

Supporting Information for:

**Coordination Chemistry of a Strongly-Donating
Hydroxylamine with Early Actinides: An Investigation of
Redox Properties and Electronic Structure**

Alex McSkimming,^{†,‡} Jing Su,^{†,§} Thibault Cheisson,[‡] Michael R. Gau,[‡] Patrick J.
Carroll,[‡] Enrique R. Batista,^{*,§} Ping Yang,^{*,§} and Eric J. Schelter^{*,‡}

[†] Alex McSkimming and Jing Su contributed equally to this work

[‡]P. Roy and Diana T. Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, 231 S
34th St., Philadelphia, Pennsylvania 19104, United States

[§]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, United States

NMR Spectra	S2
UV-Vis-NIR spectra	S4
Additional Crystallography Data	S6
Additional Electrochemistry Data	S7
Additional Computational Data	S11

NMR Spectra

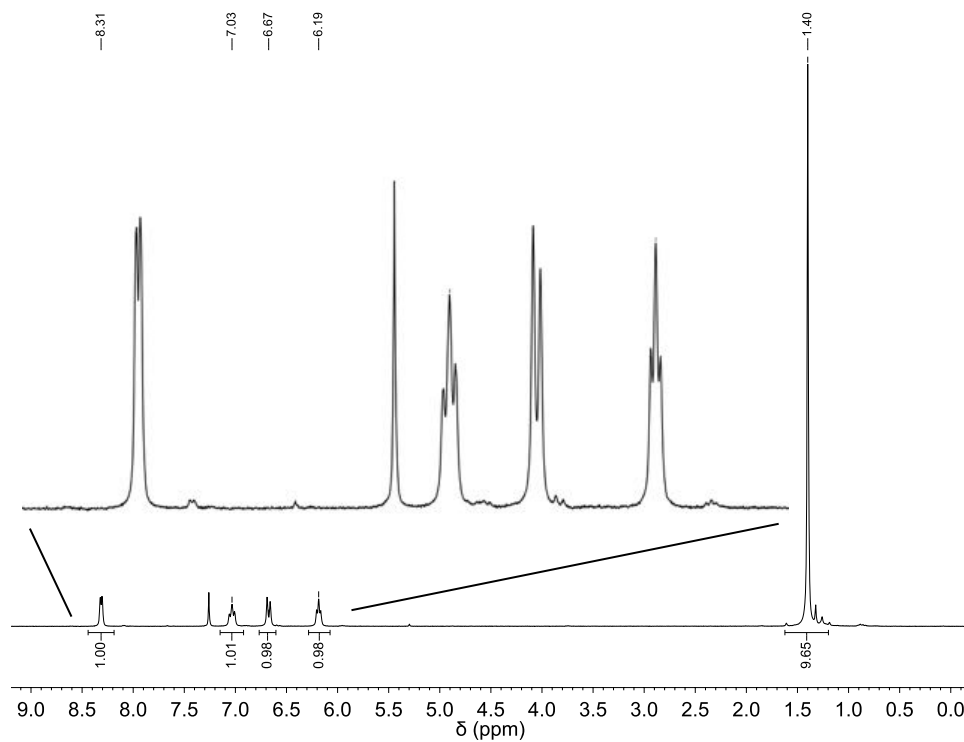


Figure S1. ^1H NMR spectrum of $[\text{Th}(\text{pyNO})_4]$ recorded at 300 MHz in CDCl_3 .

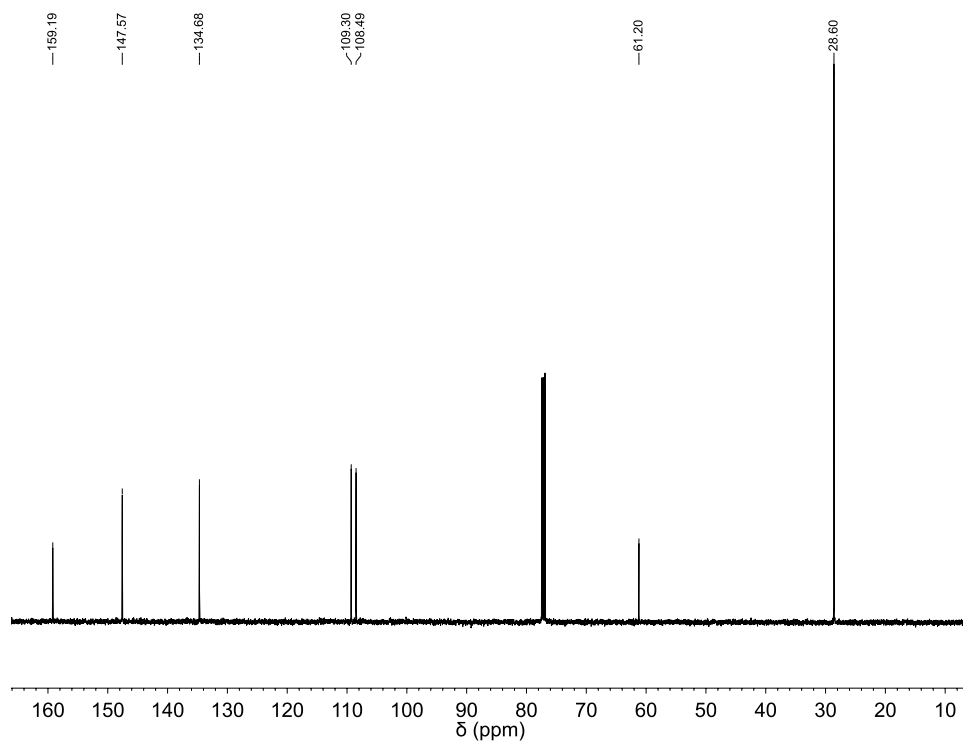


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Th}(\text{pyNO})_4]$ recorded at 126 MHz in CDCl_3 .

