Supporting Information

Complexation and Redox Chemistry of Neptunium, Plutonium and Americium with a Hydroxylaminato Ligand

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Detailed miniaturization procedure for the synthesis of $[Ce_2(PyNO)_6]$

The photographs and notes that follow demonstrate the level of planning and strategic approach that went into the experimental design and pre-optimization with cerium before attempting americium chemistry with the scare and expensive ^{243}Am isotope.

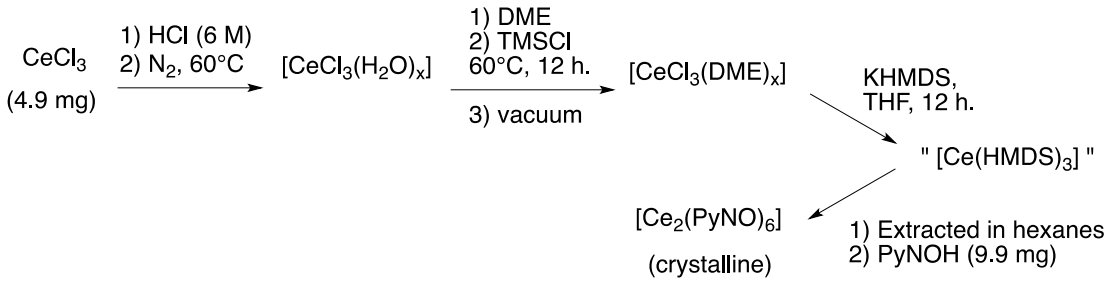


Figure S1. Overview of miniaturized procedure (~5 mg in metal content) developed for the synthesis of $Ce[N(SiMe_3)_2]_3$ and hydroxylaminato complexes from hydrated Ce salts. This protocol was then adopted for the synthesis of **3**, and Am(III)-hydroxylaminato complex. HMDS = $[N(SiMe_3)_2]^{1-}$.

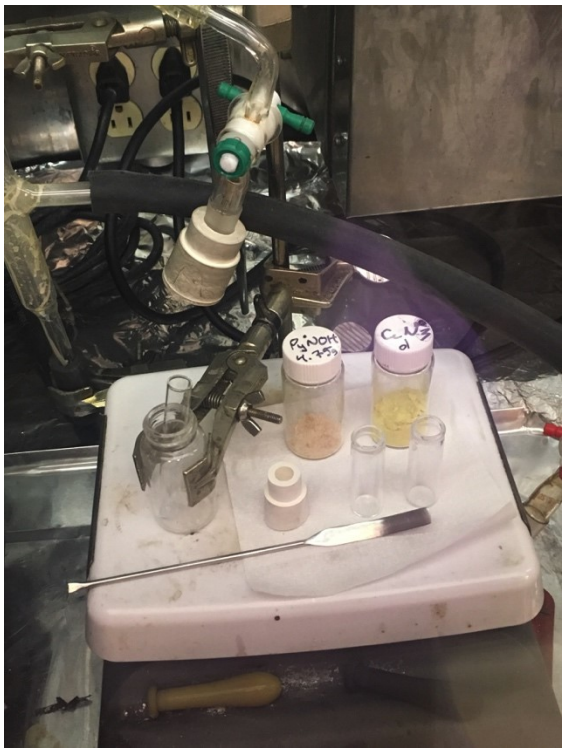


Figure S2.

Glassware:

- A small test tube (Fisher, 10 x 75 mm, #14-961-25)
- A small septum (Kimble, size 14, #774261-0014)
- Two small vials

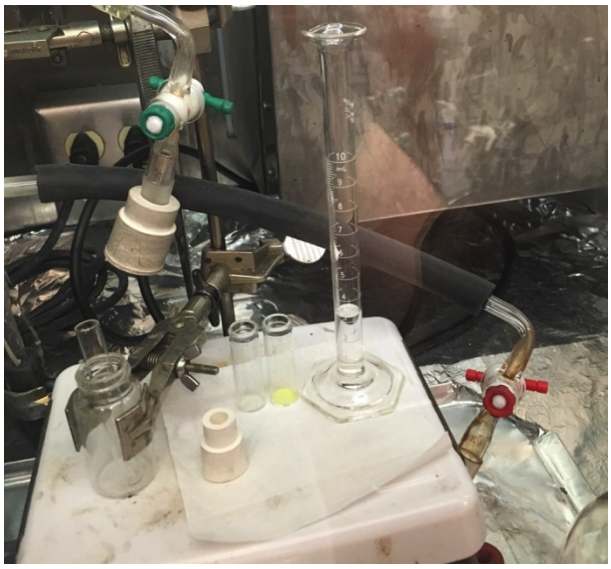


Figure S3.

PyNOH (7.1 mg, 42.7 µmol, 3 equiv.) and $Ce[N(SiMe_3)_2]_3.(Toluene)_{0.25}$ (9.2 mg, 14.3 µmol, 1 equiv.) were weighted into two separate vials.

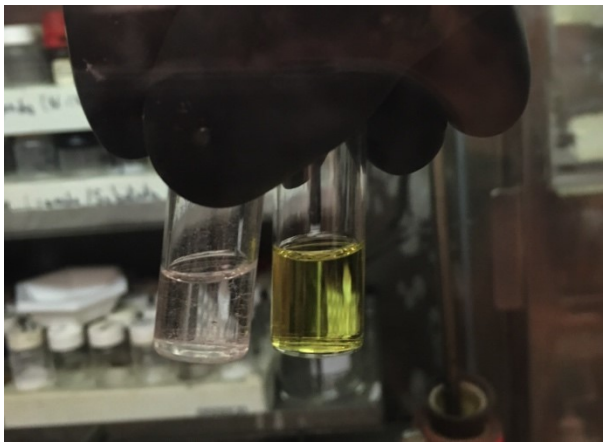
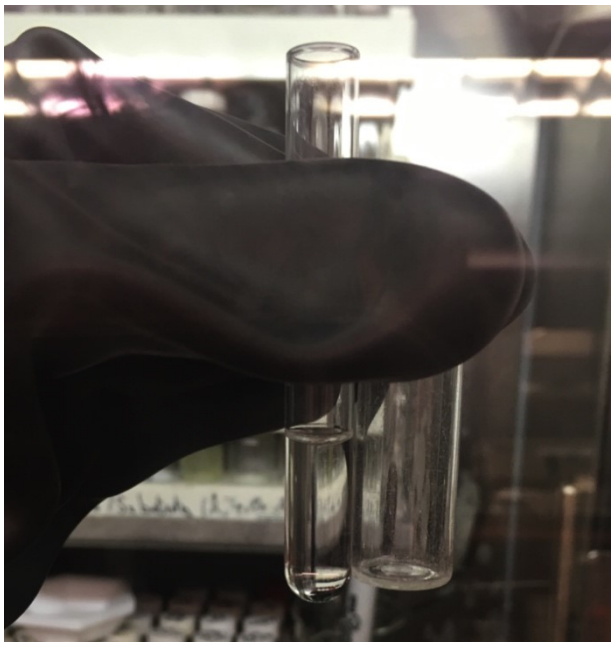


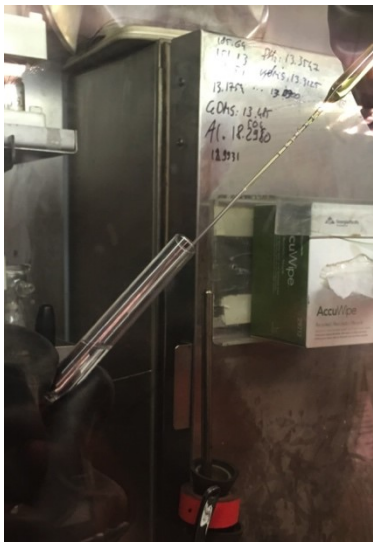
Figure S4.

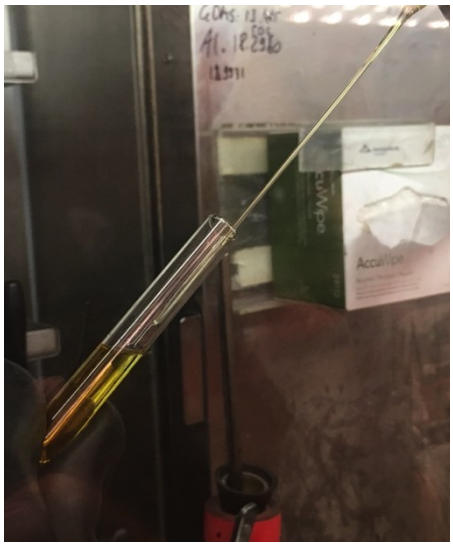
Both solids were dissolved in 1.5 mL of hexanes. Solutions were mixed with a pipette to produce clear solutions.



Figures S5-S8.

The solution of **PyNOH** was added in the test tube.





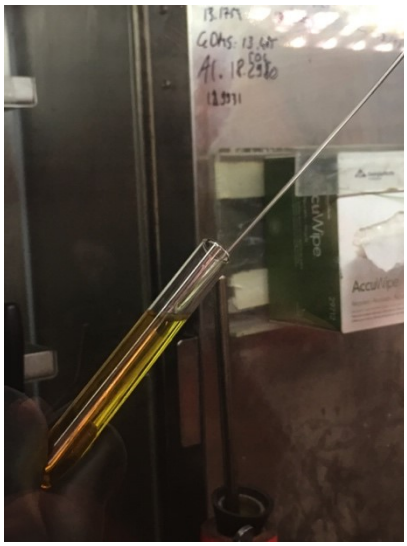
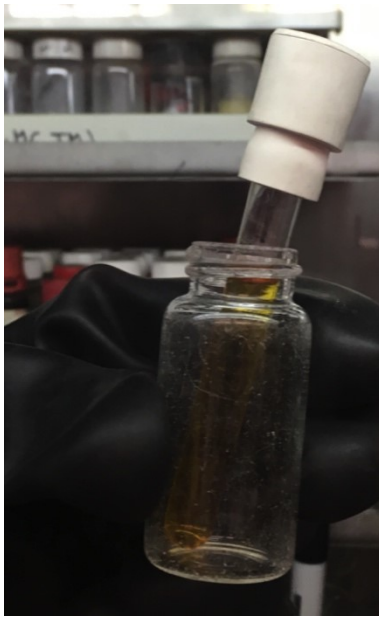
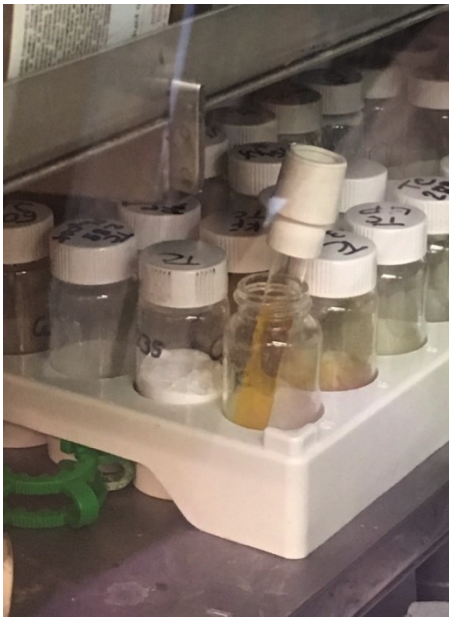


Figure S9.

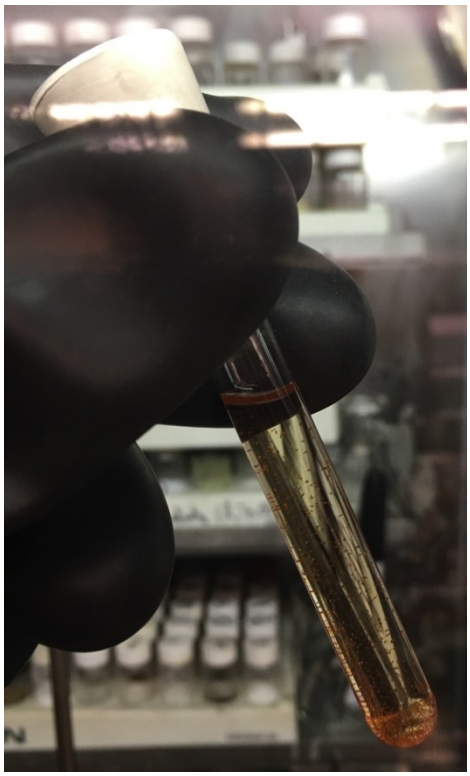
The solution of $Ce[N(SiMe_3)_2]_3$ was gently added on the top of the **PyNOH** solution leading to a clear solution.
A more careful layering can be achieved if necessary but is not required in this range of concentrations.

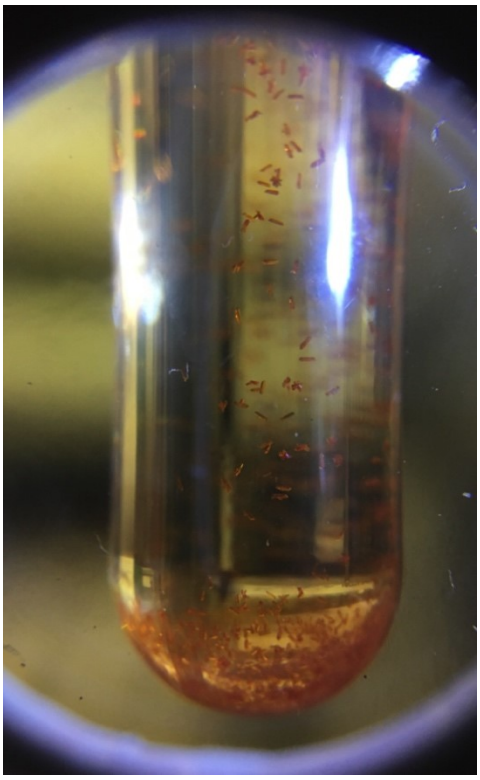




Figures S10-S11.

