZORA are at the scalar relativistic level, while SOC-ZORA includes the spin-orbit coupling (SOC) effect.

[b] α1 and α2 denote the C(t)-An-C(t) and N-An-N angles, respectively. The C(t) atoms are marked in Chart 1b.

[c] β1 and β2 are the Ar$_{cent}$-An-Ar$_{cent}$ and Pl$_{cent}$-An-Pl$_{cent}$ angles, respectively, where the subscript "cent" stands for the centroid of the cycle.

[d] γ1 is the interplanar angles between Arenes, and γ2 is between Pyrroles.

Table S5. Calculated electron-spin density of each fragment ($S_{Frag.}$) and charges ($Q_{Frag.}$) in $[AnL^2]^z$ (An = Ac~Pu, z = 0 and +1).[a]

Complexes	S_{An}	S_{Ar}	S_{Pl}	S_{other}	Q_{An}	Q_{Ar}	Q_{Pl}	Q_{other}
$[AcL^2]$	0.152	0.729	0.131	-0.012	1.907	-0.584	-0.928	-0.395
$[ThL^2]$	0.772	1.024	0.214	-0.011	1.992	-0.796	-0.896	-0.300
$[PaL^2]$	1.796	1.078	0.107	0.018	2.003	-0.840	-0.859	-0.304
$[UL^2]$	3.170	0.690	0.066	0.073	1.939	-0.747	-0.886	-0.306
$[NpL^2]$	4.453	0.508	0.028	0.012	1.869	-0.644	-0.918	-0.307
$[PuL^2]$	5.650	0.381	-0.041	0.011	1.761	-0.526	-0.944	-0.291
$[AcL^2]^+$	0.000	0.000	0.000	0.000	1.946	-0.182	-0.728	-0.036
$[ThL^2]^+$	0.395	0.468	0.111	0.026	2.095	-0.366	-0.684	-0.044
$[PaL^2]^+$	1.484	0.422	0.091	0.004	2.042	-0.342	-0.657	-0.043
$[UL^2]^+$	2.742	0.293	-0.044	0.009	2.006	-0.223	-0.643	-0.14
$[NpL^2]^+$	4.012	0.188	-0.115	-0.085	1.961	-0.255	-0.664	-0.042
$[PuL^2]^+$	5.173	-0.002	-0.187	0.016	1.923	-0.210	-0.619	-0.094

[a.] Obtained at geometries optimized by the level of theory Pri: PBE/B-I/gas.

Table S6. Electron-spin density of each fragment ($S_{Frag.}$) and charges ($Q_{Frag.}$) in $[AnL^2]^z$ (An = Ac~Pu, z = 0 and +1), obtained at geometries optimized by the level of theory ADF: PBE/B-II/gas.

Complexes	S_{An}	S_{Ar}	S_{Pl}	S_{others}	Q_{An}	Q_{Ar}	Q_{Pl}	Q_{others}
$[AcL^2]$	0.152	0.767	0.105	-0.024	0.930	0.145	-0.420	-0.655
$[ThL^2]$	0.717	1.101	0.207	-0.026	0.973	0.019	-0.329	-0.663
$[PaL^2]$	1.712	1.177	0.132	-0.021	0.934	0.032	-0.319	-0.646
$[UL^2]$	3.123	0.839	0.038	0.000	0.625	0.262	-0.264	-0.624
$[NpL^2]$	4.389	0.626	-0.023	0.008	0.722	0.244	-0.244	-0.722
$[PuL^2]$	5.622	0.418	-0.054	0.015	0.745	0.302	-0.291	-0.756
$[AcL^2]^+$	0.000	0.000	0.000	0.000	0.867	0.651	-0.144	-0.375
$[ThL^2]^+$	0.499	0.460	0.046	-0.006	0.904	0.522	0.019	-0.444
$[PaL^2]^+$	1.403	0.518	0.082	-0.003	0.802	0.563	-0.004	-0.361
$[UL^2]^+$	2.670	0.369	-0.046	0.006	0.544	0.762	0.046	-0.352
$[NpL^2]^+$	4.055	0.106	-0.183	0.022	0.526	0.783	0.036	-0.344
$[PuL^2]^+$	5.200	-0.006	-0.216	0.023	0.717	0.660	0.009	-0.386

Table S7. Bond angles (α and β in degree) and interplanar arene/pyrrolide angles (γ) of actinide complexes optimized by Priroda and ADF codes.[a]

Complexes	Approach	α1	α2	β1	β2	γ1	γ2
[AcL^2]	Pri	175.3	172.0	128.5	120.9	42.3	42.9
[ThL^2]	Pri	177.8	172.9	123.5	120.9	46.5	53.1
[PaL^2]	Pri	175.0	168.8	124.6	116.6	49.9	55.2
[UL^2]	Pri	176.7	170.4	123.6	118.1	49.9	55.3
[NpL^2]	Pri	179.2	174.4	121.9	121.8	44.7	51.3
[PuL^2]	Pri	173.5	170.6	118.7	128.7	19.6	42.0
[AcL^2]$^+$	Pri	177.6	177.4	126.8	125.3	30.4	38.0
[ThL^2]$^+$	Pri	179.3	173.5	123.1	120.2	49.7	44.9
[PaL^2]$^+$	Pri	178.7	173.2	122.8	119.6	49.1	52.8
[UL^2]$^+$	Pri	177.7	171.9	123.2	117.9	48.7	50.0
[NpL^2]$^+$	Pri	179.2	173.5	122.3	119.5	47.8	50.5
[PuL^2]$^+$	Pri	178.8	175.8	121.1	121.5	44.1	46.4
[AcL^2]	ADF	174.4	172.2	129.2	121.1	39.1	40.9
[ThL^2]	ADF	177.6	173.2	123.6	121.5	44.9	51.9
[PaL^2]	ADF	174.8	168.8	124.8	116.6	49.4	54.8
[UL^2]	ADF	174.8	168.8	124.8	116.6	49.4	54.8
[NpL^2]	ADF	176.1	173.1	119.5	125.9	25.8	45.1
[PuL^2]	ADF	174.8	171.1	120.4	128.8	15.7	41.6
[AcL^2]$^+$	ADF	176.6	177.8	127.9	125.6	25.3	36.2
[ThL^2]$^+$	ADF	178.4	173.6	123.6	124.5	28.9	45.3
[PaL^2]$^+$	ADF	178.5	173.0	122.6	119.7	48.0	51.8
[UL^2]$^+$	ADF	177.3	171.7	123.4	117.8	48.4	51.0
[NpL^2]$^+$	ADF	178.4	173.6	123.0	119.8	46.3	50.1
[PuL^2]$^+$	ADF	178.6	179.3	121.1	125.0	33.2	44.0
[UL^2(BH$_4$)]	Pri	178.2	119.8	122.6	119.6	8.0	76.8
	Expt.[b]	174.7	118.9	122.0	117.4	14.2	81.5
[UL^2(I)]	Pri	176.6	119.5	117.9	119.3	11.8	78.0
	Expt.[b]	170.7	118.3	121.4	117.0	16.4	82.2

[a] α1 and α2 denote the C(t)-An-C(t) and N-An-N angles, respectively. The C(t) atoms are marked in Chart 1b. β1 and β2 are the Ar_{cent}-An-Ar_{cent} and Pl_{cent}-An-Pl_{cent} angles, respectively, where the subscript "cent" stands for the centroid of the cycle. γ1 is the interplanar angles between arenes, and γ2 is between pyrroles.

[b] Experimental values from Refs.[10, 11].