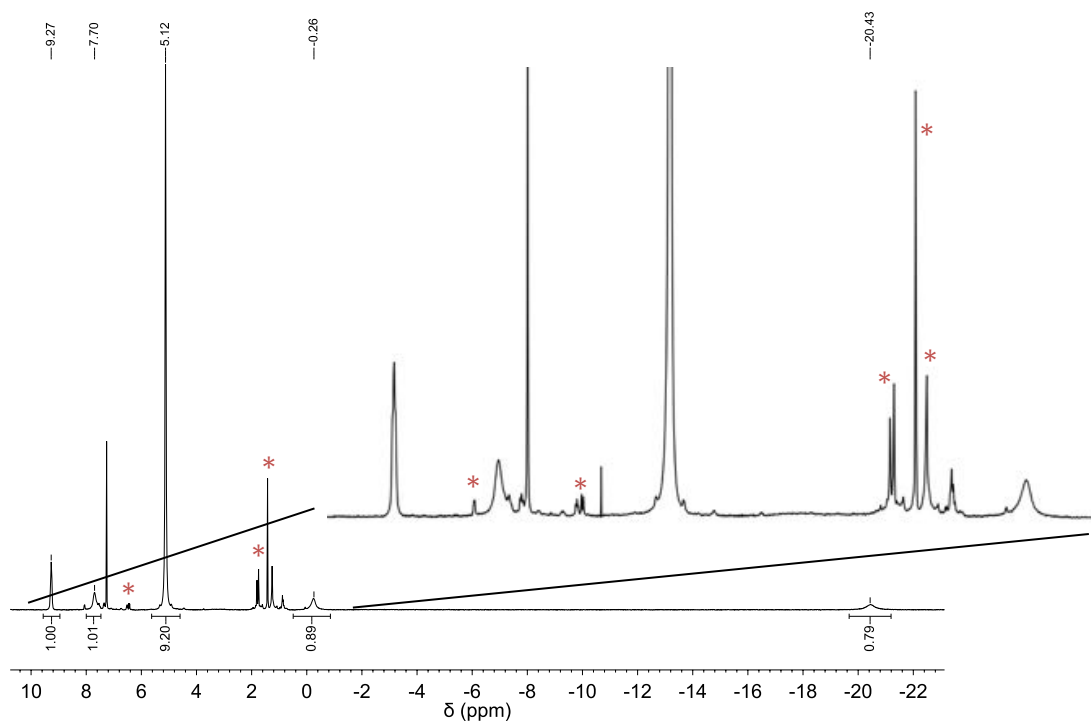


Figure S3. ^1H NMR spectrum of $[\text{U}(\text{pyNO})_4]$ recorded at 300 MHz in CDCl_3 . Asterisks indicate peaks due to decomposition product(s).

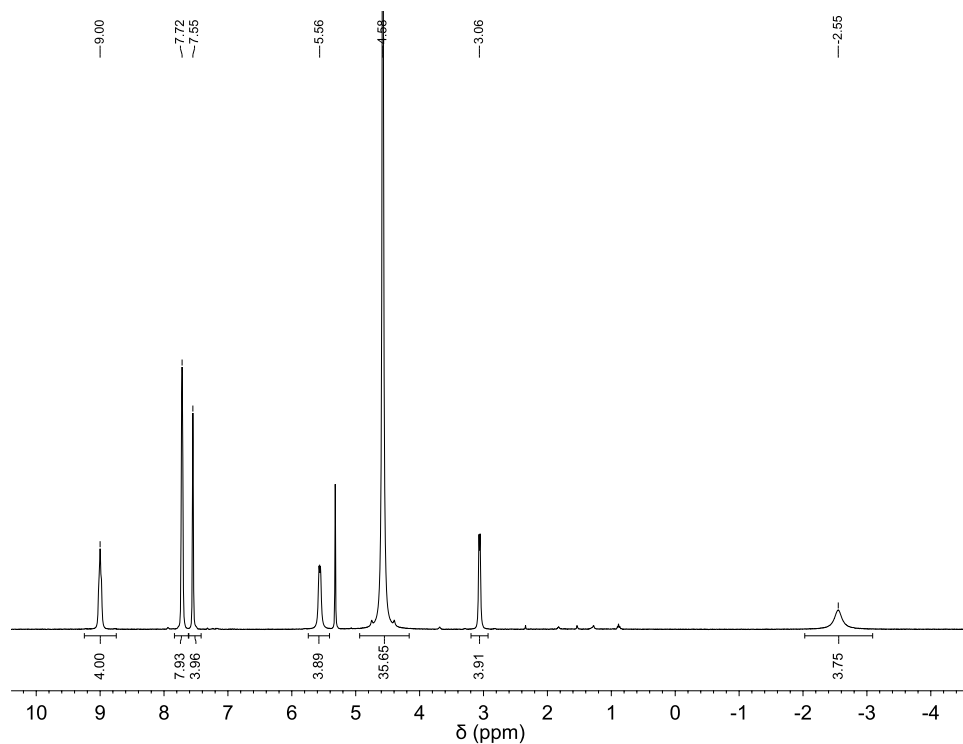


Figure S4. ^1H NMR spectrum of $[\text{U}^{\text{V}}(\text{pyNO})_4][\text{BAr}^{\text{F}}_4]$ recorded at 300 MHz in CD_2Cl_2 .

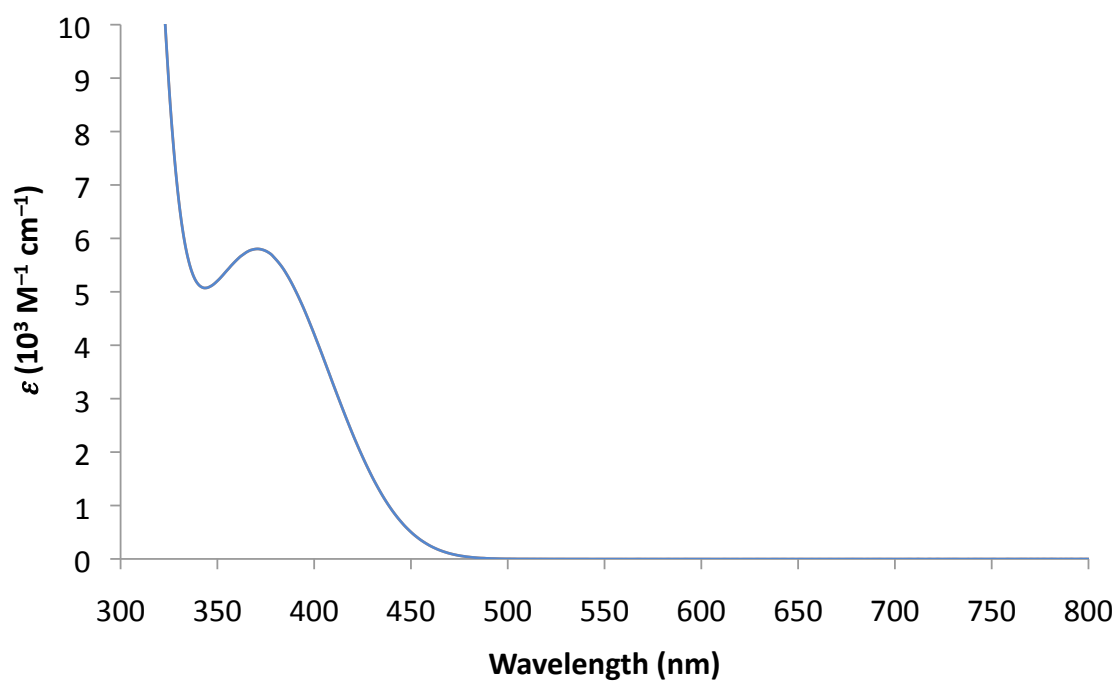


Figure S5. UV-Vis spectrum of [Th(pyNO)₄] in THF at 0.24 mmol L⁻¹ concentration.