The test tube was capped with the septum and set undisturbed for 4 hours. Crystal seeds can be observed after one hour.



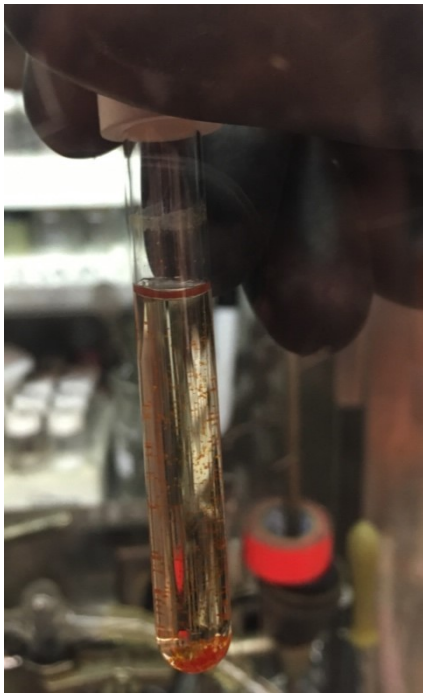


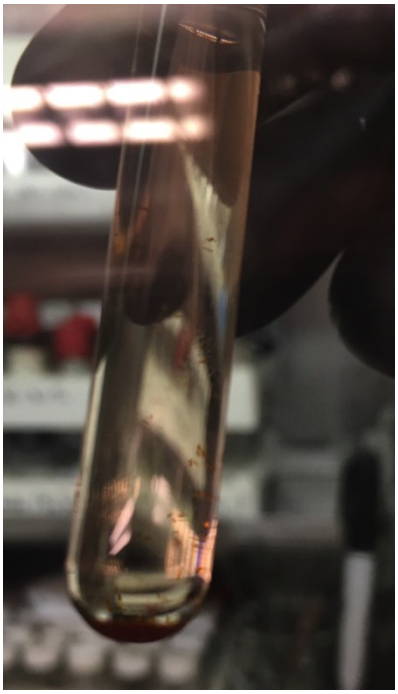
Figures S12-S13.

After 4 hours of standing, X-ray quality crystals have formed.

Figure S14.

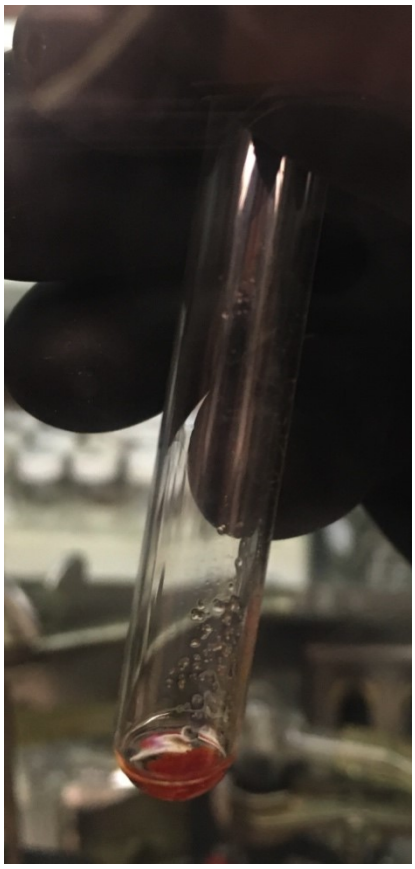
To stimulate the crystallization, the tube was placed in a freezer (- 25°C) for 5 hours.

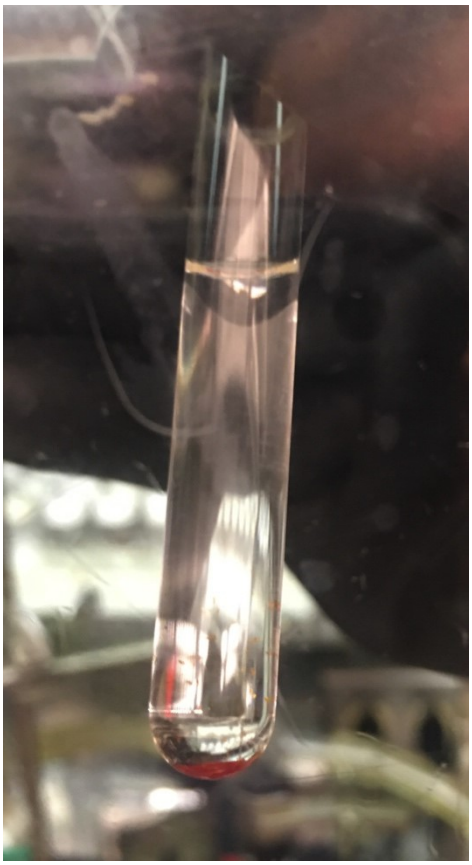




Figures S15-S16.

After 5 hours at -25°C, red crystals of **1** and a slightly yellow solution were obtained. The tube was gently shaken and tapped to detach the crystals from the walls and allowed them to fall by gravity.





Figures S17-S18.

The supernatant was carefully removed with a pipette.

The crystals were suspended in 2.5 mL of pentane, allowed to decant by gravity and the supernatant removed carefully with a pipette. This operation was repeated four times (4 x 2.5 mL).

Figures S19-S20.

Suspending the red crystals of **1** in several portions of pentane, the crystals were transferred to a (pre-weighted) small filter. The crystals were washed with 4 x 3 mL of pentane.

Crystals of **1** were dried on vacuum for 30 min directly on the filter.

Figure S21.

8.2 mg (6.4 µmol, MW = 1271.50 $g.mol^{-1}$) of crystalline **1** were collected (90 % yield).

Notes: If crystals are too small, the overall amount of hexanes can be increased to 4 mL and the reaction times extended to 6 hours for the crystals seeding and overnight refrigeration for the crystals growing. If powdered material is obtained, a more careful layering can be applied, by introducing a "buffer" layer of hexane between the two solutions. Alternatively, the layering can be facilitated in a NMR tube.

Photographs of americium hydroxylaminato complex synthesis, **3**

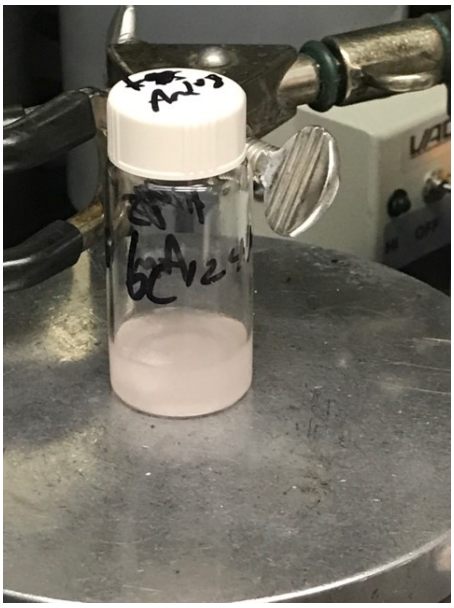


Figure S22. Putative '$AmCl_3$' residue (from an aqueous 6 M HCl stock solution that was blown to dryness and pumped *in vacuo* into a helium atmosphere drybox) suspended in DME and treated with TMS-Cl to remove scavenge residual water content.

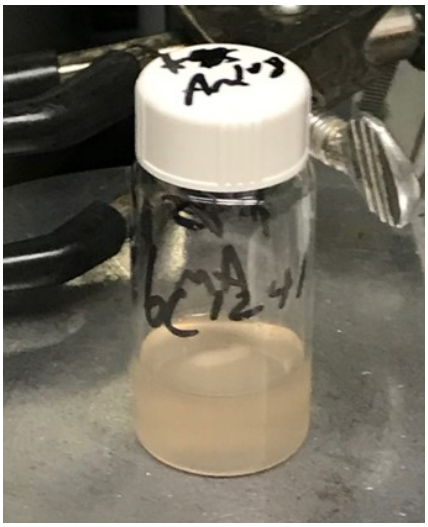


Figure S23. Following addition of $K[N(SiMe_3)_2]$ and stirring at ambient temperature overnight – a distinct color change from pale pink to peach is observed.

Figure S24. Reaction mixture, presumed to contain the intended $Am[N(SiMe_3)_2]_3$ intermediate, with volatiles removed *in vacuo*.

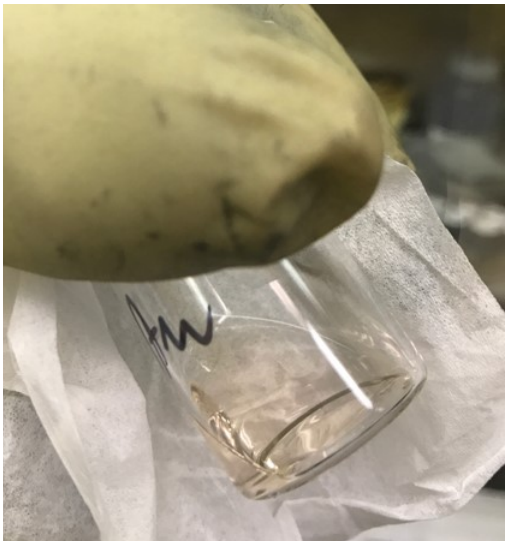


Figure S25. The putative $Am[N(SiMe_3)_2]_3$ intermediate extracted into hexanes, after filtration. This is good indicator that the reaction proceeded as planned because '$AmCl_3(DME)x$' would not be expected to exhibit appreciable solubility in hexanes.

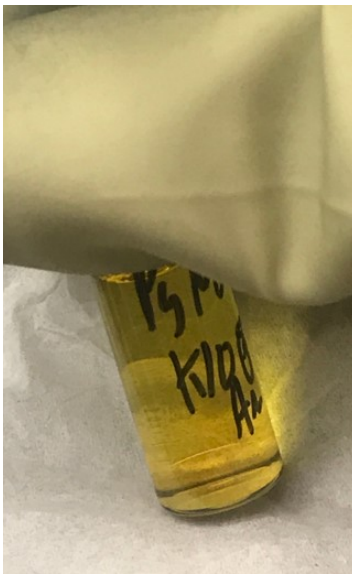


Figure S26. Reaction solution immediately after filtration of 2-(^{t}BuNOH)py in Et_2O onto a solution of the $Am[N(SiMe_3)_2]_3$ intermediate in Et_2O – the color change to yellow is very apparent.

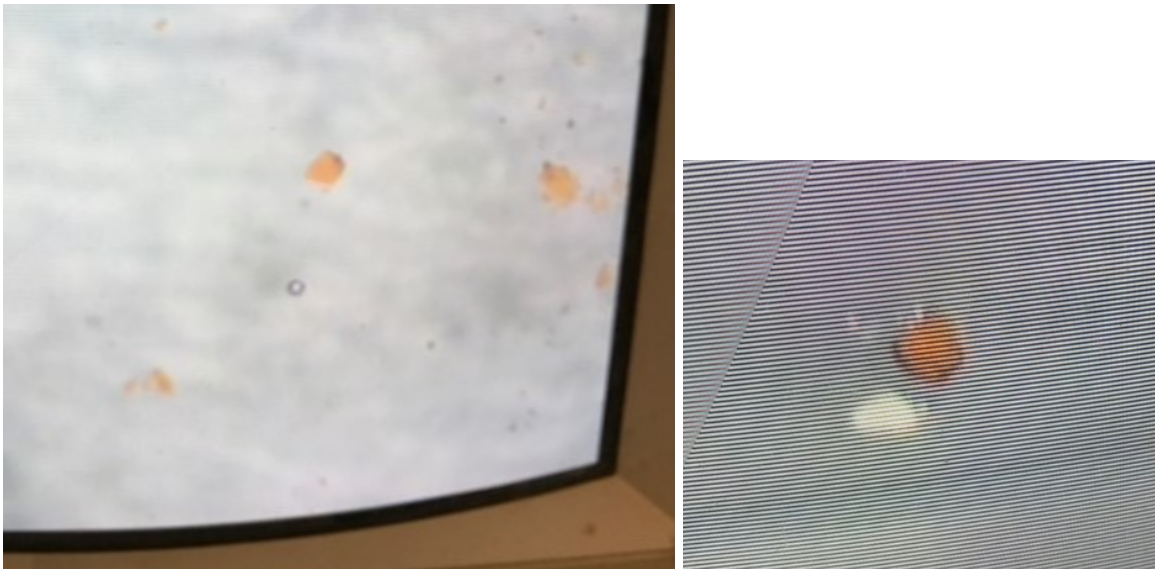


Figure S27. Small orange-yellow (amber) crystals that deposited from the solution, and were used for X-ray diffraction structural determination.

Crystallographic Data

Table S1. Crystallographic Data for **1** and **3**.