Table S8. Bond lengths [a] (Å) of $[AnL^2]^z$ (An = Ac~Pu, z = 0 and +1) optimized by Priroda and ADF codes, along with formal shortness ratio (FSR)[b].

	Appr.s	An-C(t) [c]	An-N	An-Ar_{cent} [d]	An-Pl_{cent} [d]	$FSR_{An-C(t)}$	FSR_{An-N}
$[AcL^2]$	Pri	2.926	2.756	2.658	2.669	1.005	0.960
$[ThL^2]$	Pri	2.838	2.726	2.561	2.540	1.013	0.988
$[PaL^2]$	Pri	2.768	2.708	2.460	2.543	0.999	0.992
$[UL^2]$	Pri	2.786	2.716	2.484	2.530	1.013	1.002
$[NpL^2]$	Pri	2.801	2.697	2.586	2.515	1.015	0.992
$[PuL^2]$	Pri	2.763	2.646	2.906	2.471	0.997	0.969
$[AcL^2]^+$	Pri	2.911	2.692	2.812	2.611	1.055	0.990
$[ThL^2]^+$	Pri	2.864	2.641	2.556	2.543	1.081	1.012
$[PaL^2]^+$	Pri	2.832	2.640	2.534	2.472	1.081	1.023
$[UL^2]^+$	Pri	2.803	2.608	2.517	2.486	1.078	1.019
$[NpL^2]^+$	Pri	2.821	2.622	2.556	2.472	1.081	1.020
$[PuL^2]^+$	Pri	2.844	2.598	2.635	2.470	1.085	1.007
$[AcL^2]$	ADF	2.917	2.754	2.678	2.684	1.118	1.072
$[ThL^2]$	ADF	2.836	2.734	2.579	2.553	1.013	0.990
$[PaL^2]$	ADF	2.768	2.710	2.465	2.549	0.999	0.993
$[UL^2]$	ADF	2.780	2.724	2.486	2.533	1.011	1.005
$[NpL^2]$	ADF	2.750	2.652	2.807	2.478	1.118	1.096
$[PuL^2]$	ADF	2.761	2.654	2.933	2.483	1.118	1.092
$[AcL^2]^+$	ADF	2.897	2.688	2.850	2.622	1.110	1.046
$[ThL^2]^+$	ADF	2.801	2.654	2.769	2.510	1.057	1.017
$[PaL^2]^+$	ADF	2.818	2.645	2.538	2.484	1.075	1.025
$[UL^2]^+$	ADF	2.797	2.622	2.513	2.488	1.076	1.024
$[NpL^2]^+$	ADF	2.816	2.634	2.561	2.485	1.145	1.088
$[PuL^2]^+$	ADF	2.802	2.600	2.746	2.460	1.134	1.070
$[UL^2(BH_4)]$	Pri	2.850	2.454	2.501	—	—	—
	Expt.[e]	2.845	2.464	2.591	—	—	—
$[UL^2(I)]$	Pri	2.834	2.446	2.538	3.650	—	—
	Expt.[e]	2.870	2.466	2.619	3.663	—	—

[a.] Average value.

[b.] FSR of a A-B bond is defined as $FSR_{A-B} = D_{A-B}/(R_A + R_B)$, where D_{A-B} is the optimized A-B bond length, and R_A and R_B values are the atomic radii. Pyykkö's calculations[12] showed the An^{VI} radius, Ac (1.86 Å), Th (1.75), Pa (1.72), U (1.70), Np (1.71) and Pu (1.72). Corresponding An^{III} and An^{II} radius are obtained by adding 0.15 and 0.30 Å, respectively. And radii of C and N are 0.75 and 0.71 Å, respectively.

[c.] The C(t) atoms are marked in Chart 1b.

[d.] The distance was determined between the actinide and the centroid of planar Ar or Pl, where the subscript "cent" stands for the centroid of the cycle.

[e.] Experimental values from Refs.[10, 11].

Table S9. Calculated reaction energies (in eV) while using the graphite potassium as reductant.

An =	$[AnL^2]^+ + [K(C_{24}H_{12})] = [AnL^2] + [K(C_{24}H_{12})]^+$				
	Δ_rE	Δ_rE_0	Δ_rG	Δ_rG(sol)	Δ_rG(sol-so)
Ac	0.63	0.56	0.53	0.65	0.62
Th	0.32	0.30	0.21	0.34	0.34
Pa	0.09	0.09	0.05	0.17	0.13
U	-0.01	-0.01	-0.06	0.08	0.10
Np	0.45	0.40	0.31	0.46	0.41
Pu	-0.31	-0.29	-0.34	-0.15	-0.07

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Optimized Cartesian coordinates of all complexes by Priroda code

[AcL^2]

Total energy: -27076.22910491 Hartree

C	0.23197664	-0.33130315	0.34551596
C	0.28270448	-1.00057038	1.58829518
C	1.35195126	-0.16904257	-0.69665060
N	-1.06974238	0.02733426	0.04798041
H	1.16471246	-1.38040566	2.10430725
C	-1.04851284	-1.02308195	2.08624150
C	1.12144809	-1.33854496	-1.68263221
C	1.22935904	1.20205199	-1.38945499
C	2.73541608	-0.24580344	-0.02803288
C	-1.84553580	-0.36647375	1.12257912
H	-1.36383734	-1.42340472	3.04998206
C	0.17254063	-1.20090871	-2.74814393
C	1.56277797	-2.64547656	-1.38106141
H	1.93336788	1.27717441	-2.23473863
H	1.46358635	1.99776024	-0.66415629
H	0.20580471	1.38350357	-1.74544952
H	3.52843997	-0.17719134	-0.79039344
H	2.89218115	-1.17541634	0.53987197
H	2.85185285	0.59160640	0.67774541
C	-3.37861225	-0.24892138	1.07277017
C	-3.81718907	-1.42172039	0.16438031
C	-3.91336022	-2.73806038	0.66659216
C	1.04911646	-3.81181928	-1.98934013
N	-1.23083999	-5.42722544	-0.62979626
C	-0.28047504	-2.33781255	-3.42876313
H	-0.18842047	-0.21542703	-3.04203873
H	2.24652265	-2.77004761	-0.53745964
C	-3.78126419	1.11757924	0.48499839
C	-3.98108397	-0.35948297	2.48404731
C	-3.80525869	-1.26742969	-1.26065180
H	-3.87201696	-2.87388053	1.75034652
C	-3.89007799	-3.89489209	-0.14272182
C	1.20412305	-5.19774238	-1.31996160
C	0.10217596	-3.63028139	-3.04999662
C	-1.99015969	-5.26523397	0.51442444
C	0.08754232	-5.23015242	-0.26217557
H	-0.99358289	-2.21501839	-4.25110361
H	-4.86895653	1.16252075	0.30985411
H	-3.24827142	1.32552590	-0.45308866
H	-3.50560164	1.91379818	1.19501027