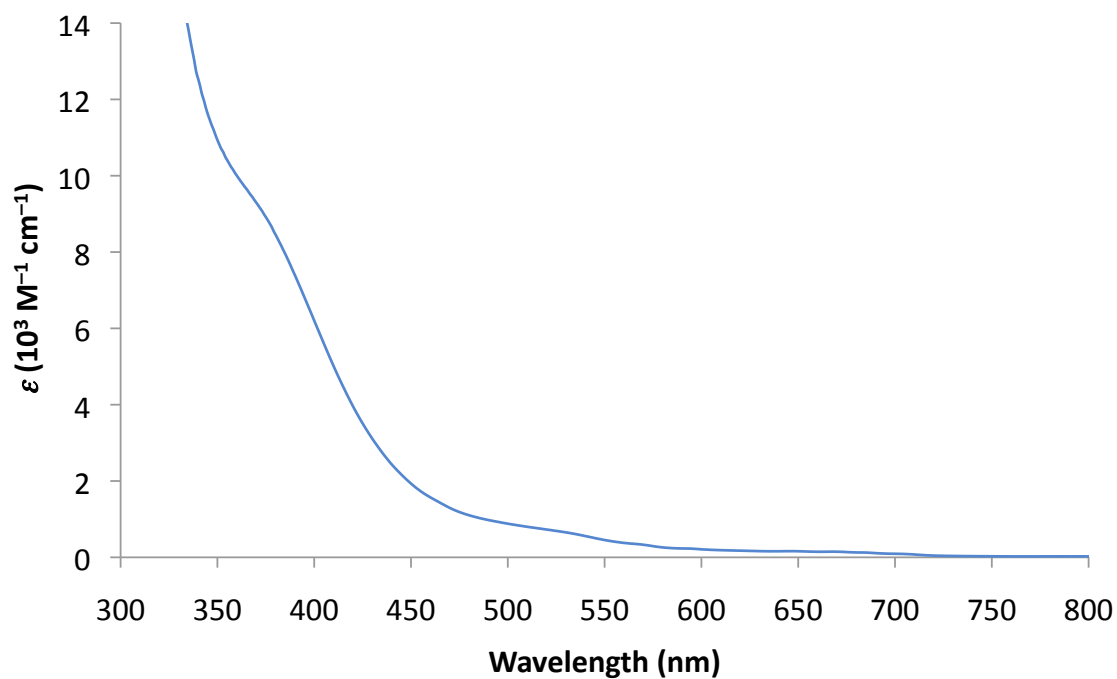


Figure S6. UV-Vis spectrum of [U(pyNO)₄] in THF at 0.24 mmol L⁻¹ concentration.

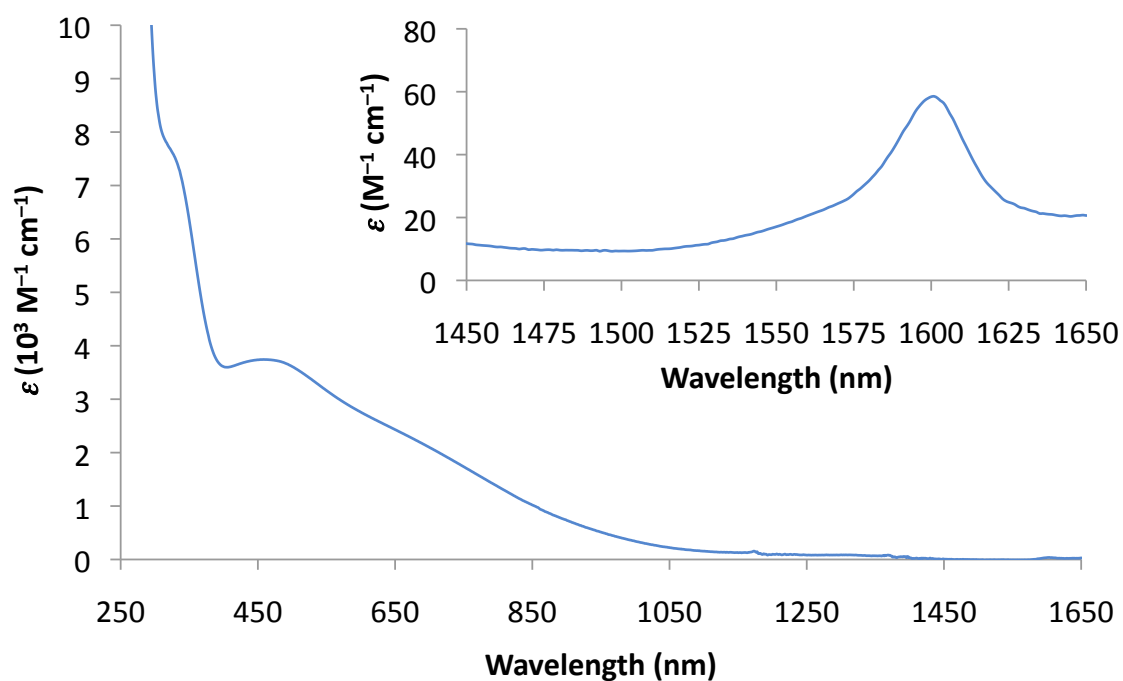


Figure S7. UV-Vis spectrum of $[U(pyNO)_4][BAr^F_4]$ in THF at 0.22 mmol L^{-1} concentration. Inset shows a close-up of the NIR region recorded at 6.4 mmol L^{-1} concentration.