Compound	**1**	**3**
Empirical Formula	$C_{36}H_{52}N_8O_4Pu$	$C_{54}H_{78}Am_2N_{12}O_6$
Formula Weight	899.86	1477.40
Temperature (K)	100(1)	100(1)
Crystal System	Monoclinic	Monoclinic
Space Group	*I*2/*c*	$P2_1/n$
***a* (Å)**	17.550(4)	12.9096(17)
***b* (Å)**	10.078(2)	16.627(2)
***c* (Å)**	21.290(5)	13.5557(18)
α (deg)	90	90
β (deg)	98.496(16)	101.1463(16)
γ (deg)	90	90
Volume (Å^3)	3724.2(14)	2854.8(7)
Z	4	2
ρ_{calcd} (Mg/m^3)	1.610	1.714
μ (mm^{-1})	1.819	2.725
R1[a] ($I > 2.0\sigma(I)$)	0.0344	0.0324
wR2 (I>2σ(I))	0.0709	0.0611

[a] Definitions: $R1 = \Sigma||F_o| - |F_c||/ \Sigma |F_o|$, $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/ \Sigma w(F_o^2)^2]^{1/2}$.

NMR spectra

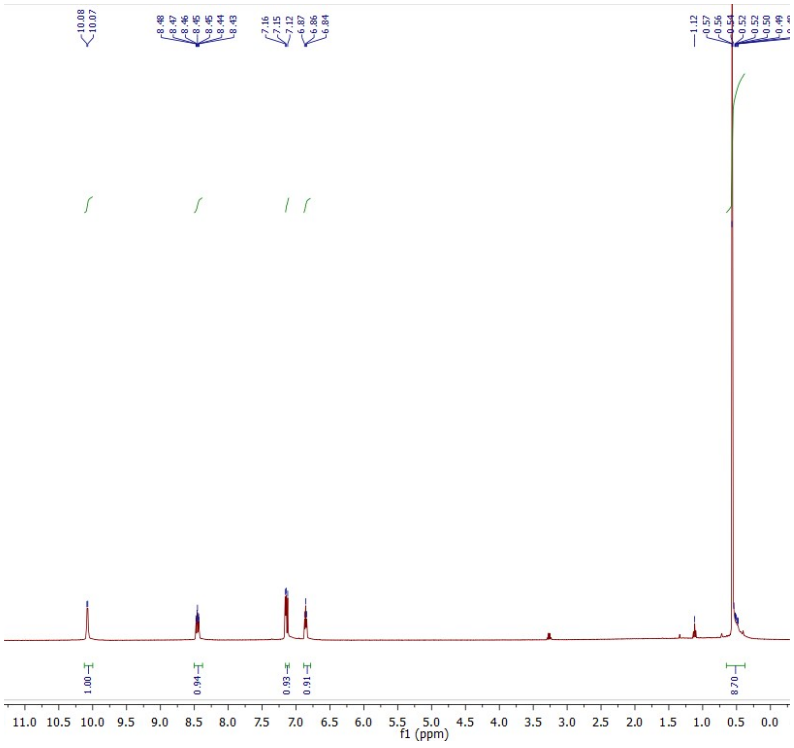


Figure S28. ^{1}H NMR spectra of **1** in C_6D_6 solution.

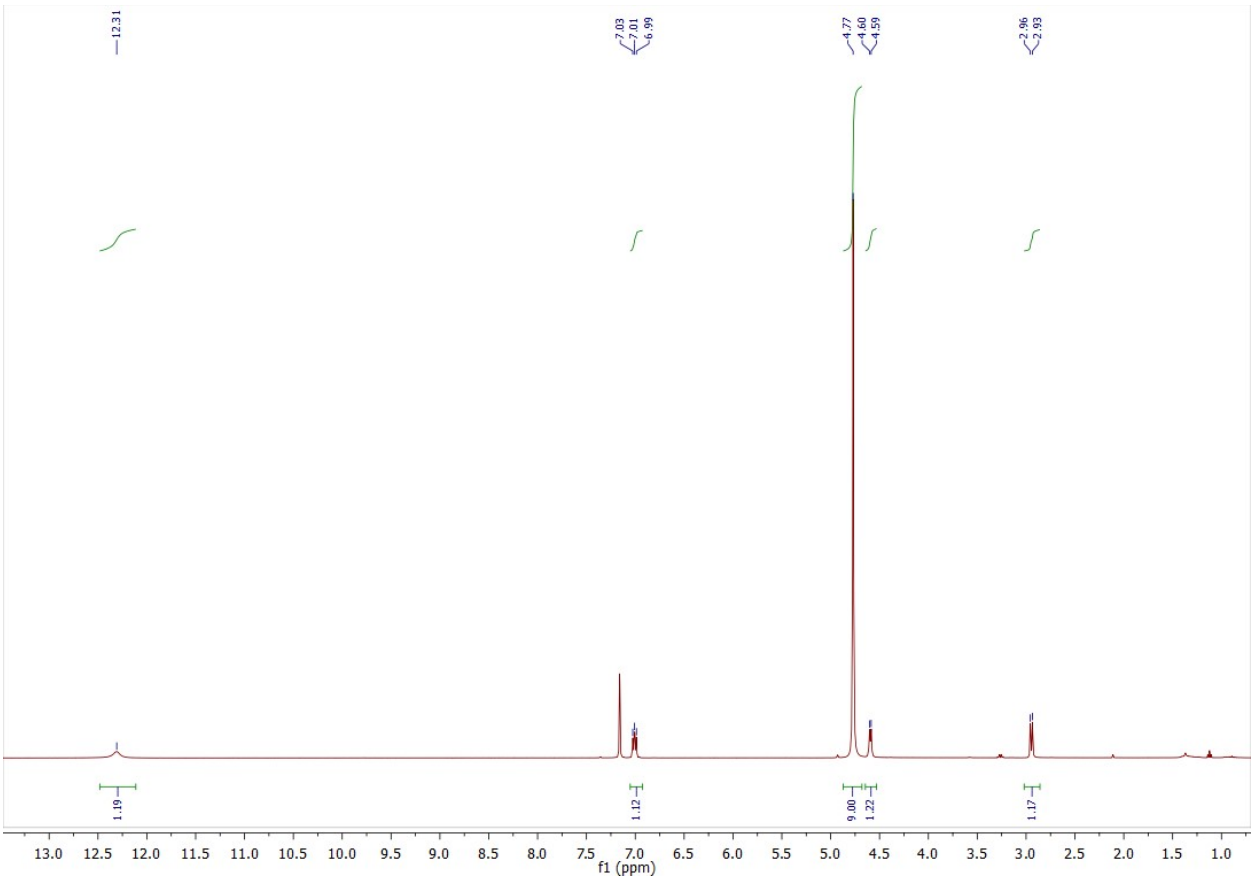


Figure S29. ^{1}H NMR spectra of **2** in C_6D_6 solution.

UV-Vis-NIR spectra

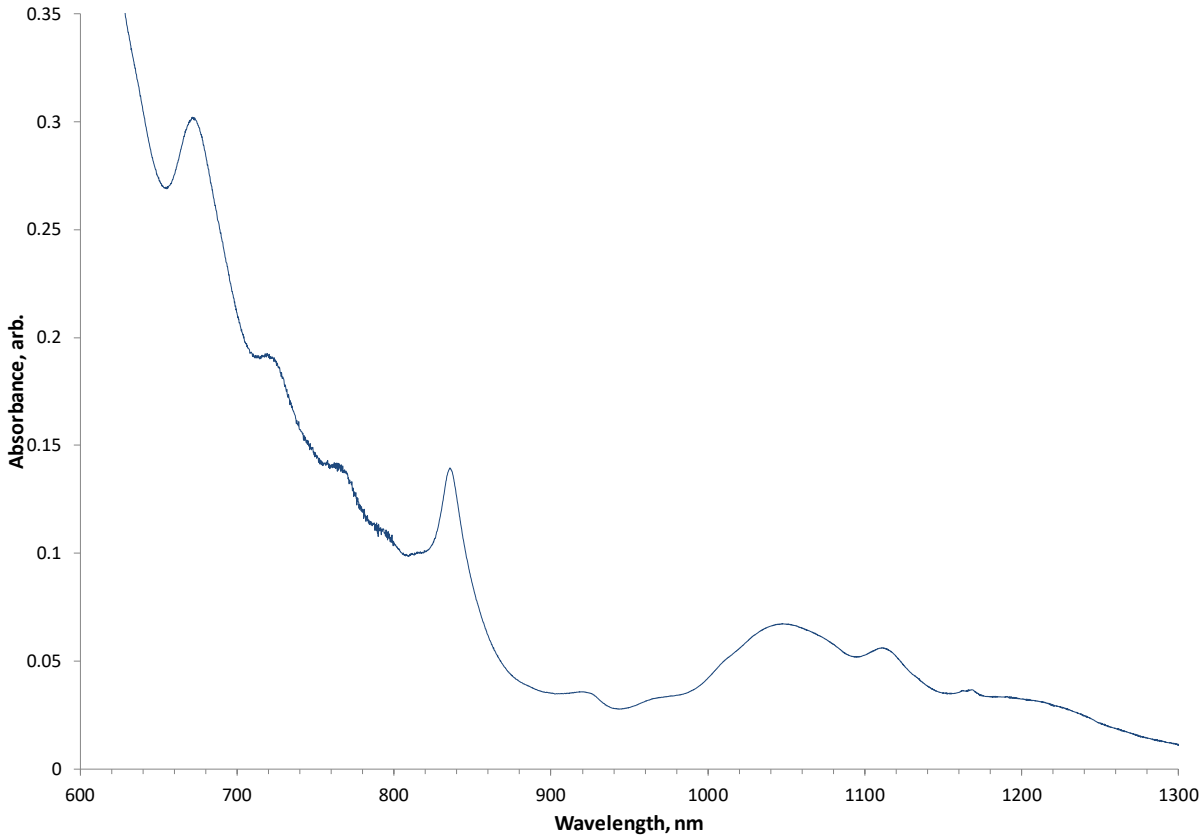


Figure S30. Vis-NIR spectrum of **1** dissolved in THF.

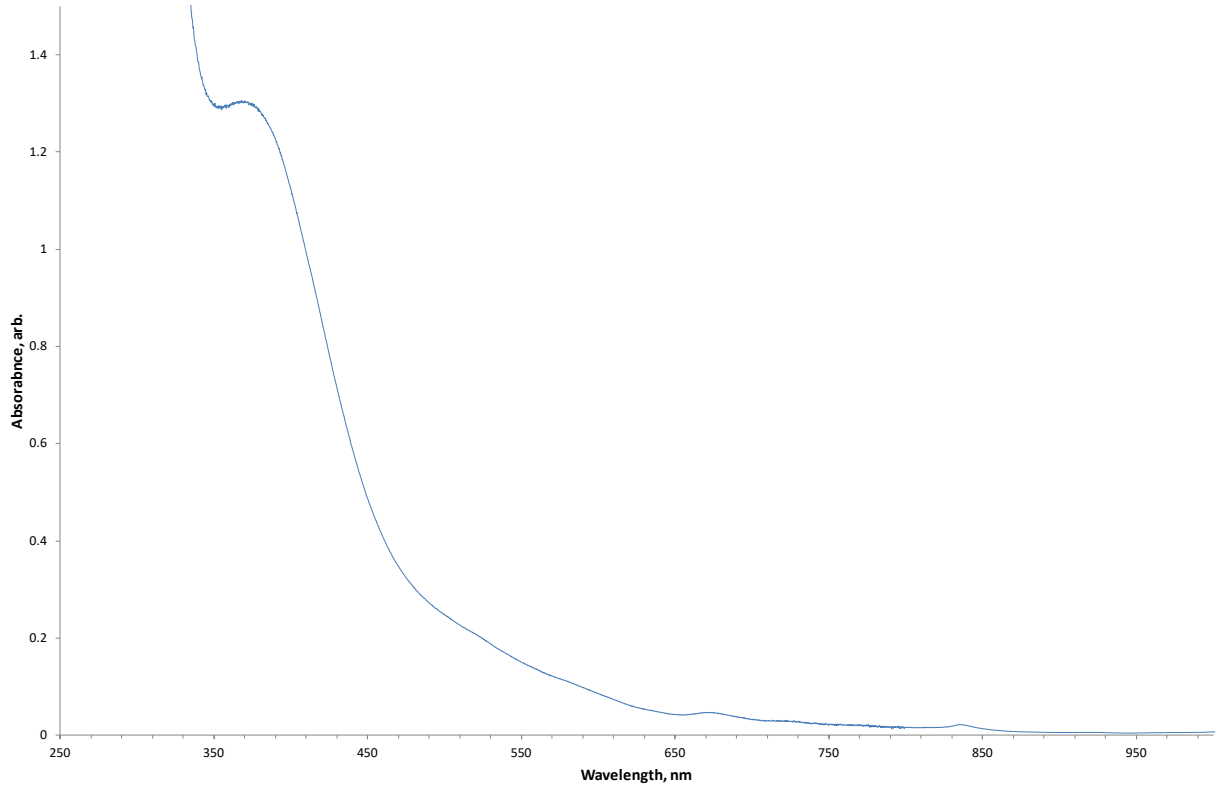


Figure S31. UV-Vis-NIR spectrum of **1** dissolved in THF, diluted to observe maxima of intense band in the UV region.