H	-5.08129122	-0.32285997	2.42961128
H	-3.63069234	0.48170306	3.10257266
H	-3.69921756	-1.28710279	3.00496496
C	-3.87555567	-2.39744408	-2.08442281
H	-3.75556157	-0.27480478	-1.70796208
C	-3.87652672	-3.69677476	-1.56229329
C	-3.52710497	-5.27757153	0.44845262
C	1.00770382	-6.34908501	-2.32533739
C	2.58460258	-5.36647264	-0.66213401
H	-0.31240311	-4.49179943	-3.57323144
C	-1.16339737	-4.91324052	1.60405827
C	0.16790205	-4.89070757	1.10644195
H	-3.88082946	-2.26230341	-3.17141563
H	-3.88089991	-4.55115813	-2.23893884
C	-4.00425860	-6.43329781	-0.45242279
C	-4.13228947	-5.48024380	1.84828752
H	1.19042976	-7.30975142	-1.81759401
H	1.71218266	-6.25638109	-3.16848488
H	-0.02206321	-6.37885720	-2.70748853
H	2.64718368	-6.35591367	-0.18252001
H	2.79048441	-4.61394260	0.11413406
H	3.37806460	-5.29296648	-1.42357690
H	-1.46200575	-4.74413824	2.63881083
H	1.06671347	-4.70148093	1.69364195
H	-3.78046533	-7.39348396	0.03955239
H	-3.47750806	-6.43636461	-1.41670780
H	-5.09143547	-6.37082688	-0.62539652
H	-3.80072949	-4.72599183	2.57798357
H	-3.83586167	-6.46593304	2.24007127
H	-5.23234227	-5.43848728	1.79452288
Ac	-1.21759989	-2.67648285	-0.46967805

[ThL^2]

Total energy: -27821.21025124 Hartree

C	0.23659738	-0.40434199	0.36148671
C	0.27329199	-1.19134083	1.53782257
C	1.32430442	-0.18400084	-0.68607508
N	-1.05295766	-0.00815754	0.08969648
H	1.14830454	-1.61689422	2.02720852
C	-1.06651501	-1.21386310	2.03959802
C	1.01582049	-1.34344552	-1.64671733
C	1.17204098	1.19508990	-1.35081947
C	2.72963453	-0.27288645	-0.06901143

C	-1.83453706	-0.43931224	1.13707383
H	-1.39206787	-1.65962670	2.97850334
C	0.02316327	-1.20955827	-2.65796560
C	1.48494931	-2.64793597	-1.34527996
H	1.84856207	1.28117201	-2.21715033
H	1.42810678	1.98290708	-0.62414304
H	0.13815533	1.37717206	-1.67373590
H	3.49700202	-0.21174672	-0.85790463
H	2.89772754	-1.20105533	0.49709171
H	2.87707577	0.56610816	0.62947903
C	-3.34864518	-0.26300362	1.06364130
C	-3.71258546	-1.42302137	0.12337867
C	-3.82814426	-2.73789014	0.64351384
C	0.94297829	-3.81043617	-1.95110471
N	-1.21235190	-5.40647687	-0.57975696
C	-0.43839850	-2.34366588	-3.34772201
H	-0.35662608	-0.22341199	-2.92647567
H	2.25094514	-2.76488085	-0.58029430
C	-3.71128414	1.11267628	0.47800404
C	-4.00043096	-0.38722294	2.45048861
C	-3.63435961	-1.26993283	-1.28938069
H	-3.89780842	-2.87010423	1.72206408
C	-3.78586182	-3.88960928	-0.18369971
C	1.17725465	-5.18473835	-1.30406923
C	-0.05000225	-3.63640164	-2.95606328
C	-1.97616518	-5.19908410	0.54594888
C	0.09568128	-5.16398272	-0.22760079
H	-1.18087071	-2.22382473	-4.14154111
H	-4.79251846	1.16895413	0.26961292
H	-3.14940600	1.32215983	-0.44217805
H	-3.45086488	1.90042521	1.20324079
H	-5.09852494	-0.35773524	2.35944053
H	-3.67824548	0.45454360	3.08385755
H	-3.72810460	-1.31385878	2.97717309
C	-3.70763365	-2.39652428	-2.12625368
H	-3.55366939	-0.27561319	-1.72943931
C	-3.70568539	-3.69624293	-1.59141799
C	-3.49730433	-5.26381911	0.44122140
C	0.95179069	-6.34910026	-2.28403502
C	2.58038581	-5.32953794	-0.69271080
H	-0.48494730	-4.50384460	-3.45320734
C	-1.17199558	-4.71388777	1.60537444
C	0.16829474	-4.69131758	1.10499917
H	-3.67439119	-2.26243483	-3.21100737

H	-3.67979634	-4.55540547	-2.26223419
C	-3.93418805	-6.43060913	-0.46138024
C	-4.15201548	-5.44558617	1.82032214
H	1.15628264	-7.30373323	-1.77295196
H	1.62954954	-6.26021484	-3.14913635
H	-0.08801310	-6.38716716	-2.63569398
H	2.67429557	-6.32064147	-0.22108957
H	2.79647476	-4.57873760	0.08176310
H	3.34927051	-5.24004271	-1.47741636
H	-1.47881529	-4.49260577	2.62670883
H	1.06242626	-4.44939318	1.67791974
H	-3.72555404	-7.38579238	0.04697632
H	-3.37803239	-6.44046626	-1.40843252
H	-5.01517187	-6.37129687	-0.67022068
H	-3.83091316	-4.69365243	2.55630598
H	-3.88414808	-6.43410897	2.22603043
H	-5.24920838	-5.38812030	1.73177716
Th	-1.19157831	-2.68594606	-0.40177429

[PaL^2]

Total energy: -28580.83728077 Hartree

C	0.23810738	-0.44724420	0.37379881
C	0.27031473	-1.25287652	1.53548649
C	1.30943552	-0.19775431	-0.68277794
N	-1.04503485	-0.03654112	0.11141469
H	1.14147081	-1.70242933	2.00972203
C	-1.06754037	-1.27604715	2.03519379
C	0.96574853	-1.34204179	-1.64701127
C	1.14442524	1.19161488	-1.32113442
C	2.72727288	-0.29783496	-0.09711283
C	-1.82877046	-0.48248741	1.14617489
H	-1.40043964	-1.74621856	2.95931240
C	-0.04390380	-1.20524568	-2.62443497
C	1.41575918	-2.64834517	-1.32223181
H	1.81452477	1.29527491	-2.19044334
H	1.40217980	1.96873811	-0.58361128
H	0.10790892	1.37372462	-1.63441780
H	3.47823879	-0.24225935	-0.90200929
H	2.90197804	-1.22577353	0.46689570
H	2.89576994	0.54098215	0.59680325
C	-3.33720849	-0.27631151	1.05393462
C	-3.67636489	-1.42068671	0.08823527
C	-3.76389370	-2.73597401	0.61433988

C	0.89319096	-3.80726216	-1.95334158
N	-1.20295546	-5.38224635	-0.55299447
C	-0.56995014	-2.34820960	-3.26764431
H	-0.43868621	-0.22022542	-2.87516885
H	2.18367554	-2.76548125	-0.56144052
C	-3.67221864	1.11011842	0.47894630
C	-4.01968976	-0.41144027	2.42477735
C	-3.55998221	-1.26511330	-1.31022214
H	-3.84064707	-2.86712264	1.69096797
C	-3.74903984	-3.88595786	-0.21731092
C	1.16283304	-5.17041399	-1.30044603
C	-0.11554800	-3.64222471	-2.92730095
C	-1.96645952	-5.15991956	0.56580208
C	0.10024706	-5.12497660	-0.20726060
H	-1.31936487	-2.22871855	-4.05180313
H	-4.75086129	1.18445692	0.26335288
H	-3.10111472	1.31904752	-0.43530579
H	-3.40582018	1.88748641	1.21313470
H	-5.11568311	-0.38678588	2.31036089
H	-3.71633175	0.42972200	3.06816829
H	-3.75430673	-1.33777624	2.95502892
C	-3.55100109	-2.39922487	-2.15314500
H	-3.45605563	-0.27173465	-1.74769696
C	-3.63193137	-3.70217503	-1.61228098
C	-3.48363755	-5.24899201	0.43754777
C	0.92211178	-6.34999752	-2.25737432
C	2.57974025	-5.29905186	-0.71809875
H	-0.56483927	-4.51148184	-3.40845615
C	-1.16614630	-4.65574160	1.61683453
C	0.17139975	-4.63311065	1.11651430
H	-3.50363363	-2.26651130	-3.23524906
H	-3.58269075	-4.56315750	-2.27956228
C	-3.89504906	-6.43168718	-0.45522707
C	-4.16625362	-5.41267572	1.80522807
H	1.12760433	-7.29711918	-1.73291346
H	1.59262860	-6.27822139	-3.12956837
H	-0.12050124	-6.38902452	-2.59948972
H	2.69402797	-6.29020623	-0.25110488
H	2.80398315	-4.54863718	0.05409614
H	3.33210335	-5.20010975	-1.51750201
H	-1.47737976	-4.40880395	2.63077425
H	1.06402397	-4.36576454	1.68013375
H	-3.67794585	-7.37848909	0.06511362
H	-3.33213442	-6.44387369	-1.39787487