Additional Crystallography Data

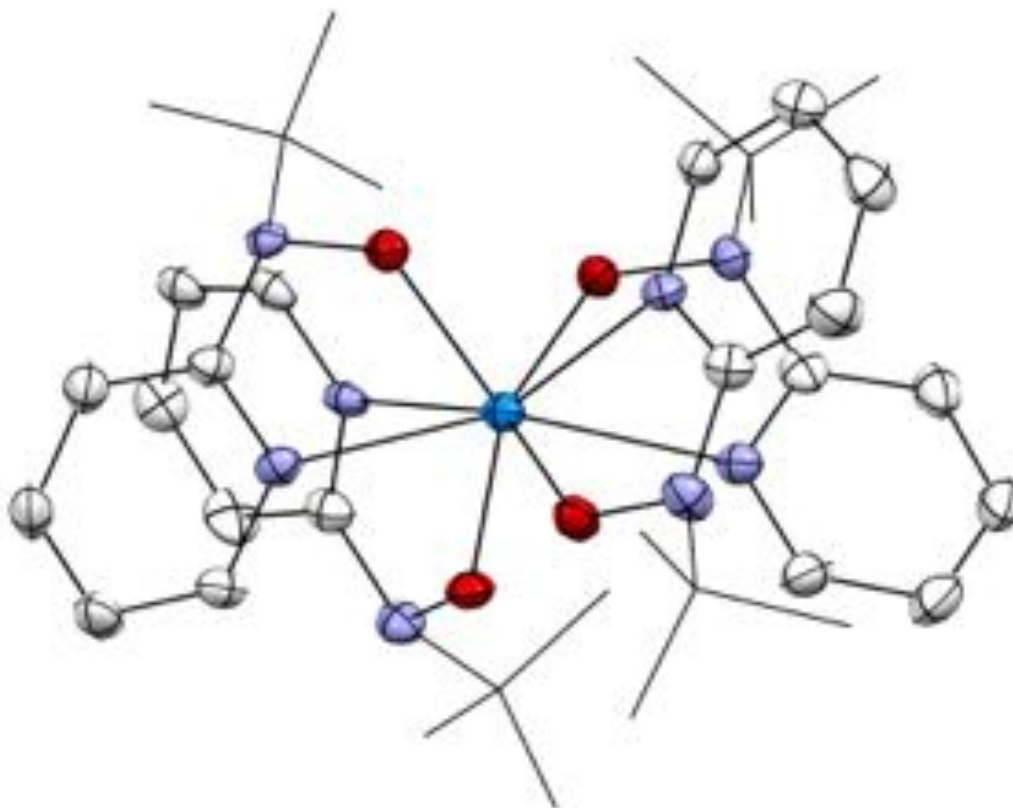


Figure S8. Thermal ellipsoid plot (50% probability) of the solid-state structure of [U(pyNO)₄][BArF₄]. O = red, N = lavender, U = light blue, unlabelled ellipsoids correspond to carbon. Hydrogen atoms and [BArF₄][−] counter-ion is omitted for clarity; *t*Bu groups are shown in wire-frame.

Additional Electrochemistry Data

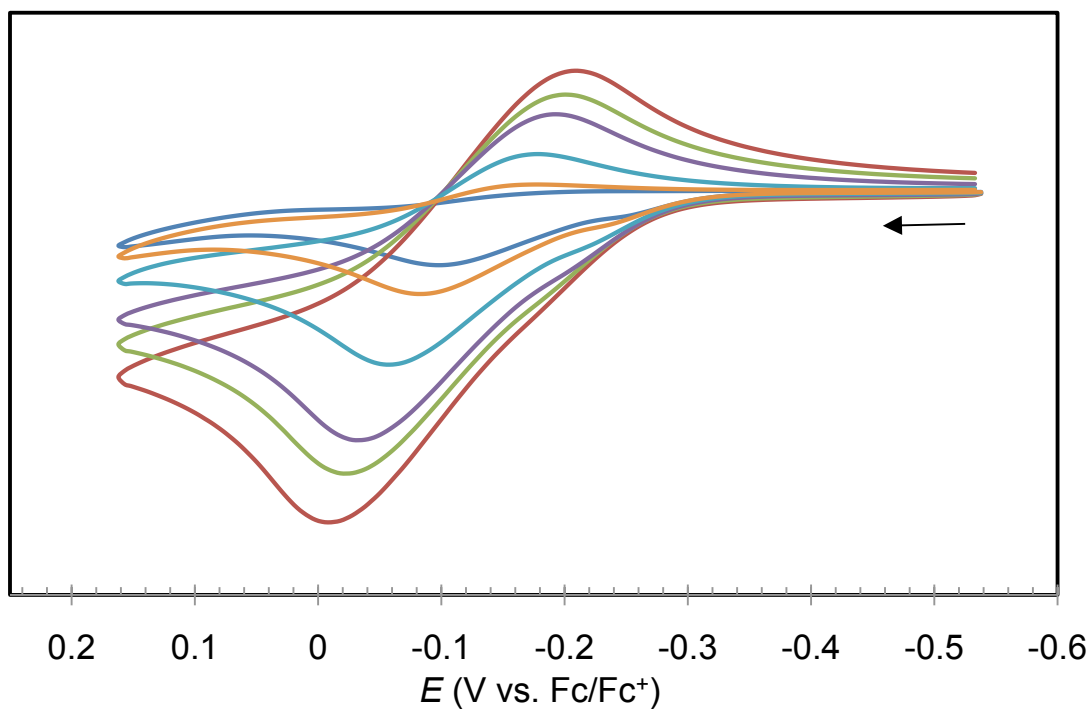


Figure S9. Scan rate dependence of the first oxidation process in cyclic voltammograms of $[\text{Th}(\text{pyNO})_4]$ in THF with $0.1\text{ M } [\text{nPr}_4\text{N}][\text{BAR}^{\text{F}}_4]$.

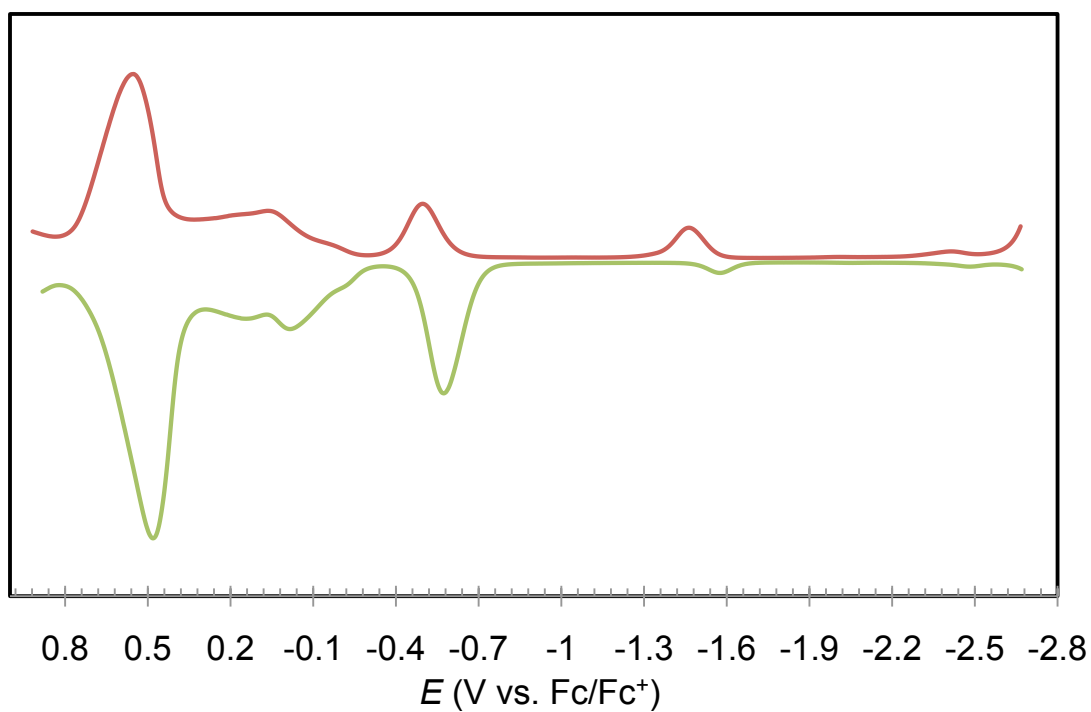


Figure S10. Differential pulse voltammograms of $[\text{Th}(\text{pyNO})_4]$ recorded in THF with $0.1\text{ M } [\text{nPr}_4\text{N}][\text{BAR}^{\text{F}}_4]$.