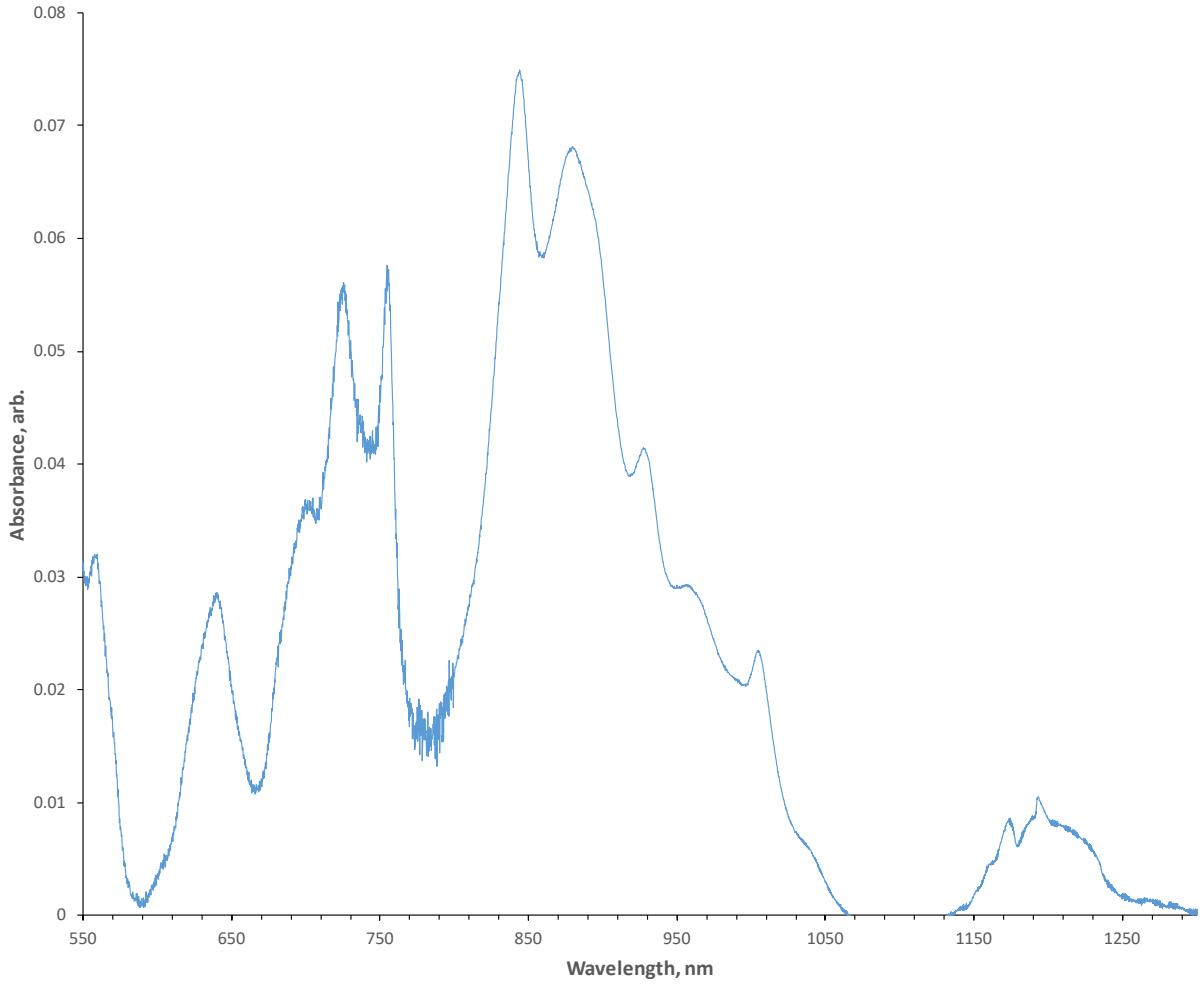


Figure S32 Vis-NIR spectrum of **2** dissolved in THF.

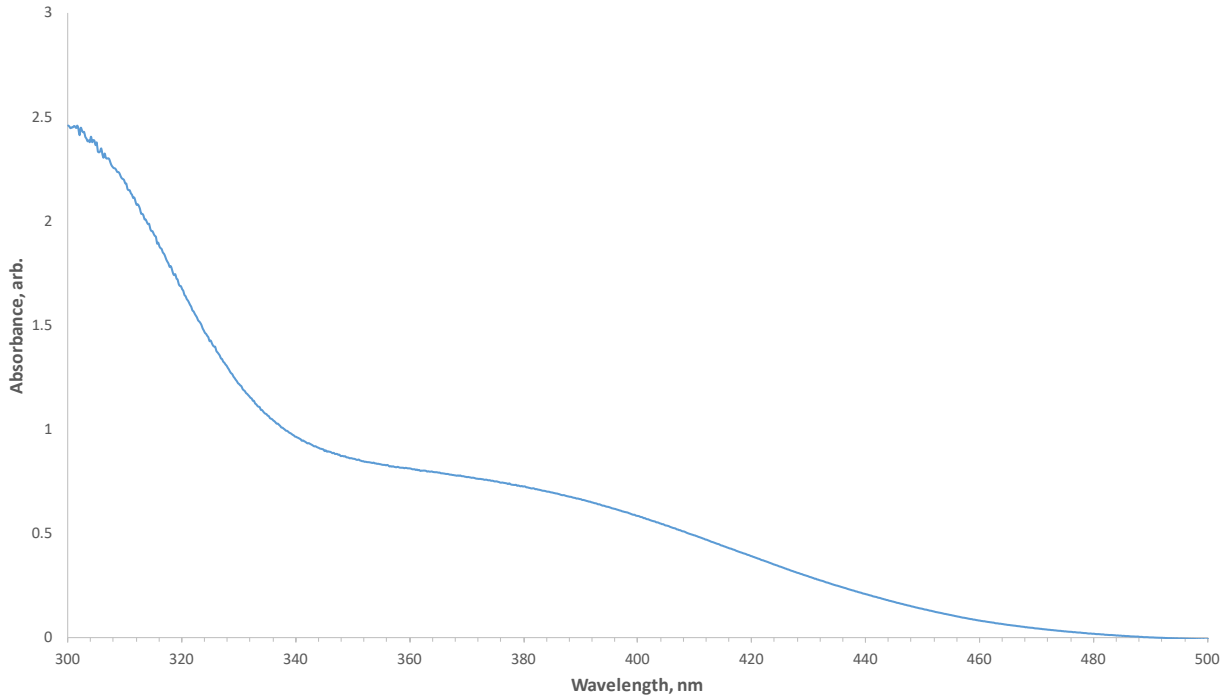
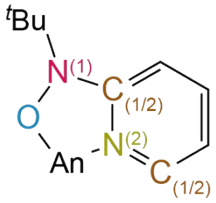


Figure S33. UV-Vis-NIR spectrum of **2** dissolved in THF, diluted to observe maxima of intense band in the UV region.

Additional computational data

Table S2. Experimental and optimized average An–O, An–N and An-C distances in Å for An[(^{t}BuNO)py]$_4^{0/-}$ (An=Np, Pu). The N1, N2, and C1/C2 atoms correspond to those shown in the illustration below.

	An-O			An-N1			An-N2			An-C1/C2		
	Calc.	XRD	EXAFS	Calc.	XRD	EXAFS	Calc.	XRD	EXAFS	Calc.	XRD	EXAFS
Pu^{IV}	2.296	2.231(4)	2.239(4)	2.546	2.500(2)	2.496(5)	3.313	3.253(4)	3.29(2)	3.430 /3.450	3.370(4) /3.436(4)	3.41(3)
Np^{IV}	2.245		2.245(9)	2.576		2.528(14)	3.297		3.30(3)	3.436 /3.499		3.45(3)
Pu^{III}	2.384			2.557			3.365			3.445 /3.464		
Np^{III}	2.356			2.558			3.355			3.453 /3.462		



An illustration showing how the nomenclature in Table S2 (regarding N1, N2, and C1/C2) correspond with atoms associated with structures from **1** and **2**.

Table S3. Optimized Am–O and Am–N bond lengths in Å of Am[(^{t}BuNO)py]$_4$ and [Am^{III}(μ_2-(^{t}BuNO)py)(2-(^{t}BuNO)py)$_2$]$_2$, and comparison with experimental values.

	Terminal An-O			Bridging An-O			Terminal An-N			Bridging An-N[a]	
	Calc.	Expt.		Calc.	Expt.		Calc.	Expt.		Calc.	Expt.
Am[(^{t}BuNO)py]$_4^-$	2.393						2.590				
[Am^{III}(μ_2-(^{t}BuNO)py)(2-(^{t}BuNO)py)$_2$]$_2$	2.329	2.297		2.430	2.416		2.544	2549		2.673 2.805	2.634 2.641

[a] The shorter and longer bridging An-N distances represent for the Am–$N_{(py)}$ and Am–$N_{(tBu)}$ modees, respectively.

Table S4. Optimized An–O and An–N bond lengths in Å of Np[(^{t}BuNO)py]$_4^{+/0/-}$, Pu[(^{t}BuNO)py]$_4^{+/0/-}$, Am[(^{t}BuNO)py]$_4^{0/-}$, and [Am^{III}(μ_2-(^{t}BuNO)py)(2-(^{t}BuNO)py)$_2$]$_2$ complexes. The average values are in parentheses.

An	An-O	An-N
	An[(^{t}BuNO)py]$_4^+$	
Np	2.191, 2.191, 2.191, 2.191 (2.191)	2.553, 2.553, 2.553, 2.553 (2.553)
Pu	2.196, 2.196, 2.293, 2.293 (2.245)	2.543, 2.543, 2.568, 2.568 (2.556)
	An[(^{t}BuNO)py]$_4$	
Np	2.245, 2.245, 2.245, 2.245 (2.245)	2.576, 2.576, 2.576, 2.576 (2.576)
Pu	2.296, 2.296, 2.296, 2.296 (2.296)	2.546, 2.546, 2.546, 2.546 (2.546)
Am	2.327, 2.327, 2.327, 2.327 (2.327)	2.581, 2.581, 2.581, 2.581 (2.581)
	An[(^{t}BuNO)py]$_4^-$	
Np	2.356, 2.356, 2.356, 2.356 (2.356)	2.558, 2.558, 2.558, 2.558 (2.558)
Pu	2.384, 2.384, 2.385, 2.385 (2.384)	2.557, 2.557, 2.557, 2.557 (2.557)
Am	2.393, 2.393, 2.393, 2.393 (2.393)	2.590, 2.590, 2.590, 2.590 (2.590)
	[An(μ_2-(^{t}BuNO)py)(2-(^{t}BuNO)py)$_2$]$_2$	
Am	2.299, 2.359, 2.409, 2.452	2.529, 2.558, 2.673, 2.805
	2.299, 2.359, 2.409, 2.451	2.529, 2.558, 2.673, 2.805

Table S5. Calculated absolute redox potentials in V of the redox couples in THF at the scalar relativistic level (E_{SR}) and at the spin-orbit relativistic level (E_{so}), respectively, and spin-orbit coupling correction ($\Delta E_{SO}=E_{SO}-E_{SR}$). The E_{SR} for $Fc^{+} \rightarrow Fc^{0}$ is calculated to be −5.436 V, and SO correction is neglected for these light transition metal compounds.[a]

	E_{SR} (V)	E_{so} (V)	ΔE_{SO} (V)
$Np[(^{t}BuNO)py]_4^{0} \rightarrow Np[(^{t}BuNO)py]_4^{-}$	–2.217	–2.151	0.056
$Pu[(^{t}BuNO)py]_4^{0} \rightarrow Pu[(^{t}BuNO)py]_4^{-}$	–2.936	–2.755	0.181
$Am[(^{t}BuNO)py]_4^{0} \rightarrow Am[(^{t}BuNO)py]_4^{-}$	–3.559	-	-
$Np[(^{t}BuNO)py]_4^{+} \rightarrow Np[(^{t}BuNO)py]_4^{0}$	–4.749	-	-
$Pu[(^{t}BuNO)py]_4^{+} \rightarrow Pu[(^{t}BuNO)py]_4^{0}$	–4.701	-	-

[a] SO correction is neglected for $Am[(^{t}BuNO)py]_4^{0} \rightarrow Am[(^{t}BuNO)py]_4^{-}$ and $An[(^{t}BuNO)py]_4^{+} \rightarrow An[(^{t}BuNO)py]_4^{0}$ (An=Np, Pu), because the electron is removed from ligand without change on the oxidation state of An center in the reduction reaction.