H	-4.97504773	-6.38943774	-0.67268765
H	-3.85081404	-4.66062238	2.54320390
H	-3.91684890	-6.40149575	2.22183483
H	-5.26101554	-5.34477858	1.69672798
Pa	-1.21593427	-2.67717624	-0.46557227

[UL^2]

Total energy: -29355.05543933 Hartree

C	0.23339917	-0.44228029	0.37018735
C	0.26833298	-1.24585802	1.53260135
C	1.31094641	-0.19909363	-0.68350182
N	-1.04710737	-0.02532737	0.10604571
H	1.14055972	-1.69135653	2.00864426
C	-1.06809421	-1.26844655	2.03201146
C	0.97014833	-1.34516331	-1.64740551
C	1.15216182	1.18888369	-1.32688777
C	2.72570539	-0.30124289	-0.09079581
C	-1.82766178	-0.47700870	1.14045660
H	-1.40082537	-1.73420304	2.95841694
C	-0.03476481	-1.20662524	-2.62993421
C	1.43051583	-2.64693591	-1.33858679
H	1.82391358	1.28932516	-2.19534300
H	1.41135107	1.96632767	-0.59032000
H	0.11621716	1.37347535	-1.64038365
H	3.48161428	-0.24877026	-0.89133586
H	2.89504257	-1.22783935	0.47708001
H	2.89156939	0.53878612	0.60211528
C	-3.33870507	-0.27754305	1.05414177
C	-3.67981473	-1.42393640	0.09075980
C	-3.78556515	-2.73513809	0.61181267
C	0.89754369	-3.80465972	-1.95303536
N	-1.20547300	-5.39327804	-0.56018155
C	-0.55226780	-2.34806767	-3.27283504
H	-0.42888347	-0.22162787	-2.88112866
H	2.19365129	-2.76468182	-0.57230655
C	-3.68179587	1.10713512	0.47912763
C	-4.01442394	-0.41443774	2.42818334
C	-3.57042884	-1.26697462	-1.30846291
H	-3.85544877	-2.86660376	1.68943646
C	-3.75224256	-3.88353016	-0.21400288
C	1.16414166	-5.16936680	-1.30094847
C	-0.10661578	-3.64014470	-2.93231011
C	-1.96552581	-5.16356773	0.55913404
C	0.09525115	-5.12867056	-0.21180599

H	-1.30840766	-2.22893279	-4.05181793
H	-4.76086586	1.17786554	0.26433231
H	-3.11044993	1.31868069	-0.43434902
H	-3.41796181	1.88485590	1.21375793
H	-5.11118542	-0.39356526	2.32004022
H	-3.71030180	0.42831168	3.06894037
H	-3.74213835	-1.33895979	2.95815163
C	-3.56790469	-2.39989529	-2.14543891
H	-3.46734165	-0.27366455	-1.74591385
C	-3.64216598	-3.70058415	-1.60999569
C	-3.48497555	-5.24802259	0.43821953
C	0.92933633	-6.34644433	-2.26269787
C	2.57825420	-5.29771215	-0.71175271
H	-0.55538101	-4.50920902	-3.41395848
C	-1.16729612	-4.66007827	1.61147935
C	0.16894586	-4.63753218	1.11162479
H	-3.51269205	-2.26738542	-3.22808736
H	-3.59383579	-4.56143294	-2.27726677
C	-3.90394858	-6.42852160	-0.45424621
C	-4.16085177	-5.41131882	1.80929052
H	1.13708691	-7.29399755	-1.74008678
H	1.60059085	-6.27093050	-3.13405492
H	-0.11324364	-6.38801666	-2.60453138
H	2.69007315	-6.28984270	-0.24649919
H	2.79723379	-4.54957018	0.06417978
H	3.33546426	-5.19671551	-1.50638967
H	-1.47866731	-4.41677661	2.62623440
H	1.06235128	-4.37373759	1.67564892
H	-3.68925572	-7.37578785	0.06607111
H	-3.34105202	-6.44302609	-1.39683869
H	-4.98414321	-6.38295393	-0.67026093
H	-3.83897416	-4.66125302	2.54654322
H	-3.91046847	-6.40100176	2.22296800
H	-5.25622500	-5.34168600	1.70768899
U	-1.20599569	-2.68079369	-0.43899514

[NpL^2]

Total energy: -30144.61423008 Hartree

C	0.23256724	-0.42373766	0.36383837
C	0.27511552	-1.19036256	1.54926579
C	1.31838082	-0.19359629	-0.68680760
N	-1.05494325	-0.03472569	0.08470630
H	1.15121740	-1.61150759	2.04095660
C	-1.06258620	-1.21310335	2.04960763

C	1.00739475	-1.34640866	-1.65552477
C	1.16018754	1.19025775	-1.34073123
C	2.72726359	-0.28378642	-0.07684858
C	-1.83108685	-0.45877517	1.13574537
H	-1.38811894	-1.65477354	2.99069498
C	0.05401083	-1.20593979	-2.68625329
C	1.45021200	-2.64851054	-1.33153481
H	1.83635447	1.28984294	-2.20588128
H	1.41256917	1.97184619	-0.60629958
H	0.12461745	1.36925264	-1.65957674
H	3.49174799	-0.21992118	-0.86834020
H	2.89904959	-1.21219324	0.48745055
H	2.87666180	0.55397960	0.62241387
C	-3.34602604	-0.27252399	1.05794893
C	-3.71302780	-1.42586941	0.10966214
C	-3.79566490	-2.73703057	0.62973191
C	0.93526342	-3.80441826	-1.96018227
N	-1.21245320	-5.37860277	-0.57847435
C	-0.44241530	-2.34376832	-3.34174602
H	-0.32932773	-0.22029582	-2.95173831
H	2.17380449	-2.76939498	-0.52685208
C	-3.69666719	1.10838088	0.47669350
C	-4.00558542	-0.39817183	2.44154347
C	-3.67483906	-1.26811623	-1.29198780
H	-3.80958082	-2.87079921	1.71030103
C	-3.78562040	-3.88376184	-0.19568364
C	1.17190077	-5.17466808	-1.30398487
C	-0.01710258	-3.63389263	-2.98723627
C	-1.97060650	-5.17995063	0.54964506
C	0.09333913	-5.14518857	-0.22152984
H	-1.18393208	-2.22352101	-4.13660951
H	-4.77722021	1.17875381	0.26925102
H	-3.13069223	1.31461264	-0.44159855
H	-3.42756688	1.88981344	1.20531615
H	-5.10326168	-0.36559602	2.34658060
H	-3.68420030	0.44219395	3.07686876
H	-3.73749639	-1.32520966	2.96937856
C	-3.69678249	-2.39761192	-2.12532980
H	-3.58929777	-0.27438159	-1.73256023
C	-3.74641936	-3.69596860	-1.59354954
C	-3.49318390	-5.25328033	0.43922404
C	0.93885027	-6.34574758	-2.27451724
C	2.57901378	-5.31759662	-0.70009742
H	-0.45480742	-4.50112631	-3.48245142