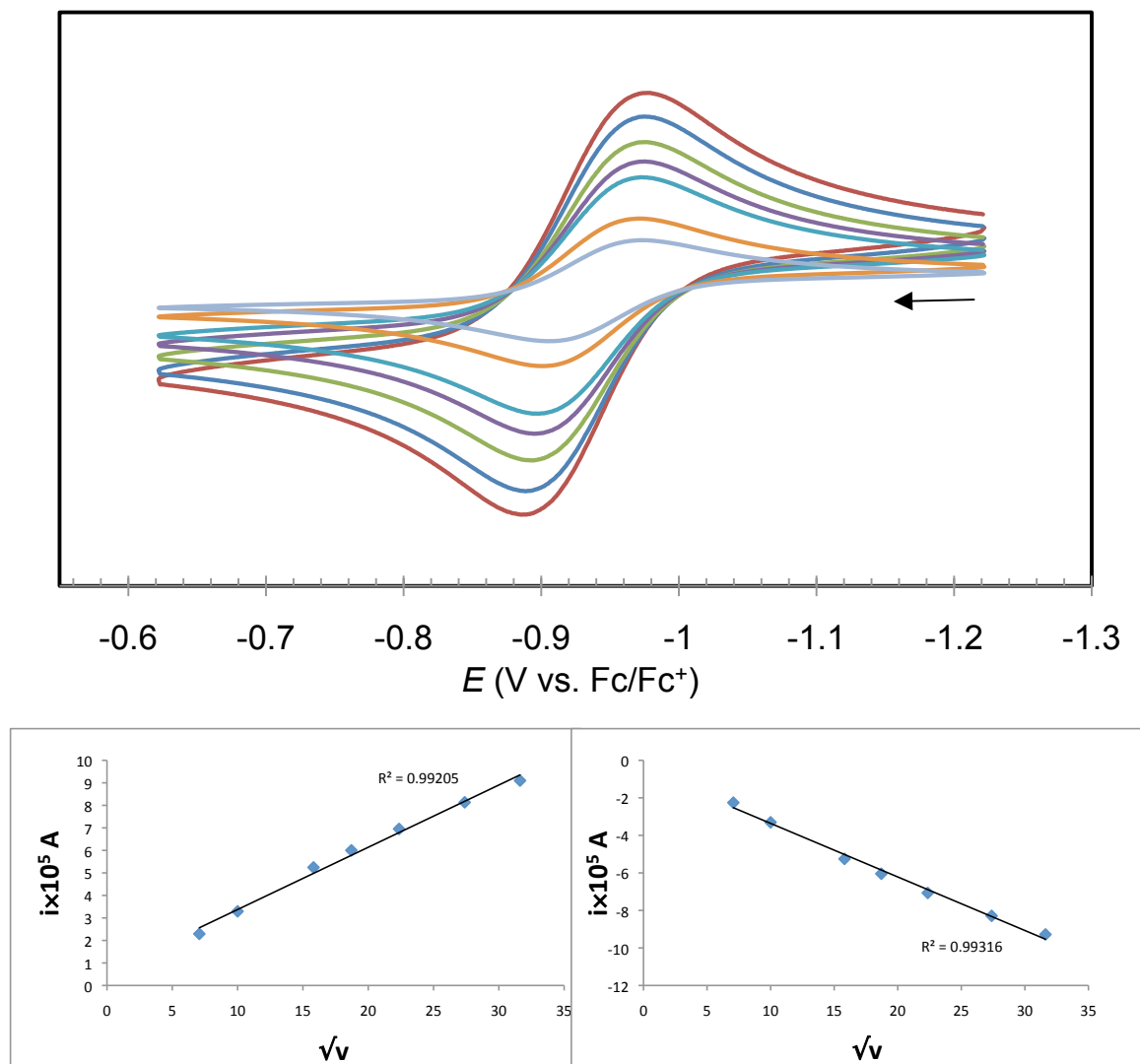


Figure S11. Scan rate dependence of the U^{IV}/U^V couple in cyclic voltammograms of $[U(pyNO)_4]$ in THF with 0.1M $[nPr_4N][BAr^F_4]$ and associated Randles-Sevcik plots.

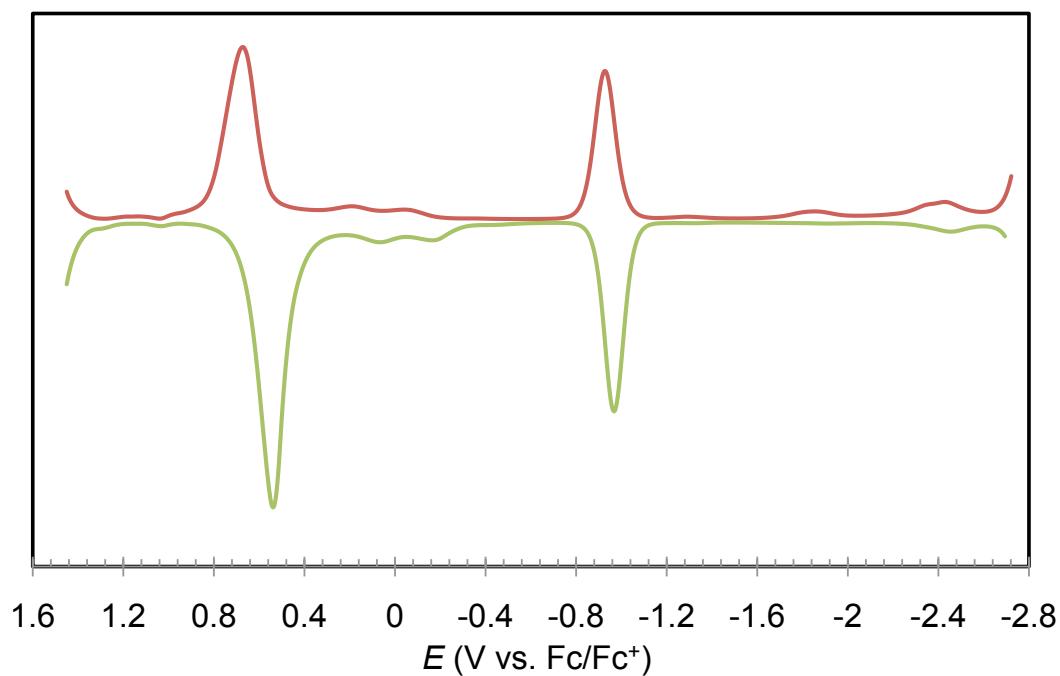


Figure S12. Differential pulse voltammograms of $[\text{U}(\text{pyNO})_4]$ recorded in THF with 0.1 M $[\text{nPr}_4\text{N}][\text{BAr}^{\text{F}}_4]$.