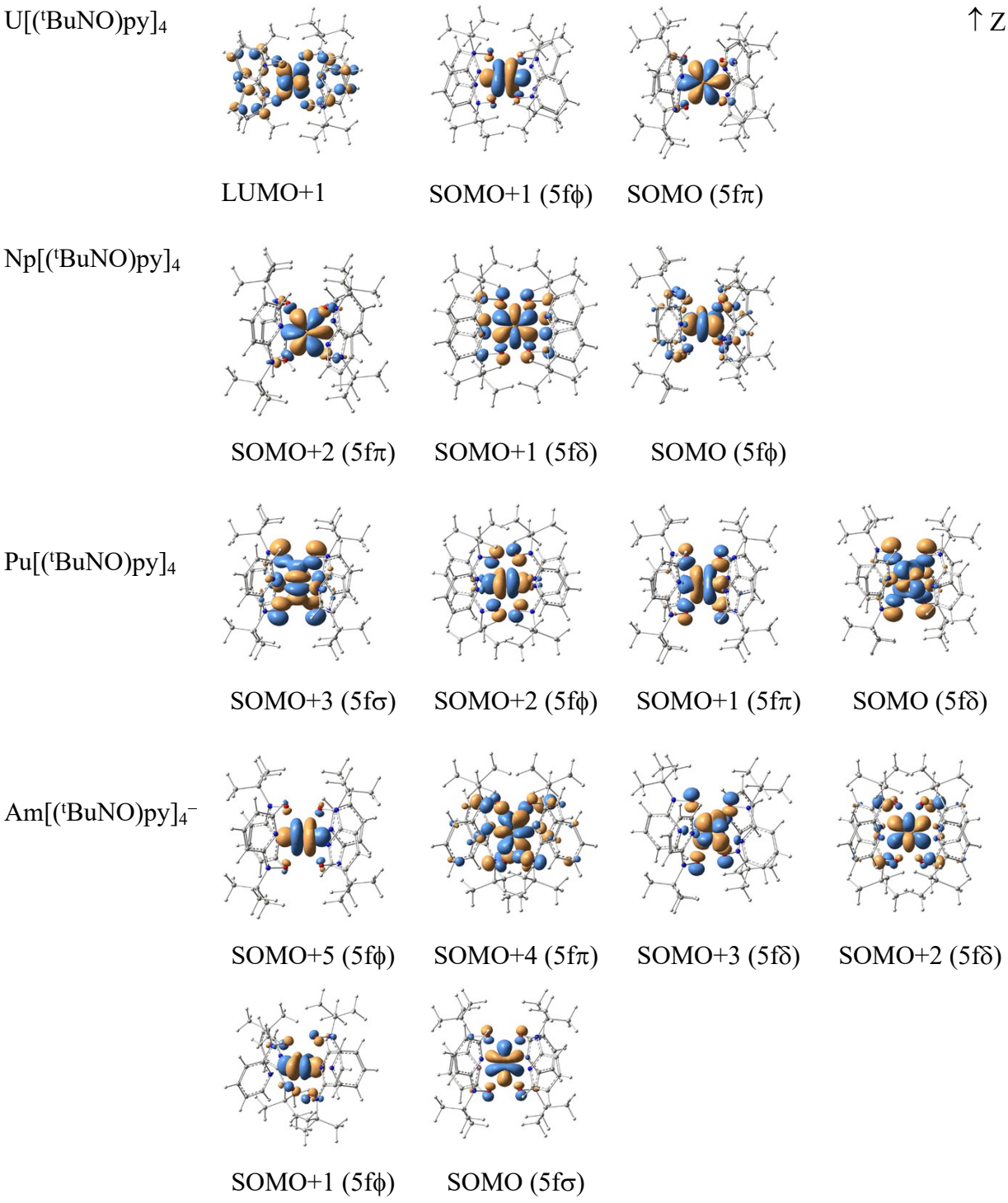


Figure S34. SOMOs in An[(ᵗBuNO)py]$_4$ (An=U, Np, Pu) and Am[(ᵗBuNO)py]$_4^-$ complexes and LUMO+1 in U[(ᵗBuNO)py]$_4$ with dominant 5f character in parentheses. The Z direction is labeled with an arrow.

Table S6. Cartesian coordinates (in Å) of optimized geometries of $Np[(^tBuNO)py]_4^{+/0/-}$, $Pu[(^tBuNO)py]_4^{+/0/-}$, $Am[(^tBuNO)py]_4^{0/-}$, and $[Am^{III}(\mu_2\text{-}(^tBuNO)py)(2\text{-}(^tBuNO)py)_2]_2$ complexes.

$Np[(^tBuNO)py]_4^-$				$Np[(^tBuNO)py]_4^0$			
O	0.81639100	1.09003500	1.92226200	O	0.86214600	1.24288800	1.65891100
O	0.81835300	-1.08843300	-1.92221800	O	0.86423100	-1.24144600	-1.65899400
O	-0.81636800	-1.09001400	1.92227500	O	-0.86214400	-1.24289000	1.65891000
O	-0.81834700	1.08843800	-1.92221700	O	-0.86423000	1.24144700	-1.65899200
N	1.79606400	2.04204800	1.96490200	N	2.01198900	1.98901500	1.69338700
N	1.93449600	1.64791700	-0.29078900	N	2.04775800	1.46597000	-0.54364600
N	1.79966400	-2.03875000	-1.96493500	N	2.01528500	-1.98571500	-1.69343200
N	1.93675700	-1.64525100	0.29094600	N	2.05004900	-1.46271800	0.54363300
N	-1.79603800	-2.04202900	1.96492300	N	-2.01198800	-1.98901500	1.69338600
N	-1.93447700	-1.64791200	-0.29077100	N	-2.04775600	-1.46596900	-0.54364700
N	-1.79966300	2.03875000	-1.96493400	N	-2.01528500	1.98571400	-1.69343100
N	-1.93674300	1.64526300	0.29095000	N	-2.05004700	1.46271700	0.54363400
C	2.42494600	2.33919500	0.79660300	C	2.61807900	2.17168300	0.48445700
C	2.48080800	1.87111500	-1.50643100	C	2.57718400	1.56066800	-1.77996000
C	3.51871600	2.76359800	-1.74686400	C	3.67729600	2.34699500	-2.09537800
C	4.03361300	3.46884400	-0.63849800	C	4.26695700	3.07795900	-1.04583100
C	3.50169000	3.26490200	0.62666900	C	3.75323500	3.00089900	0.23719100
C	2.06053200	2.64648700	3.30551600	C	2.26869600	2.73914500	2.96627900
C	3.48597300	2.29025400	3.78180000	C	3.68999900	2.43152800	3.48166700
C	1.82289500	4.17196100	3.26778300	C	2.03685700	4.24996800	2.75751800
C	1.06082600	2.04569200	4.30828000	C	1.27022800	2.24101300	4.02461700
C	2.42859500	-2.33539700	-0.79653500	C	2.62156000	-2.16748500	-0.48445600
C	2.48305400	-1.86802300	1.50667300	C	2.57952700	-1.55663500	1.77998400
C	3.52225100	-2.75900300	1.74710900	C	3.68084900	-2.34124600	2.09545400
C	4.03852100	-3.46312300	0.63866300	C	4.27174100	-3.07123600	1.04592100
C	3.50665600	-3.25956600	-0.62659000	C	3.75799900	-2.99492500	-0.23713800
C	2.06534200	-2.64246600	-3.30563900	C	2.27321800	-2.73545500	-2.96630800
C	1.06518400	-2.04269600	-4.30856700	C	1.27404700	-2.23885700	-4.02470600
C	1.82970900	-4.16826400	-3.26839900	C	2.04369500	-4.24663200	-2.75755800
C	3.49046700	-2.28423500	-3.78136200	C	3.69407500	-2.42565000	-3.48161400
C	-2.42492000	-2.33918300	0.79662700	C	-2.61807800	-2.17168200	0.48445600
C	-2.48079700	-1.87112200	-1.50640700	C	-2.57718200	-1.56066800	-1.77996100
C	-3.51870600	-2.76360900	-1.74682200	C	-3.67729500	-2.34699400	-2.09538000
C	-4.03359500	-3.46884700	-0.63844600	C	-4.26695600	-3.07795800	-1.04583200
C	-3.50166200	-3.26489200	0.62671500	C	-3.75323500	-3.00089800	0.23719000
C	-2.06052600	-2.64648300	3.30552800	C	-2.26869700	-2.73914300	2.96627900
C	-3.48599400	-2.29028400	3.78175300	C	-3.68999900	-2.43152100	3.48166800
C	-1.82288700	-4.17195400	3.26776400	C	-2.03686400	-4.24996700	2.75751800
C	-1.06086700	-2.04570500	4.30835300	C	-1.27022500	-2.24101600	4.02461500

C	-2.42858700	2.33540200	-0.79653200	C	-2.62156000	2.16748400	-0.48445500
C	-2.48303000	1.86804400	1.50667900	C	-2.57952500	1.55663500	1.77998500
C	-3.52222300	2.75902800	1.74711600	C	-3.68084700	2.34124500	2.09545600
C	-4.03849700	3.46314500	0.63867000	C	-4.27174000	3.07123500	1.04592300
C	-3.50664100	3.25957900	-0.62658500	C	-3.75799900	2.99492300	-0.23713600
C	-2.06535200	2.64246100	-3.30563800	C	-2.27321900	2.73545300	-2.96630700
C	-1.06515100	2.04274900	-4.30855800	C	-1.27404300	2.23886100	-4.02470300
C	-1.82979800	4.16827000	-3.26837900	C	-2.04370400	4.24663100	-2.75755600
C	-3.49045400	2.28416400	-3.78138300	C	-3.69407300	2.42564100	-3.48161700
H	2.03199400	1.27572400	-2.30854200	H	2.06507700	0.95958400	-2.53727300
H	3.91713400	2.89853100	-2.75521500	H	4.06033400	2.39009300	-3.11644300
H	4.85942000	4.17763800	-0.76297600	H	5.13558500	3.71596300	-1.23451100
H	3.92086400	3.80732600	1.47254100	H	4.21898100	3.57456900	1.03520900
H	3.60233800	1.19619800	3.81302400	H	3.81252400	1.34766700	3.62636700
H	3.66214900	2.68621700	4.79624100	H	3.84902500	2.92855600	4.45164600
H	4.27102600	2.68692100	3.12388900	H	4.48685700	2.76658400	2.80554800
H	2.48804800	4.69817400	2.57070300	H	2.72136800	4.69219800	2.02077600
H	1.97414700	4.60464900	4.27107800	H	2.17400300	4.78974900	3.70799000
H	0.78715000	4.37589500	2.95692700	H	1.00798200	4.42591600	2.40919900
H	0.02617900	2.26384400	4.01489100	H	0.23387100	2.44352100	3.72797600
H	1.25621100	2.48723100	5.30028300	H	1.47898200	2.76541800	4.97023900
H	1.16070700	0.95532600	4.37015100	H	1.36701800	1.16024200	4.19517900
H	2.03309600	-1.27360500	2.30886400	H	2.06641300	-0.95639700	2.53728600
H	3.92058700	-2.89366000	2.75552900	H	4.06387300	-2.38378700	3.11654700
H	4.86533600	-4.17073800	0.76315400	H	5.14135600	-3.70788300	1.23464200
H	3.92685200	-3.80112000	-1.47251400	H	4.22470800	-3.56782300	-1.03514700
H	0.03072500	-2.26225400	-4.01557200	H	0.23798400	-2.44294700	-3.72812600
H	1.26147100	-2.48370800	-5.30062600	H	1.48365900	-2.76294400	-4.97031500
H	1.16366600	-0.95218300	-4.37011900	H	1.36919500	-1.15794000	-4.19526900
H	2.49533800	-4.69377100	-2.57123800	H	2.72886500	-4.68781200	-2.02079700
H	1.98185800	-4.60048900	-4.27175800	H	2.18170100	-4.78619900	-3.70802700
H	0.79413500	-4.37365100	-2.95792900	H	1.01508000	-4.42416400	-2.40927300
H	3.60542000	-1.19001900	-3.81223600	H	3.81495000	-1.34159700	-3.62626800
H	3.66747200	-2.67967700	-4.79586100	H	3.85390500	-2.92239700	-4.45160500
H	4.27583500	-2.68006500	-3.12332500	H	4.49141300	-2.75951600	-2.80547300
H	-2.03199100	-1.27573700	-2.30852700	H	-2.06507500	-0.95958400	-2.53727400
H	-3.91713200	-2.89855200	-2.75516900	H	-4.06033200	-2.39009100	-3.11644500
H	-4.85940200	-4.17764300	-0.76291100	H	-5.13558500	-3.71596100	-1.23451300
H	-3.92082600	-3.80730600	1.47260000	H	-4.21898100	-3.57456800	1.03520800
H	-3.60238100	-1.19623000	3.81299100	H	-3.81251800	-1.34765900	3.62636800
H	-3.66220900	-2.68626900	4.79617800	H	-3.84902500	-2.92854800	4.45164800
H	-4.27100700	-2.68695600	3.12379600	H	-4.48685900	-2.76657400	2.80555100
H	-2.48802100	-4.69814700	2.57065000	H	-2.72137800	-4.69219600	2.02077700
H	-1.97417000	-4.60466700	4.27104300	H	-2.17401000	-4.78974800	3.70799000
H	-0.78713300	-4.37587800	2.95693300	H	-1.00799000	-4.42592000	2.40919700
H	-0.02620500	-2.26384100	4.01500500	H	-0.23387000	-2.44352800	3.72797300