C	-1.16653776	-4.71804430	1.61489833
C	0.17132795	-4.69549815	1.11503185
H	-3.66282250	-2.26385264	-3.21025968
H	-3.71558454	-4.55503478	-2.26435742
C	-3.91902303	-6.42739969	-0.45954031
C	-4.15456735	-5.43152424	1.81613455
H	1.14012487	-7.29609199	-1.75460754
H	1.61454854	-6.27037152	-3.14247662
H	-0.10293970	-6.38131606	-2.62023307
H	2.67446152	-6.30769989	-0.22709382
H	2.80001221	-4.56621088	0.07220948
H	3.34443330	-5.23091522	-1.48851034
H	-1.47314651	-4.50156256	2.63755066
H	1.06665353	-4.45877325	1.68865415
H	-3.70109445	-7.37752930	0.05398191
H	-3.35918788	-6.43536456	-1.40433843
H	-5.00027247	-6.38207129	-0.67031556
H	-3.83669884	-4.67903591	2.55275745
H	-3.88758036	-6.41906036	2.22433947
H	-5.25153829	-5.37566300	1.72389193
Np	-1.17954881	-2.69016154	-0.36998207

[PuL^2]

Total energy: -30949.28890383 Hartree

C	0.14110546	-0.44687479	0.32999319
C	0.24922514	-1.10115950	1.57656726
C	1.19426967	-0.19003789	-0.74923826
N	-1.16235729	-0.08985074	0.08975365
H	1.15321460	-1.48224444	2.05200485
C	-1.06150131	-1.10451796	2.14390861
C	1.04096716	-1.33463668	-1.76962155
C	0.95205467	1.19100671	-1.38265117
C	2.61604795	-0.21004211	-0.14806677
C	-1.88728671	-0.43969996	1.20678878
H	-1.33173915	-1.46848296	3.13478360
C	0.72069901	-1.17331246	-3.12499797
C	1.18592043	-2.64606691	-1.28550056
H	1.69731488	1.39577250	-2.16853892
H	1.04302437	1.96974106	-0.60891500
H	-0.05987890	1.26090939	-1.80609057
H	3.36135044	-0.03962692	-0.94183218
H	2.85655804	-1.17088562	0.33268681
H	2.71827407	0.58464505	0.60849379

C	-3.41099124	-0.28038191	1.17572145
C	-3.78923713	-1.43941572	0.23127264
C	-3.93737760	-2.74933151	0.75761788
C	0.96880156	-3.78847811	-2.07476915
N	-1.31558806	-5.32055901	-0.55878850
C	0.54502137	-2.29700551	-3.94058688
H	0.59350922	-0.17473029	-3.54775694
H	1.47748459	-2.78477012	-0.23856619
C	-3.80370305	1.09677294	0.61105845
C	-4.01839619	-0.42403213	2.57945866
C	-3.64659359	-1.29054234	-1.16736456
H	-4.06159447	-2.87864903	1.83153429
C	-3.86083852	-3.89784118	-0.07293881
C	1.04820558	-5.15483647	-1.36659083
C	0.64963567	-3.59433437	-3.42610785
C	-2.02621688	-5.21266471	0.61552215
C	0.00474754	-5.10875351	-0.24900233
H	0.29168054	-2.15832025	-4.99564302
H	-4.89125908	1.14797565	0.43703834
H	-3.27322813	1.31610546	-0.32525135
H	-3.52522197	1.88102268	1.33339715
H	-5.11923025	-0.41922922	2.52419875
H	-3.69695722	0.42326035	3.20543587
H	-3.70537783	-1.34546108	3.09322813
C	-3.62419733	-2.41615147	-2.00838839
H	-3.49596997	-0.29972733	-1.59636879
C	-3.71720105	-3.70948568	-1.46674140
C	-3.55636101	-5.27165892	0.55816539
C	0.72978914	-6.32249679	-2.31648600
C	2.46464535	-5.36547368	-0.78989313
H	0.46778543	-4.44999524	-4.07945090
C	-1.16942469	-4.84515105	1.67995280
C	0.14259012	-4.78589885	1.11860398
H	-3.51088371	-2.28581909	-3.08814381
H	-3.62082011	-4.57294802	-2.12520019
C	-4.02409338	-6.44498433	-0.32168639
C	-4.16380711	-5.43933940	1.95921103
H	0.77054225	-7.27087640	-1.75767202
H	1.46659662	-6.37146880	-3.13482701
H	-0.28185663	-6.22778338	-2.73577069
H	2.51415690	-6.32381680	-0.24819440
H	2.75938250	-4.56475979	-0.09402565
H	3.20357166	-5.38358875	-1.60736251
H	-1.42467763	-4.71936888	2.73179455

H	1.06406768	-4.58519288	1.66545653
H	-3.79575197	-7.39621297	0.18565576
H	-3.50141361	-6.45967805	-1.28748763
H	-5.11170683	-6.38983516	-0.49421353
H	-3.80094350	-4.69081784	2.67963849
H	-3.89659693	-6.43093827	2.35721959
H	-5.26263512	-5.36645674	1.91286516
Pu	-1.39929593	-2.71859347	-0.08766353

$[AcL^2]^+$

Total energy: -27076.08567549 Hartree

C	0.22758601	-0.34196569	0.33134558
C	0.28598621	-0.96522168	1.59503675
C	1.36069634	-0.16373123	-0.69951902
N	-1.08056177	-0.02802868	0.01610095
H	1.17338360	-1.29479317	2.13519951
C	-1.04885516	-0.98752248	2.09389075
C	1.16440398	-1.34267812	-1.68664734
C	1.21886971	1.20411728	-1.39372105
C	2.73847361	-0.22276608	-0.01537620
C	-1.85159663	-0.37684106	1.10833800
H	-1.35467348	-1.33732999	3.07977526
C	0.35383213	-1.20032168	-2.82924627
C	1.56625411	-2.65188795	-1.33398676
H	1.94384973	1.30194396	-2.21755654
H	1.41879271	2.00053776	-0.66056015
H	0.20171418	1.37013831	-1.77517558
H	3.53700800	-0.13341405	-0.76866189
H	2.90986232	-1.15127687	0.54968000
H	2.83466040	0.61427029	0.69258255
C	-3.38752889	-0.24350440	1.07447126
C	-3.85200026	-1.42736911	0.18822684
C	-3.88368872	-2.74382541	0.70400269
C	1.09117459	-3.80932063	-1.99328691
N	-1.23749799	-5.36706331	-0.64547907
C	-0.05808922	-2.32796571	-3.54976024
H	0.02197589	-0.20976213	-3.14446337
H	2.17540234	-2.78167694	-0.43571088
C	-3.77605445	1.11963045	0.47118954
C	-3.97749613	-0.33438246	2.49346287
C	-3.99556888	-1.27470320	-1.20421358
H	-3.74866105	-2.88104650	1.78000199
C	-3.92418004	-3.89439917	-0.11733678