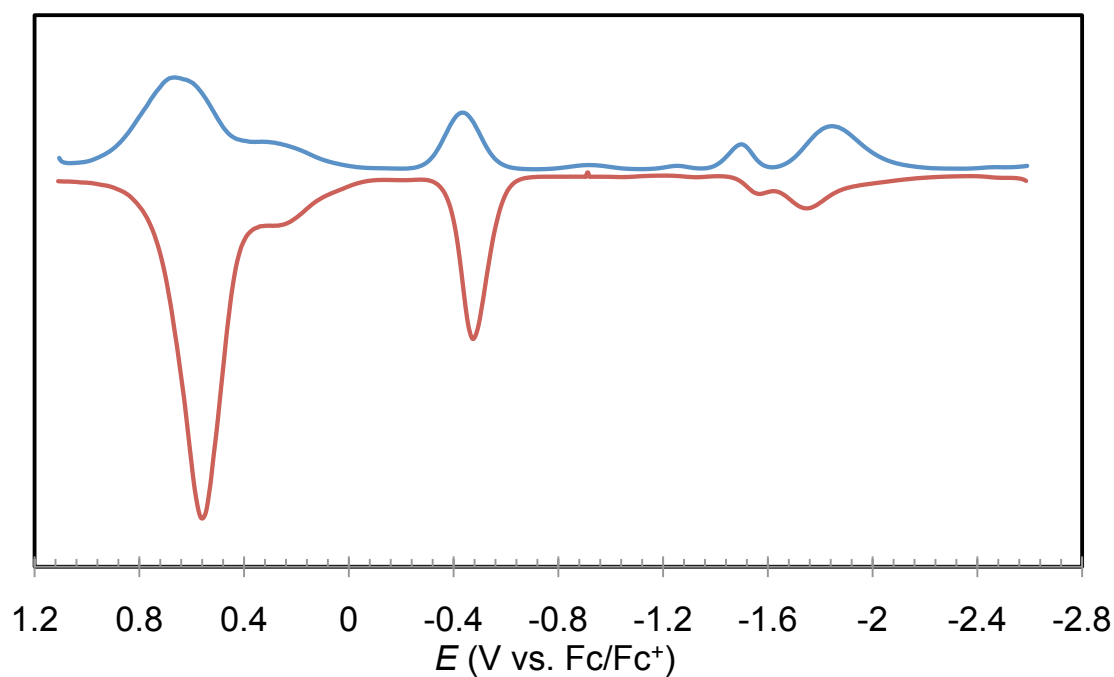


Figure S13. Differential pulse voltammograms of $[\text{Ce}(\text{pyNO})_4]$ recorded in THF with 0.1 M $[\text{nPr}_4\text{N}][\text{BAr}^{\text{F}}_4]$.

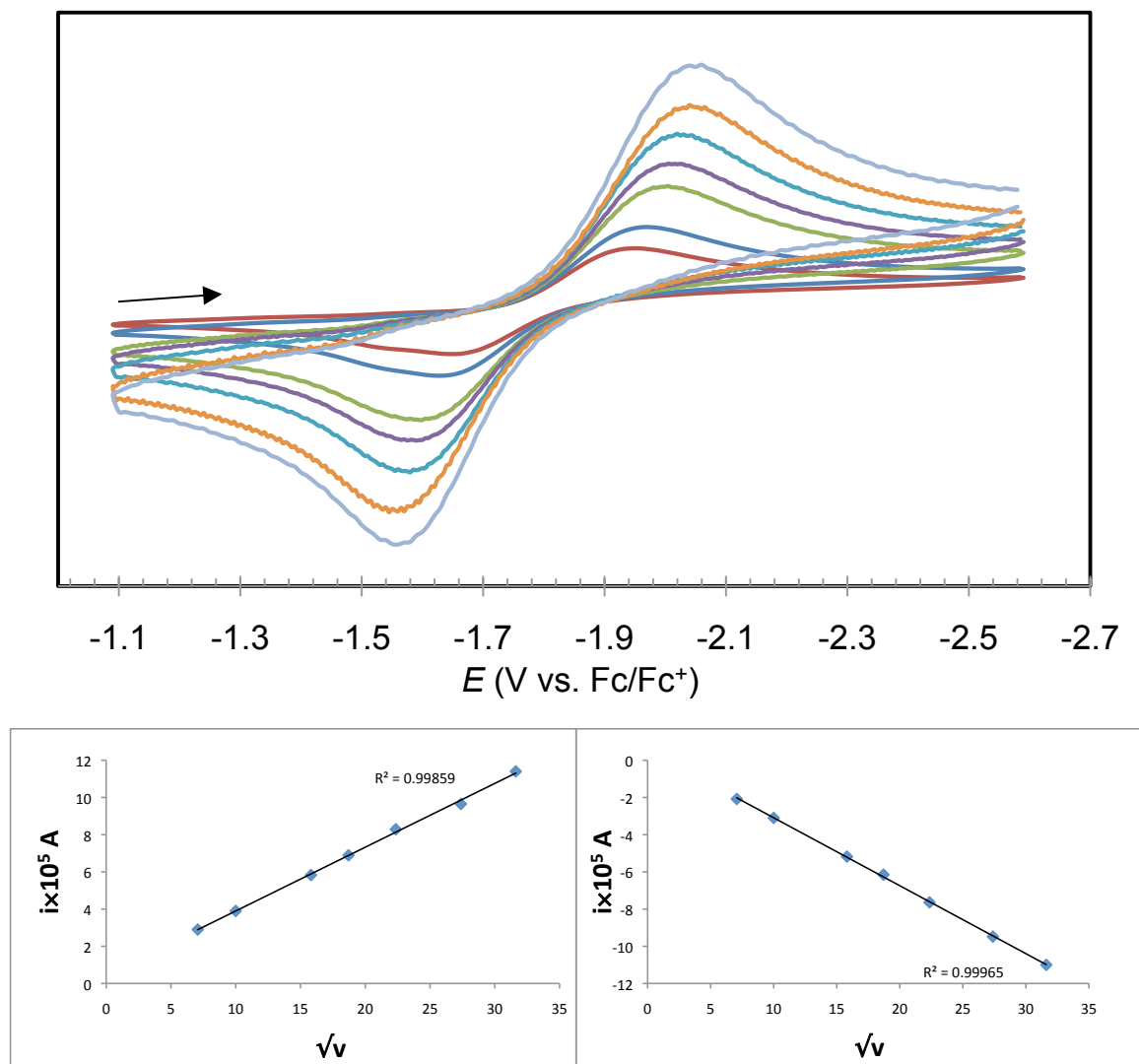


Figure S14. Scan rate dependence of the $\text{Ce}^{\text{III}}/\text{Ce}^{\text{IV}}$ couple in cyclic voltammograms of $[\text{Ce}(\text{pyNO})_4]$ in THF with 0.1M $[\text{nPr}_4\text{N}][\text{BAR}^{\text{F}}_4]$ and associated Randles-Sevcik plots.