H	-1.25629100	-2.48727300	5.30033600	H	-1.47898100	-2.76541900	4.97023800
H	-1.16075800	-0.95534100	4.37025000	H	-1.36701200	-1.16024400	4.19517700
H	-2.03306700	1.27363100	2.30887000	H	-2.06641100	0.95639600	2.53728700
H	-3.92055100	2.89369300	2.75553800	H	-4.06387100	2.38378600	3.11654900
H	-4.86530700	4.17076500	0.76316200	H	-5.14135400	3.70788200	1.23464500
H	-3.92683600	3.80113300	-1.47250900	H	-4.22470800	3.56782300	-1.03514400
H	-0.03070700	2.26235600	-4.01554700	H	-0.23798200	2.44295600	-3.72812000
H	-1.26144700	2.48375900	-5.30061600	H	-1.48365500	2.76294700	-4.97031200
H	-1.16357800	0.95223100	-4.37011900	H	-1.36918500	1.15794300	-4.19526700
H	-2.49546300	4.69373300	-2.57121800	H	-2.72887800	4.68780800	-2.02079700
H	-1.98195900	4.60049900	-4.27173400	H	-2.18171000	4.78619800	-3.70802500
H	-0.79423900	4.37370700	-2.95789400	H	-1.01509100	4.42416800	-2.40926800
H	-3.60535200	1.18994200	-3.81226600	H	-3.81494200	1.34158800	-3.62627100
H	-3.66746300	2.67960400	-4.79588200	H	-3.85390300	2.92238800	-4.45160900
H	-4.27585100	2.67995100	-3.12335500	H	-4.49141500	2.75950300	-2.80547800
Np	0.00000800	0.00000600	0.00007500	Np	0.00000100	0.00000000	-0.00005400
$Np[(^tBuNO)py]_4^+$				$Pu[(^tBuNO)py]_4^-$			
O	1.01479800	1.25192500	1.48502900	O	-1.34861000	0.00826400	1.96618100
O	1.01665500	-1.25039300	-1.48502200	O	0.08594000	1.34624400	-1.96624400
O	-1.01476100	-1.25187900	1.48512200	O	1.34861000	-0.00826400	1.96618100
O	-1.01670900	1.25031600	-1.48503800	O	-0.08594000	-1.34624400	-1.96624400
N	2.07963100	2.08832500	1.41018300	N	-2.70809600	0.03043900	1.99799700
N	1.90430500	1.50013800	-0.80086500	N	-2.53979600	0.06447900	-0.29223000
N	2.08276000	-2.08517500	-1.41021500	N	0.16212800	2.70393900	-1.99564800
N	1.90661400	-1.49727800	0.80084200	N	0.00000000	2.54078000	0.28951900
N	-2.07959100	-2.08829000	1.41035000	N	2.70809600	-0.03043900	1.99799700
N	-1.90434000	-1.50020300	-0.80073000	N	2.53979600	-0.06447900	-0.29223000
N	-2.08280400	2.08510900	-1.41023100	N	-0.16212800	-2.70393900	-1.99564800
N	-1.90660200	1.49729000	0.80084200	N	0.00000000	-2.54078000	0.28951900
C	2.55591500	2.25476700	0.13739300	C	-3.36742900	0.07174800	0.81132700
C	2.29273800	1.58964700	-2.09305000	C	-3.08793900	0.10372200	-1.52334300
C	3.32114300	2.40808400	-2.53268000	C	-4.45472600	0.15106200	-1.77253700
C	3.99834800	3.17945600	-1.56837800	C	-5.31181400	0.16293600	-0.64951700
C	3.62794100	3.11147600	-0.23681900	C	-4.78836300	0.12518800	0.63095900
C	2.45611200	2.83717500	2.66218300	C	-3.32837000	0.00226500	3.36025700
C	3.92314600	2.53415500	3.02505800	C	-4.11322900	1.30663400	3.61928200
C	2.19603300	4.34448100	2.47083200	C	-4.20870100	-1.25556400	3.52584300
C	1.56303400	2.33412200	3.80648200	C	-2.19815000	-0.08126300	4.39984500
C	2.55937700	-2.25086700	-0.13745100	C	0.08859700	3.36628400	-0.81210400
C	2.29523100	-1.58618800	2.09301200	C	-0.07098700	3.09173700	1.51796700
C	3.32494500	-2.40300200	2.53259700	C	-0.06266600	4.45955300	1.76599600
C	4.00334700	-3.17327500	1.56825800	C	0.01733800	5.31474700	0.64435400
C	3.63278900	-3.10586500	0.23671100	C	0.09050800	4.78837300	-0.63341800
C	2.46046000	-2.83328200	-2.66229000	C	0.26587400	3.32068500	-3.35577100
C	1.56647000	-2.33164400	-3.80649300	C	0.36002300	2.18643800	-4.39017800
C	2.20293800	-4.34104700	-2.47108400	C	1.55582400	4.16167300	-3.47027300

C	3.92695900	-2.52773700	-3.02520400	C	-1.00217600	4.14447600	-3.66872700
C	-2.55591700	-2.25479300	0.13758300	C	3.36742900	-0.07174800	0.81132700
C	-2.29281300	-1.58977000	-2.09290000	C	3.08793900	-0.10372200	-1.52334300
C	-3.32122800	-2.40823100	-2.53246300	C	4.45472600	-0.15106200	-1.77253700
C	-3.99839900	-3.17956300	-1.56810600	C	5.31181400	-0.16293600	-0.64951700
C	-3.62795100	-3.11152300	-0.23656100	C	4.78836300	-0.12518800	0.63095900
C	-2.45602600	-2.83706400	2.66240900	C	3.32837000	-0.00226500	3.36025700
C	-3.92302300	-2.53396800	3.02537300	C	4.11322900	-1.30663400	3.61928200
C	-2.19600700	-4.34439000	2.47113100	C	4.20870100	1.25556400	3.52584300
C	-1.56285600	-2.33397700	3.80661800	C	2.19815000	0.08126300	4.39984500
C	-2.55938300	2.25085000	-0.13746200	C	-0.08859700	-3.36628400	-0.81210400
C	-2.29518500	1.58625300	2.09301800	C	0.07098700	-3.09173700	1.51796700
C	-3.32488000	2.40309600	2.53259700	C	0.06266600	-4.45955300	1.76599600
C	-4.00329600	3.17334200	1.56824700	C	-0.01733800	-5.31474700	0.64435400
C	-3.63277200	3.10587700	0.23669200	C	-0.09050800	-4.78837300	-0.63341800
C	-2.46054100	2.83318500	-2.66231200	C	-0.26587400	-3.32068500	-3.35577100
C	-1.56659000	2.33153000	-3.80654100	C	-0.36002300	-2.18643800	-4.39017800
C	-2.20301900	4.34095200	-2.47113200	C	-1.55582400	-4.16167300	-3.47027300
C	-3.92705600	2.52763900	-3.02516200	C	1.00217600	-4.14447600	-3.66872700
H	1.73160400	0.95684400	-2.78510300	H	-2.35177300	0.09680300	-2.33395400
H	3.59098700	2.44315500	-3.58912500	H	-4.83776200	0.18205600	-2.79508100
H	4.82038200	3.83695700	-1.86271200	H	-6.39882700	0.20530600	-0.77973300
H	4.15661900	3.70818300	0.50223900	H	-5.46758800	0.14255100	1.48156500
H	4.07018000	1.45143000	3.15350000	H	-3.43956400	2.16990500	3.50810800
H	4.17632800	3.02883400	3.97484600	H	-4.51741200	1.31275800	4.64569800
H	4.64321400	2.88309000	2.27369300	H	-4.95259000	1.45134600	2.92610100
H	2.80513000	4.79405000	1.67559900	H	-5.05196800	-1.29223800	2.82372400
H	2.42556700	4.88056500	3.40404800	H	-4.61886700	-1.30099400	4.54883300
H	1.13758400	4.52185100	2.22831500	H	-3.59877700	-2.15624900	3.35843900
H	0.49986400	2.52067200	3.60636600	H	-1.59044100	-0.98293900	4.25562000
H	1.84368100	2.87450000	4.72228400	H	-2.65224000	-0.10603900	5.40507800
H	1.69879000	1.25943200	3.98918700	H	-1.52350300	0.78036000	4.32889100
H	1.73312700	-0.95427100	2.78508800	H	-0.14338800	2.35704000	2.32682200
H	3.59488300	-2.43765900	3.58903100	H	-0.12310500	4.84502200	2.78631100
H	4.82644300	-3.82946300	1.86255200	H	0.01675100	6.40275100	0.77319900
H	4.16241100	-3.70170300	-0.50237100	H	0.13959000	5.46643100	-1.48373200
H	0.50363100	-2.52003000	-3.60633300	H	1.24395200	1.56039000	-4.21468900
H	1.84799100	-2.87145000	-4.72236300	H	0.43120200	2.63743900	-5.39457000
H	1.70037800	-1.25670500	-3.98909800	H	-0.51747900	1.53069400	-4.34690400
H	2.81280200	-4.78967100	-1.67590800	H	1.58883600	5.00895400	-2.77310500
H	2.43336800	-4.87664500	-3.40435700	H	1.65723400	4.56251400	-4.49291600
H	1.14479400	-4.52023900	-2.22857000	H	2.42955000	3.52616300	-3.26057100
H	4.07214400	-1.44475000	-3.15355100	H	-1.88888900	3.49651000	-3.59595500
H	4.18094700	-3.02189800	-3.97504600	H	-0.95332100	4.55072100	-4.69319800
H	4.64764300	-2.87551100	-2.27389100	H	-1.15005400	4.98630200	-2.97890300
H	-1.73170200	-0.95699700	-2.78499800	H	2.35177300	-0.09680300	-2.33395400

H	-3.59110400	-2.44335000	-3.58889700	H	4.83776200	-0.18205600	-2.79508100
H	-4.82043700	-3.83708300	-1.86238600	H	6.39882700	-0.20530600	-0.77973300
H	-4.15660400	-3.70820300	0.50253500	H	5.46758800	-0.14255100	1.48156500
H	-4.07000900	-1.45122900	3.15375000	H	3.43956400	-2.16990500	3.50810800
H	-4.17615000	-3.02857100	3.97521400	H	4.51741200	-1.31275800	4.64569800
H	-4.64316100	-2.88293000	2.27408800	H	4.95259000	-1.45134600	2.92610100
H	-2.80516000	-4.79398600	1.67595500	H	5.05196800	1.29223800	2.82372400
H	-2.42550800	-4.88041400	3.40438900	H	4.61886700	1.30099400	4.54883300
H	-1.13757600	-4.52181000	2.22856700	H	3.59877700	2.15624900	3.35843900
H	-0.49970800	-2.52060100	3.60645400	H	1.59044100	0.98293900	4.25562000
H	-1.84348000	-2.87427200	4.72247600	H	2.65224000	0.10603900	5.40507800
H	-1.69854200	-1.25926600	3.98925200	H	1.52350300	-0.78036000	4.32889100
H	-1.73307100	0.95435600	2.78510400	H	0.14338800	-2.35704000	2.32682200
H	-3.59479000	2.43779700	3.58903600	H	0.12310500	-4.84502200	2.78631100
H	-4.82637600	3.82955300	1.86253600	H	-0.01675100	-6.40275100	0.77319900
H	-4.16240200	3.70169500	-0.50240100	H	-0.13959000	-5.46643100	-1.48373200
H	-0.50374000	2.51987200	-3.60640000	H	-1.24395200	-1.56039000	-4.21468900
H	-1.84810800	2.87136100	-4.72239800	H	-0.43120200	-2.63743900	-5.39457000
H	-1.70054200	1.25659900	-3.98916100	H	0.51747900	-1.53069400	-4.34690400
H	-2.81286900	4.78958500	-1.67595000	H	-1.58883600	-5.00895400	-2.77310500
H	-2.43347100	4.87653600	-3.40440900	H	-1.65723400	-4.56251400	-4.49291600
H	-1.14487100	4.52015100	-2.22864400	H	-2.42955000	-3.52616300	-3.26057100
H	-4.07224600	1.44465300	-3.15350400	H	1.88888900	-3.49651000	-3.59595500
H	-4.18108800	3.02180200	-3.97499100	H	0.95332100	-4.55072100	-4.69319800
H	-4.64770700	2.87541100	-2.27381500	H	1.15005400	-4.98630200	-2.97890300
Np	-0.00000600	-0.00001200	0.00002000	Pu	0.00000000	0.00000000	-0.00046400
$Pu[(^tBuNO)py]_4^0$				$Pu[(^tBuNO)py]_4^+$			
O	0.73776200	1.14269700	1.84978700	O	-0.63589200	1.31205100	1.60533300
O	0.73966700	-1.14145900	-1.84975500	O	1.54852600	0.23072600	-1.70491500
O	-0.73779300	-1.14272500	1.84977300	O	0.63589200	-1.31205100	1.60533300
O	-0.73965200	1.14143800	-1.84976400	O	-1.54852600	-0.23072600	-1.70491500
N	1.70555600	2.09229400	1.92023900	N	-0.71399900	2.64385400	1.67334200
N	1.96472300	1.59138100	-0.30169400	N	-0.26674400	2.49521000	-0.57771400
N	1.70902900	-2.08945300	-1.92022800	N	2.80513700	0.73363300	-1.65984800
N	1.96723800	-1.58830300	0.30176200	N	2.28336700	0.91404900	0.57415600
N	-1.70558500	-2.09232300	1.92021400	N	0.71399900	-2.64385400	1.67334200
N	-1.96472600	-1.59141100	-0.30171900	N	0.26674400	-2.49521000	-0.57771400
N	-1.70902000	2.08942700	-1.92024600	N	-2.80513700	-0.73363300	-1.65984800
N	-1.96725400	1.58826900	0.30174000	N	-2.28336700	-0.91404900	0.57415600
C	2.39627600	2.33095400	0.76960600	C	-0.53030500	3.31389100	0.48538200
C	2.57628900	1.74102800	-1.49535500	C	-0.09640200	3.04837400	-1.79861700
C	3.63185000	2.61348100	-1.72015800	C	-0.17216600	4.41191700	-2.04437300
C	4.08436100	3.37499600	-0.62321900	C	-0.42343600	5.25836600	-0.94872100
C	3.48310900	3.24501100	0.61574700	C	-0.60123900	4.72366300	0.31615300
C	1.86286500	2.78855400	3.24076600	C	-1.11218500	3.23556500	3.00835600
C	3.25413800	2.48716600	3.83586900	C	0.00000000	4.17635600	3.51301600