C	1.21154609	-5.20301694	-1.32565961
C	0.28128919	-3.61986159	-3.12957252
C	-1.99437636	-5.25104366	0.50463613
C	0.08445047	-5.21598861	-0.27322834
H	-0.68028166	-2.19879475	-4.44068573
H	-4.86587329	1.18547408	0.32351016
H	-3.26197467	1.31136770	-0.48101277
H	-3.47214697	1.91838941	1.16501321
H	-5.07632260	-0.27423196	2.44873048
H	-3.60900203	0.50638942	3.10043921
H	-3.71198767	-1.26172317	3.02313735
C	-4.12517823	-2.39814642	-2.02981375
H	-3.98186551	-0.27871948	-1.64978645
C	-4.06664006	-3.69449731	-1.50389064
C	-3.53509813	-5.28344529	0.45022244
C	0.99381446	-6.34874745	-2.33211451
C	2.58628963	-5.39392271	-0.65976046
H	-0.10642009	-4.48171372	-3.67509217
C	-1.16427953	-4.94620429	1.60314311
C	0.17052805	-4.92379062	1.10371152
H	-4.24540399	-2.26101210	-3.10883846
H	-4.10725935	-4.55082678	-2.17898912
C	-3.99787275	-6.43352474	-0.46417249
C	-4.12921843	-5.50686628	1.85273709
H	1.14443966	-7.31061609	-1.81842246
H	1.71560176	-6.28262491	-3.16187675
H	-0.02955130	-6.35763337	-2.73256126
H	2.62802644	-6.38203323	-0.17707597
H	2.81070084	-4.64262723	0.11238432
H	3.38239510	-5.34525804	-1.41929884
H	-1.45583131	-4.83070598	2.64696616
H	1.07194518	-4.78756027	1.70102553
H	-3.74568752	-7.39352347	0.01182166
H	-3.48931229	-6.41697973	-1.43824125
H	-5.08863722	-6.39804517	-0.61523293
H	-3.81393596	-4.75375411	2.59055701
H	-3.81492864	-6.49024216	2.23393223
H	-5.22932654	-5.49003281	1.80249046
Ac	-1.18005943	-2.68982817	-0.37110217

$[ThL^2]^+$

Total energy: -27821.05571051 Hartree

C	0.23526585	-0.43206330	0.34774316

C	0.28147205	-1.13555124	1.57115993
C	1.33055647	-0.19583606	-0.69537991
N	-1.06759766	-0.08783720	0.04797602
H	1.16190645	-1.51951448	2.08625313
C	-1.05311304	-1.15804193	2.07090822
C	1.01337233	-1.34451235	-1.66887984
C	1.17947692	1.19192409	-1.34375393
C	2.73240245	-0.29997172	-0.07465115
C	-1.84244794	-0.46709870	1.12575950
H	-1.36703512	-1.56217682	3.03321683
C	-0.00169647	-1.20702360	-2.66338145
C	1.49066410	-2.64112618	-1.40185993
H	1.87244141	1.29457910	-2.19405673
H	1.42148251	1.96937486	-0.60269717
H	0.15260823	1.38039184	-1.68483985
H	3.50117199	-0.23595926	-0.86070974
H	2.90050645	-1.22919327	0.49052449
H	2.88417504	0.53569029	0.62542588
C	-3.35987084	-0.27527296	1.06075244
C	-3.72574481	-1.42411399	0.10462411
C	-3.87323271	-2.73151874	0.60394242
C	0.94067805	-3.80381351	-1.97272419
N	-1.22207378	-5.31790575	-0.60005733
C	-0.47835860	-2.34493236	-3.32825848
H	-0.38093716	-0.22136577	-2.93294254
H	2.24672997	-2.75959019	-0.62401980
C	-3.71291393	1.10950258	0.48899825
C	-4.00572846	-0.41510647	2.44805332
C	-3.61627686	-1.26667943	-1.31018663
H	-3.92999740	-2.86444183	1.68554348
C	-3.79884369	-3.88316480	-0.20138318
C	1.18380300	-5.17125304	-1.31031008
C	-0.07375764	-3.63613914	-2.96326049
C	-1.98229485	-5.16832886	0.54247750
C	0.09603519	-5.13319793	-0.23380715
H	-1.22264334	-2.22496640	-4.12120627
H	-4.79651681	1.18220555	0.30387626
H	-3.16850870	1.32531590	-0.44017429
H	-3.43190005	1.88706160	1.21605057
H	-5.10314206	-0.38257416	2.36080845
H	-3.68519295	0.42293724	3.08556187
H	-3.73372638	-1.34296563	2.97363987
C	-3.66011432	-2.39661667	-2.13804071
H	-3.53560725	-0.27299588	-1.75072782

C	-3.68839301	-3.69548085	-1.61238744
C	-3.50766265	-5.25051464	0.44172076
C	0.95783134	-6.34834421	-2.27599538
C	2.58451622	-5.30258707	-0.69223455
H	-0.50790761	-4.50289703	-3.46149332
C	-1.16193194	-4.77536591	1.62248139
C	0.17310417	-4.75275670	1.12380273
H	-3.62245220	-2.26267929	-3.22328736
H	-3.66277826	-4.55398271	-2.28343210
C	-3.93368632	-6.43011060	-0.45070151
C	-4.15627282	-5.41820287	1.82459061
H	1.14894440	-7.29541607	-1.74807012
H	1.65014164	-6.28087340	-3.13033158
H	-0.07561232	-6.38849768	-2.64572059
H	2.68242022	-6.29090064	-0.21775984
H	2.80157868	-4.55030345	0.08113463
H	3.35436259	-5.21763265	-1.47524798
H	-1.45963642	-4.60028079	2.65623175
H	1.07012383	-4.55755479	1.71131446
H	-3.70372906	-7.37707847	0.06168725
H	-3.39408775	-6.44201382	-1.40723217
H	-5.01798776	-6.39310508	-0.64226120
H	-3.83605307	-4.66478984	2.56010521
H	-3.88973053	-6.40401010	2.23523251
H	-5.25296718	-5.36505138	1.73839376
Th	-1.19758130	-2.68378510	-0.41589463

$[PaL^2]^+$ Total energy: -28580.67413954 Hartree

C	0.22958624	-0.46991373	0.34308080
C	0.26456181	-1.26038227	1.51388292
C	1.32326145	-0.19961316	-0.68824827
N	-1.06244752	-0.09035423	0.06232942
H	1.14011711	-1.67110140	2.01434812
C	-1.07730402	-1.28287384	2.01548090
C	0.99233080	-1.34738589	-1.65116304
C	1.15738032	1.18995781	-1.32574479
C	2.72823638	-0.29929494	-0.07430477
C	-1.84191527	-0.50476838	1.11728415
H	-1.39761160	-1.71382154	2.96280854
C	-0.01026097	-1.20891347	-2.64471242
C	1.46880552	-2.64440151	-1.36890173
H	1.84434765	1.30232045	-2.17960932
H	1.39960540	1.96424371	-0.58152875