Additional Computational Data

Table S1. Optimized M–O and M–N bond lengths in Å of $[M(\text{pyNO})_4]^{-/0}$ (M=Ce, Th and U) and $[\text{U}(\text{pyNO})_4]^+$. The average values are in parentheses.

M	M-O	M-N
$[\text{M}(\text{pyNO})_4]^-$		
Ce	2.40, 2.40, 2.40, 2.40 (2.40)	2.71, 2.71, 2.71, 2.71 (2.71)
Th	2.36, 2.36, 2.32, 2.32 (2.34)	2.69, 2.69, 2.60, 2.60 (2.64)
U	2.34, 2.34, 2.34, 2.34 (2.34)	2.64, 2.64, 2.64, 2.64 (2.64)
$[\text{M}(\text{pyNO})_4]$		
Ce	2.25, 2.25, 2.25, 2.25 (2.25)	2.63, 2.63, 2.63, 2.63 (2.63)
Th	2.32, 2.32, 2.32, 2.32 (2.32)	2.67, 2.67, 2.67, 2.67 (2.67)
U	2.25, 2.25, 2.25, 2.25 (2.25)	2.62, 2.62, 2.62, 2.62 (2.62)
$[\text{U}(\text{pyNO})_4]^+$		
U	2.16, 2.16, 2.16, 2.16 (2.16)	2.56, 2.56, 2.57, 2.57 (2.57)

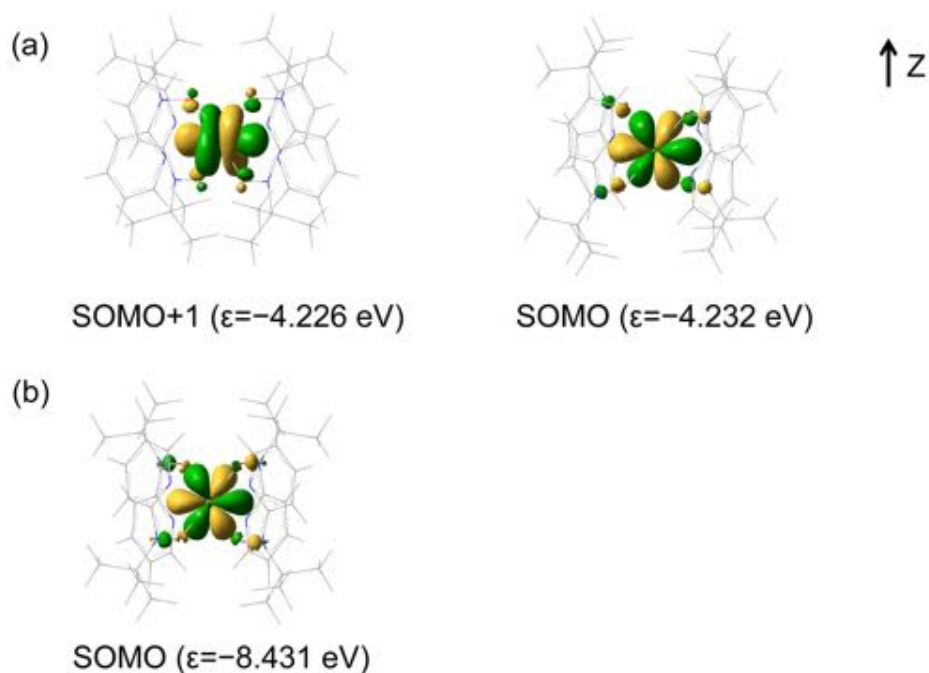


Figure S15. Envelop of Singly occupied molecular orbitals (SOMOs) for (a) $[\text{U}(\text{pyNO})_4]$ and (b) $[\text{U}(\text{pyNO})_4]^+$ with contour values of 0.03 au and Z direction labeled in arrow. The orbital energies are given in parentheses.

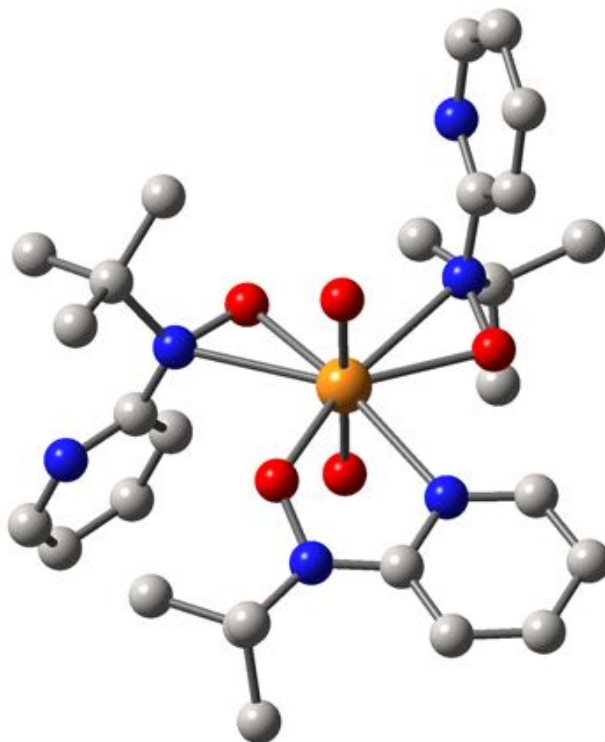


Figure S16. The optimized geometrical structure of $[\text{UO}_2(\text{pyNO})_3]^-$. The hydrogen atoms are not shown for clarity.