C	1.61148000	4.30206600	3.07942100	C	-2.47597000	3.94283200	2.88217800
C	0.80020500	2.23323800	4.20264900	C	-1.26131700	2.08203600	4.01159800
C	2.40002400	-2.32713500	-0.76955100	C	3.23075200	1.07501100	-0.40004700
C	2.57895800	-1.73705400	1.49545700	C	2.60133600	1.22093400	1.85017600
C	3.63586700	-2.60786200	1.72029000	C	3.84310800	1.70189900	2.24026000
C	4.08962600	-3.36863100	0.62335000	C	4.81851100	1.87199100	1.24080300
C	3.48825500	-3.23952600	-0.61564900	C	4.52717800	1.56155800	-0.07700000
C	1.86744900	-2.78539500	-3.24079000	C	3.58944600	0.72775400	-2.94678700
C	0.80406400	-2.23149200	-4.20268100	C	2.66031800	0.23391900	-4.06655700
C	1.61818600	-4.29927800	-3.07960700	C	4.77612400	-0.25034900	-2.83363400
C	3.25831700	-2.48195400	-3.83580300	C	4.03936700	2.16144700	-3.29043400
C	-2.39629600	-2.33098800	0.76957300	C	0.53030500	-3.31389100	0.48538200
C	-2.57627000	-1.74105500	-1.49539400	C	0.09640200	-3.04837400	-1.79861700
C	-3.63182400	-2.61350600	-1.72022300	C	0.17216600	-4.41191700	-2.04437300
C	-4.08435400	-3.37502600	-0.62329700	C	0.42343600	-5.25836600	-0.94872100
C	-3.48312700	-3.24504700	0.61568000	C	0.60123900	-4.72366300	0.31615300
C	-1.86286300	-2.78855400	3.24075900	C	1.11218500	-3.23556500	3.00835600
C	-3.25409800	-2.48713500	3.83594100	C	0.00000000	-4.17635600	3.51301600
C	-1.61145000	-4.30207200	3.07948000	C	2.47597000	-3.94283200	2.88217800
C	-0.80015500	-2.23317900	4.20254900	C	1.26131700	-2.08203600	4.01159800
C	-2.40002500	2.32710200	-0.76957800	C	-3.23075200	-1.07501100	-0.40004700
C	-2.57899400	1.73702000	1.49542500	C	-2.60133600	-1.22093400	1.85017600
C	-3.63590400	2.60783300	1.72023800	C	-3.84310800	-1.70189900	2.24026000
C	-4.08964000	3.36860800	0.62329300	C	-4.81851100	-1.87199100	1.24080300
C	-3.48824900	3.23950200	-0.61569600	C	-4.52717800	-1.56155800	-0.07700000
C	-1.86745700	2.78539000	-3.24079600	C	-3.58944600	-0.72775400	-2.94678700
C	-0.80401400	2.23162700	-4.20270700	C	-2.66031800	-0.23391900	-4.06655700
C	-1.61834600	4.29928800	-3.07953400	C	-4.77612400	0.25034900	-2.83363400
C	-3.25829700	2.48186500	-3.83582800	C	-4.03936700	-2.16144700	-3.29043400
H	2.16800200	1.11175200	-2.29203800	H	0.11292000	2.33593800	-2.60130000
H	4.08962300	2.69485700	-2.70751300	H	-0.03600400	4.80339800	-3.05354200
H	4.91892300	4.07281300	-0.74031400	H	-0.47923900	6.34123600	-1.08573000
H	3.85176500	3.83177600	1.45417000	H	-0.78804100	5.38603100	1.15722400
H	3.38332600	1.40134000	3.96003500	H	0.95656100	3.63744200	3.58495300
H	3.34987100	2.95843000	4.82693900	H	-0.26004900	4.54380700	4.51704900
H	4.08216800	2.85146700	3.21334400	H	0.15944100	5.05451500	2.87477600
H	2.33102600	4.79700500	2.41418900	H	-2.46747200	4.79805300	2.19444700
H	1.67118100	4.79739800	4.06146800	H	-2.78637700	4.31718900	3.86923800
H	0.60439100	4.47327500	2.67060000	H	-3.24149200	3.23435100	2.53238600
H	-0.21495400	2.42423900	3.83137600	H	-2.04691300	1.37882200	3.70664400
H	0.92154500	2.73345300	5.17643100	H	-1.53763100	2.51134200	4.98599300
H	0.90731200	1.15028000	4.34277300	H	-0.32550900	1.52034800	4.13405600
H	2.16962700	-1.10846700	2.29214900	H	1.79810000	1.05524400	2.57202800
H	4.09370200	-2.68856700	2.70767100	H	4.04674800	1.93306200	3.28694200
H	4.92525200	-4.06516900	0.74047500	H	5.81402600	2.24488200	1.49515900
H	3.85786100	-3.82570700	-1.45405900	H	5.28940300	1.68843700	-0.84135200

H	-0.21084700	-2.42399300	-3.83150800	H	2.30932200	-0.78989400	-3.88317000
H	0.92619600	-2.73141300	-5.17651300	H	3.22520800	0.24366600	-5.01015900
H	0.90962900	-1.14836300	-4.34266700	H	1.78185900	0.88252600	-4.18504600
H	2.33839800	-4.79327100	-2.41439400	H	5.50382600	0.03402200	-2.06238800
H	1.67862000	-4.79443100	-4.06169900	H	5.31279600	-0.29288500	-3.79351600
H	0.61132100	-4.47193900	-2.67084300	H	4.41542000	-1.26343800	-2.60113000
H	3.38593700	-1.39593500	-3.95989900	H	3.16786700	2.82893900	-3.36498300
H	3.35477700	-2.95301700	-4.82689700	H	4.55283300	2.16165100	-4.26364500
H	4.08685000	-2.84508800	-3.21327000	H	4.73066000	2.59488700	-2.55663800
H	-2.16796600	-1.11177500	-2.29206600	H	-0.11292000	-2.33593800	-2.60130000
H	-4.08957700	-2.69487800	-2.70758800	H	0.03600400	-4.80339800	-3.05354200
H	-4.91891300	-4.07284400	-0.74041300	H	0.47923900	-6.34123600	-1.08573000
H	-3.85180400	-3.83182000	1.45408600	H	0.78804100	-5.38603100	1.15722400
H	-3.38327200	-1.40130300	3.96007200	H	-0.95656100	-3.63744200	3.58495300
H	-3.34976700	-2.95835500	4.82703800	H	0.26004900	-4.54380700	4.51704900
H	-4.08217400	-2.85145400	3.21349300	H	-0.15944100	-5.05451500	2.87477600
H	-2.33101000	-4.79706600	2.41430800	H	2.46747200	-4.79805300	2.19444700
H	-1.67109400	-4.79735400	4.06155500	H	2.78637700	-4.31718900	3.86923800
H	-0.60437500	-4.47327900	2.67062400	H	3.24149200	-3.23435100	2.53238600
H	0.21498300	-2.42418500	3.83122200	H	2.04691300	-1.37882200	3.70664400
H	-0.92143000	-2.73334500	5.17636200	H	1.53763100	-2.51134200	4.98599300
H	-0.90727000	-1.15021400	4.34262200	H	0.32550900	-1.52034800	4.13405600
H	-2.16967900	1.10843100	2.29212300	H	-1.79810000	-1.05524400	2.57202800
H	-4.09375600	2.68854000	2.70761200	H	-4.04674800	-1.93306200	3.28694200
H	-4.92526200	4.06515200	0.74040500	H	-5.81402600	-2.24488200	1.49515900
H	-3.85782900	3.82568800	-1.45411600	H	-5.28940300	-1.68843700	-0.84135200
H	0.21087800	2.42420400	-3.83152200	H	-2.30932200	0.78989400	-3.88317000
H	-0.92618700	2.73158100	-5.17651800	H	-3.22520800	-0.24366600	-5.01015900
H	-0.90947800	1.14849500	-4.34274500	H	-1.78185900	-0.88252600	-4.18504600
H	-2.33861900	4.79317100	-2.41430300	H	-5.50382600	-0.03402200	-2.06238800
H	-1.67881800	4.79448600	-4.06160100	H	-5.31279600	0.29288500	-3.79351600
H	-0.61150400	4.47202800	-2.67074700	H	-4.41542000	1.26343800	-2.60113000
H	-3.38583200	1.39584000	-3.95996500	H	-3.16786700	-2.82893900	-3.36498300
H	-3.35478600	2.95295800	-4.82690500	H	-4.55283300	-2.16165100	-4.26364500
H	-4.08686100	2.84491300	-3.21328500	H	-4.73066000	-2.59488700	-2.55663800
Pu	-0.00000400	-0.00001300	0.00002100	Pu	0.00000000	0.00000000	-0.16450400
$Am[(^tBuNO)py]_4^-$				$Am[(^tBuNO)py]_4^0$			
O	0.26155900	-1.39860300	1.92341500	O	0.78613497	1.16476799	1.85517885
O	-1.41907800	0.10944700	-1.92355000	O	0.78806421	-1.16346268	-1.85518660
O	-0.26155900	1.39860300	1.92341500	O	-0.78614156	-1.16477270	1.85517513
O	1.41907800	-0.10944700	-1.92355000	O	-0.78805429	1.16345627	-1.85519179
N	0.53413100	-2.72931600	1.88261000	N	1.59742287	2.24309220	1.84382897
N	0.00000000	-2.56651500	-0.34823800	N	1.94599703	1.65860248	-0.35254427
N	-2.77137400	0.23733000	-1.88255800	N	1.60105283	-2.24050508	-1.84383294
N	-2.55152700	-0.27571100	0.34827100	N	1.94854881	-1.65559748	0.35259837
N	-0.53413100	2.72931600	1.88261000	N	-1.59743006	-2.24309571	1.84382246

N	0.00000000	2.56651500	-0.34823800	N	-1.94599404	-1.65860750	-0.35255234
N	2.77137400	-0.23733000	-1.88255800	N	-1.60103990	2.24050089	-1.84384098
N	2.55152700	0.27571100	0.34827100	N	-1.94854794	1.65559238	0.35258841
C	0.32492200	-3.38543100	0.71059400	C	2.30510566	2.46716337	0.69362803
C	-0.23470900	-3.11001900	-1.55503500	C	2.58769443	1.78277310	-1.53049757
C	-0.16021700	-4.47246300	-1.83064400	C	3.59986670	2.70436227	-1.76956545
C	0.16293900	-5.32397100	-0.75156200	C	3.97877813	3.53654883	-0.69750910
C	0.39970700	-4.80410500	0.50820300	C	3.34885445	3.42780520	0.53028222
C	0.96954400	-3.34257900	3.17806000	C	1.67616161	3.02937179	3.12286533
C	-0.13921300	-4.26252300	3.73421600	C	3.05084397	2.81739435	3.79111825
C	2.31310100	-4.08223100	3.00331400	C	1.37627191	4.51807102	2.85436524
C	1.20012000	-2.20627300	4.18892400	C	0.59087145	2.49863763	4.07346289
C	-3.40091700	-0.04182100	-0.71055400	C	2.30902605	-2.46350957	-0.69360382
C	-3.06631900	-0.56742600	1.55520500	C	2.59037070	-1.77881379	1.53058338
C	-4.42880100	-0.64106500	1.83088700	C	3.60401764	-2.69878061	1.76965163
C	-5.31038200	-0.41315300	0.75163200	C	3.98434821	-3.53027426	0.69755985
C	-4.81930600	-0.12194500	-0.50828500	C	3.35432496	-3.42246567	-0.53026248
C	-3.42797900	0.60459400	-3.17783500	C	1.68106680	-3.02662523	-3.12288496
C	-2.32315300	0.95913900	-4.18775300	C	0.59486427	-2.49766362	-4.07342729
C	-4.31001900	1.85914400	-3.00222300	C	1.38364333	-4.51582636	-2.85441785
C	-4.22102800	-0.59741000	-3.73562600	C	3.05537671	-2.81234997	-3.79117155
C	-0.32492200	3.38543100	0.71059400	C	-2.30510813	-2.46716846	0.69361836
C	0.23470900	3.11001900	-1.55503500	C	-2.58768423	-1.78277836	-1.53050960
C	0.16021700	4.47246300	-1.83064400	C	-3.59985485	-2.70436743	-1.76958408
C	-0.16293900	5.32397100	-0.75156200	C	-3.97877230	-3.53655418	-0.69753020
C	-0.39970700	4.80410500	0.50820300	C	-3.34885588	-3.42781081	0.53026485
C	-0.96954400	3.34257900	3.17806000	C	-1.67616484	-3.02937195	3.12286099
C	0.13921300	4.26252300	3.73421600	C	-3.05084219	-2.81739202	3.79112461
C	-2.31310100	4.08223100	3.00331400	C	-1.37626826	-4.51807201	2.85437042
C	-1.20012000	2.20627300	4.18892400	C	-0.59087042	-2.49862645	4.07344625
C	3.40091700	0.04182100	-0.71055400	C	-2.30901827	2.46350415	-0.69361594
C	3.06631900	0.56742600	1.55520500	C	-2.59037852	1.77880918	1.53056854
C	4.42880100	0.64106500	1.83088700	C	-3.60402813	2.69877581	1.76962770
C	5.31038200	0.41315300	0.75163200	C	-3.98435278	3.53026707	0.69753154
C	4.81930600	0.12194500	-0.50828500	C	-3.35432047	3.42245753	-0.53028600
C	3.42797900	-0.60459400	-3.17783500	C	-1.68106122	3.02662591	-3.12288978
C	2.32315300	-0.95913900	-4.18775300	C	-0.59490936	2.49763583	-4.07347601
C	4.31001900	-1.85914400	-3.00222300	C	-1.38358278	4.51581547	-2.85442220
C	4.22102800	0.59741000	-3.73562600	C	-3.05540432	2.81240517	-3.79112388
H	-0.49915200	-2.37800600	-2.32665200	H	2.24219323	1.09198994	-2.30632576
H	-0.35874900	-4.85579200	-2.83399600	H	4.08033946	2.76762876	-2.74750835
H	0.21505600	-6.40881200	-0.89716700	H	4.78382782	4.26720448	-0.82101500
H	0.61460200	-5.48482300	1.33026800	H	3.67627901	4.05585225	1.35578090
H	-1.06849700	-3.68548600	3.85646600	H	3.21497586	1.74556258	3.97909591
H	0.15031000	-4.66332000	4.72041400	H	3.08590460	3.34304188	4.75859471
H	-0.36119500	-5.11393300	3.07607600	H	3.88975270	3.18229022	3.18314920