H	0.12726184	1.37447941	-1.65842306
H	3.49369496	-0.22826337	-0.86304133
H	2.90306598	-1.22880258	0.48747188
H	2.87801989	0.53523351	0.62754578
C	-3.35106828	-0.27841879	1.05878768
C	-3.69879815	-1.42677238	0.10221264
C	-3.83450844	-2.73401435	0.61379190
C	0.91984320	-3.80309865	-1.95631222
N	-1.21650481	-5.31910967	-0.58656001
C	-0.49385606	-2.34533710	-3.30932412
H	-0.39420068	-0.22264893	-2.90648015
H	2.23569225	-2.76200651	-0.60455192
C	-3.68522685	1.10836003	0.48455712
C	-4.00550810	-0.41283047	2.44238189
C	-3.59797110	-1.27006097	-1.30373956
H	-3.90840469	-2.86551090	1.69240752
C	-3.77120864	-3.88259192	-0.20215408
C	1.17667553	-5.16855895	-1.30539808
C	-0.08207655	-3.63592794	-2.94610144
C	-1.97787642	-5.13037927	0.54346365
C	0.09341233	-5.09530567	-0.23124059
H	-1.24079611	-2.22518328	-4.09889876
H	-4.76741588	1.19243290	0.29630417
H	-3.13574391	1.31880869	-0.44255608
H	-3.39874257	1.88316235	1.21234254
H	-5.10228465	-0.37351203	2.34965022
H	-3.68322808	0.42480496	3.07955592
H	-3.74125694	-1.34064679	2.97104239
C	-3.63526025	-2.39920575	-2.13486753
H	-3.50917251	-0.27596302	-1.74252014
C	-3.66951073	-3.69716959	-1.60457017
C	-3.49737655	-5.24757523	0.44282532
C	0.93507761	-6.34844208	-2.26154375
C	2.58064846	-5.30372176	-0.69600444
H	-0.52110070	-4.50420365	-3.43804251
C	-1.17554561	-4.64087461	1.59866996
C	0.16623208	-4.61817327	1.09686552
H	-3.59310453	-2.26601564	-3.21942442
H	-3.63517749	-4.55764242	-2.27319130
C	-3.90766028	-6.43048877	-0.44997022
C	-4.15234925	-5.41711675	1.82235642
H	1.12408047	-7.29371983	-1.72974766
H	1.62242496	-6.29014300	-3.12051301
H	-0.10069202	-6.38497139	-2.62448200

H	2.67660811	-6.29169066	-0.22040025
H	2.80526697	-4.55145001	0.07457150
H	3.34628369	-5.22430934	-1.48376048
H	-1.47683488	-4.43647675	2.62492174
H	1.06067592	-4.39368888	1.67592939
H	-3.67340818	-7.37490045	0.06507516
H	-3.36363893	-6.44063375	-1.40380996
H	-4.99127446	-6.40199821	-0.64655596
H	-3.83835522	-4.66319182	2.55933186
H	-3.88359416	-6.40211255	2.23347962
H	-5.24890046	-5.36899333	1.73106853
Pa	-1.19399588	-2.68520809	-0.40679460

$[UL^2]^+$ Total energy: -29354.88866568 Hartree

C	0.23349349	-0.48681756	0.35141885
C	0.27262681	-1.24823171	1.53689087
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
C	-1.83861901	-0.52184878	1.12599894
H	-1.38796228	-1.69601474	2.98841526
C	-0.01413097	-1.20884412	-2.65352952
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
H	3.48631518	-0.23515632	-0.88455087
H	2.90952865	-1.23885835	0.46947378
H	2.88402286	0.52469772	0.61296804
C	-3.34678201	-0.28719876	1.05421588
C	-3.69627391	-1.42705004	0.08793456
C	-3.80782259	-2.73344061	0.60286714
C	0.90844021	-3.79970627	-1.96477856
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
C	-3.66541945	1.10565216	0.48488407
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
H	1.06858718	-4.41730243	1.69635441
H	-3.64586406	-7.36935910	0.06992341
H	-3.33979590	-6.43696834	-1.40133303
H	-4.97043881	-6.41249302	-0.65024361
H	-3.85368996	-4.65002209	2.55292881
H	-3.89748931	-6.38916634	2.22905642
H	-5.25684878	-5.35574940	1.71240069
U	-1.20270002	-2.68204385	-0.43009214

$[NpL^2]^+$

Total energy: -30144.46431324 Hartree

C	0.22828719	-0.48134275	0.34650493
C	0.26925218	-1.24516436	1.53267943
C	1.32015403	-0.20739841	-0.69058979
N	-1.06295939	-0.10839598	0.05983418
H	1.14656752	-1.65246606	2.03321496
C	-1.06792013	-1.26776403	2.03268240
C	0.99637317	-1.34746250	-1.66694239
C	1.14943241	1.18694288	-1.31746763
C	2.72728396	-0.30593686	-0.07983224
C	-1.83773571	-0.51622943	1.11906756
H	-1.38920342	-1.69532553	2.98140878
C	0.01364284	-1.20762146	-2.67010766
C	1.45706373	-2.64391661	-1.36985530
H	1.84013926	1.31146186	-2.16661644
H	1.38362031	1.95563156	-0.56503808
H	0.11973373	1.36801692	-1.65292116
H	3.49142848	-0.22898051	-0.86919702
H	2.90615798	-1.23675853	0.47832195
H	2.87526255	0.52628359	0.62498226
C	-3.34965798	-0.28633525	1.05556274
C	-3.71207645	-1.42702152	0.09362537
C	-3.82622200	-2.73320994	0.60560716
C	0.92408099	-3.79963787	-1.97113128
N	-1.21610014	-5.30107294	-0.58437754
C	-0.48235670	-2.34421259	-3.32499153
H	-0.37309494	-0.22123937	-2.92865922
H	2.20006618	-2.76350128	-0.58246208
C	-3.67345840	1.10542587	0.48593879
C	-4.00741975	-0.41978965	2.43842305
C	-3.63310350	-1.26917438	-1.30655110
H	-3.86646399	-2.86606541	1.68591679
C	-3.78443180	-3.87918737	-0.21066197
C	1.17409813	-5.16034829	-1.30495131
C	-0.05785262	-3.63308903	-2.97099135
C	-1.97353991	-5.12003861	0.54792121
C	0.09250663	-5.08500243	-0.22456642
H	-1.22488615	-2.22387950	-4.11857821
H	-4.75508603	1.19997434	0.29945566
H	-3.12220033	1.31324284	-0.44062943
H	-3.37937822	1.87513046	1.21597391
H	-5.10381900	-0.37429914	2.34474538
H	-3.68142058	0.41546221	3.07665058

H	-3.74858606	-1.34923998	2.96670742
C	-3.65491873	-2.39771139	-2.13880325
H	-3.54028681	-0.27466495	-1.74438861
C	-3.70468759	-3.69462528	-1.60751736
C	-3.49574609	-5.23926743	0.44099940
C	0.92732567	-6.34714864	-2.25202092
C	2.58013971	-5.29572133	-0.69873866
H	-0.49930035	-4.50235581	-3.45972724
C	-1.16805760	-4.66028473	1.61183930
C	0.16913383	-4.63763689	1.11188481
H	-3.61903827	-2.26417640	-3.22346581
H	-3.66659409	-4.55575958	-2.27562264
C	-3.89562850	-6.42862420	-0.44886924
C	-4.15469275	-5.40958027	1.81924526
H	1.11106909	-7.28852327	-1.71172278
H	1.61576293	-6.30042531	-3.11080300
H	-0.10868611	-6.38076530	-2.61416360
H	2.67449366	-6.28196695	-0.21950485
H	2.80869723	-4.54130917	0.06845341
H	3.34418939	-5.22184916	-1.48848966
H	-1.47085708	-4.45933674	2.63850667
H	1.06496475	-4.41653934	1.69043122
H	-3.65192788	-7.36900103	0.06898924
H	-3.35073845	-6.43550423	-1.40209842
H	-4.97955595	-6.41186448	-0.64497490
H	-3.84625193	-4.65387378	2.55662394
H	-3.88233030	-6.39284968	2.23186386
H	-5.25117445	-5.36714673	1.72510047
Np	-1.19145285	-2.68603455	-0.40049966

$[PuL^2]^+$

Total energy: -30949.11093064 Hartree

C	0.23293830	-0.47261776	0.35035588
C	0.27867477	-1.19870545	1.55952898
C	1.32526543	-0.20803382	-0.69152227
N	-1.06313218	-0.12916132	0.05108632
H	1.15887924	-1.58613672	2.07161283
C	-1.05931819	-1.21734929	2.06304156
C	1.02594582	-1.34641418	-1.68206436
C	1.15099878	1.18713836	-1.31774823
C	2.73070796	-0.29826691	-0.07391835
C	-1.83791793	-0.51165718	1.12544576
H	-1.37577402	-1.62545281	3.02214711

C	0.07323770	-1.20628681	-2.71239867
C	1.47826418	-2.64197531	-1.37785666
H	1.84642041	1.31701582	-2.16222600
H	1.37532631	1.95642007	-0.56295194
H	0.12220382	1.36181069	-1.65993332
H	3.49761900	-0.21256113	-0.85959832
H	2.91387231	-1.23090254	0.48002503
H	2.86999003	0.53179675	0.63522310
C	-3.35216818	-0.28906314	1.05625675
C	-3.73968898	-1.43042623	0.10007577
C	-3.84763032	-2.73514479	0.61317830
C	0.94939977	-3.79546035	-1.98363632
N	-1.21981394	-5.27909497	-0.58598658
C	-0.39692927	-2.33737174	-3.39463029
H	-0.30955592	-0.21900347	-2.97529000
H	2.19664773	-2.76454750	-0.56754721
C	-3.67123820	1.10291202	0.48267361
C	-4.00681657	-0.41300138	2.44215269
C	-3.71163018	-1.27190111	-1.30240306
H	-3.85415851	-2.86830326	1.69480970
C	-3.81674312	-3.87930012	-0.20262533
C	1.17664802	-5.15767684	-1.30550629
C	0.00444218	-3.62454138	-3.01839409
C	-1.97536423	-5.12967666	0.55157511
C	0.09635608	-5.09092502	-0.22113481
H	-1.11703064	-2.21390370	-4.20848864
H	-4.75321365	1.20320268	0.30108019
H	-3.12315465	1.30286854	-0.44769746
H	-3.36896410	1.87401499	1.20786775
H	-5.10299892	-0.35956746	2.35089992
H	-3.67286443	0.42129637	3.07749883
H	-3.75430229	-1.34374879	2.97137345
C	-3.76521038	-2.39562186	-2.13537423
H	-3.63033068	-0.27607470	-1.74051414
C	-3.77729550	-3.69130829	-1.59975390
C	-3.50019398	-5.23896392	0.44373757
C	0.92366496	-6.34420504	-2.25236171
C	2.58145146	-5.30324663	-0.69727388
H	-0.42854722	-4.49399466	-3.51517481
C	-1.16196380	-4.71187563	1.62638324
C	0.17780239	-4.69375729	1.12753779
H	-3.75964359	-2.26235671	-3.22089940
H	-3.74509226	-4.55264543	-2.26865758
C	-3.89700862	-6.42888477	-0.44826208

C	-4.15402268	-5.41897636	1.82393350
H	1.09794077	-7.28651360	-1.71055214
H	1.61501608	-6.30425374	-3.10918314
H	-0.11174267	-6.36905264	-2.61743603
H	2.66798258	-6.28861791	-0.21478106
H	2.81548527	-4.54730275	0.06686337
H	3.34626473	-5.23767655	-1.48693305
H	-1.46133224	-4.53287627	2.65857095
H	1.07495910	-4.49404269	1.71217015
H	-3.64481607	-7.36958421	0.06489260
H	-3.35617852	-6.42827802	-1.40404371
H	-4.98186252	-6.41857445	-0.63958593
H	-3.85185456	-4.66065504	2.56142208
H	-3.87138187	-6.40018202	2.23462190
H	-5.25099834	-5.38681406	1.73231609
Pu	-1.17449271	-2.69204365	-0.35538059

[$K(C_{24}H_{12})$]

Total energy: -1523.260785 Hartree

K 2.50223501 -2.60353807 1.91615846
C 1.28651404 -2.88879857 -1.06178767
C 2.33877296 -3.73690072 -0.83885431
C 3.27252244 -4.38778540 -0.35213644
C 3.56671083 -0.41881362 0.09951683
C 2.11354853 -0.56474340 -0.08466852
C 1.23299619 -1.54975082 -0.64821535
C 4.90878425 -1.16573670 -0.03568562
C 3.94743216 0.97729073 0.16795051
C 5.31255041 1.13799184 -0.09199788
C 5.88920943 -0.11791514 -0.26157668
C 5.99438105 2.36054417 -0.14058098
C 5.20141346 3.51812869 0.10752632
C 3.83781520 3.39318414 0.35321766
C 3.17288827 2.13118100 0.36515033
C 1.77741954 1.88751941 0.51235148
C 1.32026056 0.62231587 0.27187081
C 4.28373739 -4.66266224 0.54995522
C 5.15525098 -3.66743198 0.94245485
C 5.54739896 -2.42557392 0.20559715
C 6.94463334 -2.54527423 -0.12322936
C 7.79887446 -1.51681324 -0.47793544
C 7.27555658 -0.20887208 -0.46895446
C 7.39755603 2.26081765 -0.42343483

C 8.00087560 1.02832000 -0.58158075
H 0.23634550 0.46901134 0.28297195
H 1.07533996 2.69618247 0.73754796
H 0.36615033 -3.29655380 -1.49558008
H 0.22800057 -1.13715663 -0.78814887
H 5.66355853 4.50969133 0.10119632
H 3.24110913 4.29384597 0.52966031
H 4.38140486 -5.66185865 0.99539901
H 5.90189765 -3.95724555 1.69273324
H 7.36566600 -3.55051433 -0.02477755
H 8.85457024 -1.71574684 -0.68294602
H 7.99886512 3.17174745 -0.50356167
H 9.07600965 0.97896935 -0.78156163

$[K(C_{24}H_{12})]^{+}$
Total energy: -1523.094310 Hartree
K 3.30132701 -1.74653987 2.59961576
C 1.13293624 -2.93142965 -0.86746246
C 1.96967195 -3.64194951 -0.03132092
C 2.89176589 -4.09692997 0.63430151
C 3.55032051 -0.48283383 -0.06264949
C 2.14709043 -0.59045449 -0.38535262
C 1.30130553 -1.59091274 -1.04320627
C 4.91051159 -1.22540104 -0.18402900
C 3.92251540 0.89761623 0.20618554
C 5.29806483 1.07473124 0.05904543
C 5.88363669 -0.15525051 -0.24363749
C 5.96948279 2.29692528 0.12615481
C 5.15234625 3.43401388 0.42643319
C 3.78314286 3.29875745 0.55618873
C 3.12196754 2.03434653 0.39625896
C 1.72965350 1.81387031 0.28892523
C 1.31408444 0.57635892 -0.13983891
C 4.16937131 -4.46937989 1.01796511
C 5.27719685 -3.77272658 0.60857468
C 5.56929050 -2.51092347 -0.06943180
C 6.97088543 -2.55420729 -0.47165484
C 7.79227047 -1.48598708 -0.72282758
C 7.26429286 -0.19478417 -0.49005329
C 7.37285854 2.24666212 -0.15232281
C 7.98478194 1.04441847 -0.45555838
H 0.24635502 0.44274836 -0.33495959
H 1.00494950 2.61751882 0.44632115

H 0.30676344 -3.43682973 -1.37724905
H 0.55114427 -1.12250305 -1.68982004
H 5.61038887 4.42220011 0.52351980
H 3.16999973 4.18422274 0.74626120
H 4.32773366 -5.41581207 1.54686938
H 6.20564236 -4.30069713 0.85231093
H 7.41018918 -3.55388506 -0.52680984
H 8.83496378 -1.64131892 -1.01101574
H 7.96345174 3.16662371 -0.13665745
H 9.05590233 1.02679734 -0.67502953