H	2.26571000	-4.91977100	2.29569200	H	2.10289355	5.00371836	2.19081814
H	2.65140400	-4.48113300	3.97439700	H	1.37485515	5.07199126	3.80634533
H	3.07548900	-3.37909600	2.63562500	H	0.38128085	4.62353470	2.39664951
H	1.97659600	-1.51537800	3.83590100	H	-0.41165466	2.61843514	3.64162166
H	1.52232700	-2.65201900	5.14543600	H	0.64233009	3.07404115	5.01127378
H	0.28707100	-1.62082900	4.34789800	H	0.73475635	1.43495059	4.29858286
H	-2.30984800	-0.75063900	2.32679900	H	2.24370018	-1.08865103	2.30644091
H	-4.78829600	-0.87952800	2.83436700	H	4.08453123	-2.76133641	2.74762027
H	-6.39444900	-0.47954200	0.89719000	H	4.79058022	-4.25962550	0.82106310
H	-5.51927800	0.01662000	-1.33061200	H	3.68282237	-4.04991107	-1.35579114
H	-1.72133400	1.80595200	-3.83332000	H	-0.40743905	-2.61910195	-3.64152564
H	-2.80090900	1.23201800	-5.14415700	H	0.64721426	-3.07297943	-5.01124212
H	-1.64143300	0.11568400	-4.34746000	H	0.73699618	-1.43374177	-4.29855050
H	-5.13788700	1.71993900	-2.29532400	H	2.11107332	-5.00029225	-2.19089324
H	-4.74279900	2.15287700	-3.97329900	H	1.38312994	-5.06972205	-3.80641323
H	-3.69455100	2.69336700	-2.63329500	H	0.38883289	-4.62294688	-2.39669293
H	-3.54585700	-1.45794700	-3.85850600	H	3.21772690	-1.74024120	-3.97911801
H	-4.65071700	-0.35239300	-4.72172000	H	3.09128328	-3.33790436	-4.75866797
H	-5.04328000	-0.91169400	-3.07802400	H	3.89490710	-3.17587632	-3.18323937
H	0.49915200	2.37800600	-2.32665200	H	-2.24217778	-1.09199566	-2.30633584
H	0.35874900	4.85579200	-2.83399600	H	-4.08032145	-2.76763407	-2.74753002
H	-0.21505600	6.40881200	-0.89716700	H	-4.78382082	-4.26721027	-0.82104129
H	-0.61460200	5.48482300	1.33026800	H	-3.67628570	-4.05585916	1.35575985
H	1.06849700	3.68548600	3.85646600	H	-3.21497375	-1.74555933	3.97909712
H	-0.15031000	4.66332000	4.72041400	H	-3.08589340	-3.34303309	4.75860495
H	0.36119500	5.11393300	3.07607600	H	-3.88975641	-3.18229233	3.18316650
H	-2.26571000	4.91977100	2.29569200	H	-2.10288943	-5.00372891	2.19083030
H	-2.65140400	4.48113300	3.97439700	H	-1.37484393	-5.07198516	3.80635464
H	-3.07548900	3.37909600	2.63562500	H	-0.38127858	-4.62353373	2.39665127
H	-1.97659600	1.51537800	3.83590100	H	0.41165316	-2.61842486	3.64159927
H	-1.52232700	2.65201900	5.14543600	H	-0.64232125	-3.07402133	5.01126271
H	-0.28707100	1.62082900	4.34789800	H	-0.73475712	-1.43493761	4.29855716
H	2.30984800	0.75063900	2.32679900	H	-2.24371390	1.08864685	2.30642909
H	4.78829600	0.87952800	2.83436700	H	-4.08454955	2.76133201	2.74759247
H	6.39444900	0.47954200	0.89719000	H	-4.79058750	4.25961659	0.82102737
H	5.51927800	-0.01662000	-1.33061200	H	-3.68281317	4.04989858	-1.35582064
H	1.72133400	-1.80595200	-3.83332000	H	0.40741341	2.61903562	-3.64160904
H	2.80090900	-1.23201800	-5.14415700	H	-0.64727253	3.07296308	-5.01128327
H	1.64143300	-0.11568400	-4.34746000	H	-0.73708523	1.43372141	-4.29860548
H	5.13788700	-1.71993900	-2.29532400	H	-2.11097805	5.00029984	-2.19087261
H	4.74279900	-2.15287700	-3.97329900	H	-1.38308095	5.06971699	-3.80641411
H	3.69455100	-2.69336700	-2.63329500	H	-0.38875525	4.62290171	-2.39672650
H	3.54585700	1.45794700	-3.85850600	H	-3.21780072	1.74030374	-3.97907191
H	4.65071700	0.35239300	-4.72172000	H	-3.09133075	3.33796905	-4.75861434
H	5.04328000	0.91169400	-3.07802400	H	-3.89489640	3.17595777	-3.18315332
Am	0.00000000	0.00000000	-0.00024500	Am	0.00000128	-0.00000283	0.00000203

$[Am^{III}(\mu_2\text{-}(^t\text{BuNO})py)(2\text{-}(^t\text{BuNO})py)_2]_2$			
Am	1.95796900	0.06586600	-0.18709000
N	3.42127700	1.68842400	-1.46149100
N	2.75382000	3.24711700	0.10408800
N	4.10278400	-0.25405500	1.16993700
N	4.54639000	-2.06180600	-0.19216100
N	0.82054400	-0.75185700	2.24338600
N	-0.98647600	0.75911600	2.53722900
O	2.10445000	2.19378700	0.67029000
O	3.39037400	-1.69562100	-0.82852700
O	0.15690000	-0.98148200	1.02312200
C	4.16632800	1.32227900	-2.52743700
H	4.05118700	0.27414200	-2.82297700
C	5.01889700	2.17237800	-3.21416400
H	5.58672700	1.82043900	-4.07697600
C	5.12437400	3.49726200	-2.73812200
H	5.79794200	4.20844300	-3.22575400
C	4.39625100	3.90614800	-1.63741600
H	4.52124900	4.91943600	-1.26265000
C	3.52028000	2.97903000	-0.98847700
C	2.54080200	4.58456300	0.75516500
C	3.84233500	5.05819000	1.43601700
H	4.17945200	4.30685100	2.16615900
H	3.66549500	6.00304300	1.97442600
H	4.66610000	5.22671300	0.72930600
C	1.46309300	4.42142300	1.83909400
H	0.51791600	4.05687300	1.41639700
H	1.28858700	5.40547000	2.30263900
H	1.76984900	3.71297100	2.61788300
C	2.01443700	5.60618900	-0.27395500
H	2.70753200	5.79678700	-1.10309400
H	1.82102700	6.56878500	0.22538600
H	1.06718900	5.24950900	-0.70564300
C	4.43364000	0.58144400	2.17872800
H	3.72090100	1.39910200	2.32920000
C	5.56787200	0.44734500	2.96622700
H	5.77971400	1.15319900	3.77135800
C	6.43200400	-0.62698600	2.66516000
H	7.34682500	-0.78237500	3.24527300
C	6.14174900	-1.48921600	1.62523300
H	6.83243700	-2.29859100	1.40235100
C	4.94776000	-1.29332800	0.85670800
C	5.24694500	-3.28485300	-0.71304600
C	4.43204900	-3.86074900	-1.88141500
H	3.39956400	-4.08307700	-1.58469400
H	4.91505800	-4.79396400	-2.21114100

H	4.40835700	-3.16960900	-2.73454600
C	6.64144800	-2.91266800	-1.26206000
H	6.54208800	-2.13829100	-2.03769300
H	7.11304500	-3.79696800	-1.71975100
H	7.32904500	-2.52841200	-0.49814100
C	5.31395600	-4.37148900	0.38177700
H	5.83845400	-4.04734900	1.28952800
H	5.83388000	-5.26292200	-0.00395500
H	4.29645700	-4.67075200	0.67525500
C	-1.55779100	1.78726400	3.20509100
H	-2.50917900	2.11815200	2.78152800
C	-0.98932600	2.39777900	4.31787100
H	-1.50463200	3.21935300	4.82004900
C	0.27809400	1.95894500	4.72997700
H	0.79606900	2.44586900	5.56142300
C	0.89649600	0.92226600	4.04270500
H	1.91249000	0.61835500	4.28817800
C	1.02184900	-2.08876200	2.97296700
C	-0.33586200	-2.59876900	3.48070200
H	-1.05928900	-2.66149900	2.65629500
H	-0.75200200	-1.93773500	4.25730400
H	-0.22505300	-3.60312100	3.91966900
C	2.01104400	-1.94503700	4.13847900
H	2.26238700	-2.95170300	4.50704200
H	1.58725000	-1.39194300	4.98833100
H	2.94717900	-1.46185800	3.81942800
C	1.60677300	-3.07752400	1.95547200
H	0.91369900	-3.24269900	1.12178900
H	1.79154300	-4.03910500	2.46019600
H	2.56168800	-2.71691400	1.54643700
C	0.21548700	0.30348500	2.96980300
Am	-1.95775500	-0.06571600	0.18713300
N	-3.42118200	-1.68825600	1.46141600
N	-2.75373900	-3.24695000	-0.10415200
N	-4.10250200	0.25370600	-1.17021400
N	-4.54686400	2.06108800	0.19213200
N	-0.82043400	0.75224200	-2.24323600
N	0.98659300	-0.75870000	-2.53704200
O	-2.10401300	-2.19369100	-0.67006100
O	-3.39070400	1.69528600	0.82841500
O	-0.15676600	0.98191100	-1.02298400
C	-4.16629800	-1.32205800	2.52729900
H	-4.05114000	-0.27391500	2.82280700
C	-5.01892200	-2.17211800	3.21400300
H	-5.58680900	-1.82014300	4.07676200
C	-5.12432400	-3.49704300	2.73805200

H	-5.79784800	-4.20822700	3.22574100
C	-4.39614100	-3.90598100	1.63740700
H	-4.52101300	-4.91933300	1.26277800
C	-3.52020400	-2.97886300	0.98841600
C	-2.54084900	-4.58434900	-0.75536800
C	-3.84250900	-5.05796100	-1.43599200
H	-4.17978800	-4.30658800	-2.16602400
H	-3.66573500	-6.00277500	-1.97449100
H	-4.66614300	-5.22655500	-0.72915000
C	-1.46339600	-4.42110300	-1.83953000
H	-0.51811300	-4.05661000	-1.41702600
H	-1.28902400	-5.40510200	-2.30322700
H	-1.77032800	-3.71256600	-2.61818000
C	-2.01422300	-5.60603100	0.27357100
H	-2.70713900	-5.79667800	1.10285000
H	-1.82089200	-6.56860100	-0.22585200
H	-1.06689500	-5.24933700	0.70507300
C	-4.43299600	-0.58176900	-2.17913900
H	-3.71990300	-1.39909100	-2.32975100
C	-5.56731200	-0.44806700	-2.96658900
H	-5.77882800	-1.15386100	-3.77186000
C	-6.43200900	0.62572400	-2.66522900
H	-7.34698900	0.78069700	-3.24520200
C	-6.14213800	1.48789800	-1.62514700
H	-6.83332100	2.29676900	-1.40196400
C	-4.94794500	1.29254400	-0.85680600
C	-5.24781500	3.28391800	0.71303400
C	-4.43287900	3.86024000	1.88115200
H	-3.40059600	4.08309800	1.58411300
H	-4.91627900	4.79319300	2.21104100
H	-4.40850100	3.16910500	2.73428400
C	-6.64203800	2.91118400	1.26238000
H	-6.54217800	2.13698900	2.03813100
H	-7.11399000	3.79533600	1.71999200
H	-7.32956800	2.52645100	0.49863900
C	-5.31551700	4.37042300	-0.38186800
H	-5.84015900	4.04603700	-1.28944700
H	-5.83565600	5.26169700	0.00394700
H	-4.29821300	4.67004600	-0.67565600
C	1.55801700	-1.78680200	-3.20489100
H	2.50930500	-2.11765500	-2.78105200
C	0.98973700	-2.39719400	-4.31782600
H	1.50512000	-3.21870600	-4.82002700
C	-0.27761300	-1.95828800	-4.73008200
H	-0.79545500	-2.44510000	-5.56167700
C	-0.89613600	-0.92168200	-4.04281000

H	-1.91209300	-0.61778400	-4.28843900
C	-1.02198400	2.08916200	-2.97266900
C	0.33564800	2.59944200	-3.48034000
H	1.05905000	2.66218800	-2.65591000
H	0.75190600	1.93856600	-4.25701600
H	0.22468900	3.60383000	-3.91918900
C	-2.01117400	1.94542500	-4.13819500
H	-2.26271200	2.95209500	-4.50660500
H	-1.58727600	1.39254600	-4.98813500
H	-2.94720200	1.46201200	-3.81919800
C	-1.60705600	3.07773300	-1.95506200
H	-0.91396700	3.24298400	-1.12140500
H	-1.79205300	4.03930700	-2.45971000
H	-2.56185700	2.71689400	-1.54595800
C	-0.21531200	-0.30300200	-2.96972200