Table S2. Experimental and calculated bond lengths for $[\text{UO}_2(\text{pyNO})_3]^-$

	U=O ^b	U-O _{pyNO} ^c	U-N
Calc.	1.80, 1.80 (1.80)	2.33, 2.34, 2.31 (2.33)	2.69, 2.70, 2.65 (2.68)
Expt.	1.81, 1.80 (1.80)	2.30, 2.32, 2.29 (2.30)	2.58, 2.59, 2.60 (2.59)

Table S3. Calculated absolute redox potentials 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 ($\Delta E_{\text{SO}} = E_{\text{SO}} - E_{\text{SR}}$). The E_{SR} for $\text{Fc}^+ \rightarrow \text{Fc}^0$ is calculated to be -5.436 V, and SOC correction is neglected for these light transition metal compounds.^a

	E_{SR} (V)	E_{so} (V)	ΔE_{SO} (V)
$[\text{Ce}(\text{pyNO})_4]^0 \rightarrow [\text{Ce}(\text{pyNO})_4]^-$	-3.225	-3.352	-0.127
$[\text{U}(\text{pyNO})_4]^0 \rightarrow [\text{U}(\text{pyNO})_4]^-$	-1.636	-1.649	-0.013
$[\text{U}(\text{pyNO})_4]^+ \rightarrow [\text{U}(\text{pyNO})_4]^0$	-4.163	-4.457	-0.294

^a The E_{SR} for $[\text{Th}(\text{pyNO})_4]^0 \rightarrow [\text{Th}(\text{pyNO})_4]^-$ is calculated to be -1.337 V, and SO correction is neglected because the Th center is of $5f^0$ configuration with oxidation state of +4 in both complexes of $[\text{Th}(\text{pyNO})_4]^0$ and $[\text{Th}(\text{pyNO})_4]^-$.

Table S4. Cartesian coordinates (in Å) of optimized geometries of $[\text{M}(\text{pyNO})_4]^{-/0}$ (M = Ce, Th and U), $[\text{U}(\text{pyNO})_4]^+$ and $[\text{UO}_2(\text{pyNO})_3]^-$.

[Ce(pyNO) ₄] [−]				[Ce(pyNO) ₄] ⁰			
Ce	-0.00000500	-0.00000400	-0.00366800	Ce	0.00000700	0.00000500	0.00000200
O	1.00207900	1.20646500	1.81874900	O	0.92734900	1.15967100	1.69524200
O	1.00381000	-1.19810800	-1.81893200	O	0.92916000	-1.15820200	-1.69525400
O	-1.00209400	-1.20647500	1.81874600	O	-0.92732600	-1.15965600	1.69525300
O	-1.00381500	1.19810300	-1.81893300	O	-0.92915700	1.15820800	-1.69525000
N	1.97563600	2.16265600	1.79098200	N	1.94323800	2.07226600	1.71752400
N	2.05532600	1.71470000	-0.45650600	N	2.00567800	1.62140900	-0.52533900
N	1.98102900	-2.15081000	-1.79116000	N	1.94646100	-2.06922100	-1.71752400
N	2.05005600	-1.71616500	0.45951700	N	2.00816800	-1.61830500	0.52534000
N	-1.97564800	-2.16266900	1.79097400	N	-1.94321000	-2.07225700	1.71754000
N	-2.05533300	-1.71471000	-0.45651300	N	-2.00566900	-1.62139800	-0.52532300
N	-1.98103200	2.15080700	-1.79116200	N	-1.94645400	2.06923100	-1.71751600
N	-2.05007100	1.71615200	0.45951300	N	-2.00815000	1.61831800	0.52534800
C	2.55622100	2.42263000	0.59826200	C	2.52151800	2.32711300	0.51655300
C	2.56600600	1.89346100	-1.67753500	C	2.51622300	1.78618000	-1.75494400
C	3.59299700	2.77437200	-1.97530400	C	3.55108900	2.65132200	-2.05004400
C	4.12028400	3.51075400	-0.90186400	C	4.08904900	3.38898900	-0.98369700
C	3.62457100	3.34987900	0.37165600	C	3.59266400	3.23997800	0.29111600
C	2.28345800	2.81304000	3.09864400	C	2.19391900	2.75391900	3.02591700
C	3.72582600	2.48479200	3.54087700	C	3.63279900	2.47307100	3.50509000
C	2.03270200	4.33467900	3.02442800	C	1.90696400	4.26481300	2.90962600
C	1.32671400	2.24246500	4.15841000	C	1.22789900	2.17040700	4.06884700
C	2.55571400	-2.41792900	-0.59686800	C	2.52515100	-2.32315300	-0.51656200
C	2.55712600	-1.90060800	1.68132000	C	2.51896600	-1.78228700	1.75494500
C	3.58354800	-2.78240800	1.97820600	C	3.55522700	-2.64576700	2.05002700
C	4.11448900	-3.51374900	0.90321300	C	4.09439300	-3.38252700	0.98365900
C	3.62287100	-3.34653000	-0.37117000	C	3.59777600	-3.23428300	-0.29115200
C	2.29027400	-2.79886500	-3.09962000	C	2.19831200	-2.75039600	-3.02593100
C	1.33918600	-2.22204900	-4.16114600	C	1.23133600	-2.16844800	-4.06885200
C	2.03397000	-4.31982100	-3.03011000	C	1.91388500	-4.26177200	-2.90968900
C	3.73508100	-2.47443600	-3.53680400	C	3.63674600	-2.46713400	-3.50502000
C	-2.55623100	-2.42264400	0.59825200	C	-2.52150100	-2.32709700	0.51657400
C	-2.56600700	-1.89346800	-1.67754500	C	-2.51623000	-1.78616800	-1.75492100
C	-3.59299500	-2.77437900	-1.97532300	C	-3.55110700	-2.65130500	-2.05000300
C	-4.12028700	-3.51076300	-0.90188700	C	-4.08906500	-3.38895900	-0.98364500
C	-3.62458000	-3.34989300	0.37163600	C	-3.59266300	-3.23994600	0.29116100
C	-2.28345700	-2.81304300	3.09864400	C	-2.19390600	-2.75393000	3.02592100
C	-3.72582200	-2.48480300	3.54089500	C	-3.63286400	-2.47324800	3.50495300

C	-2.03266800	-4.33467900	3.02445900	C	-1.90679100	-4.26479300	2.90964300
C	-1.32670600	-2.24242800	4.15838100	C	-1.22804100	-2.17032600	4.06894600
C	-2.55572300	2.41792200	-0.59687100	C	-2.52514000	2.32316400	-0.51655200
C	-2.55714800	1.90059000	1.68131500	C	-2.51894200	1.78230100	1.75495600
C	-3.58357200	2.78238800	1.97819800	C	-3.55520500	2.64577700	2.05004200
C	-4.11450700	3.51373400	0.90320600	C	-4.09438300	3.38253000	0.98367500
C	-3.62288100	3.34652100	-0.37117500	C	-3.59777200	3.23428400	-0.29113900
C	-2.29027200	2.79887100	-3.09961800	C	-2.19830600	2.75040200	-3.02592500
C	-1.33918400	2.22206100	-4.16114800	C	-1.23141600	2.16835800	-4.06887100
C	-2.03396400	4.31982700	-3.03009500	C	-1.91375500	4.26175900	-2.90973000
C	-3.73508000	2.47445100	-3.53680500	C	-3.63678200	2.46724000	-3.50494800
H	2.11004800	1.27399300	-2.44554600	H	2.04988200	1.17526600	-2.52091400
H	3.96862400	2.87848200	-2.98674800	H	3.92636900	2.74840200	-3.06137400
H	4.93332800	4.21443400	-1.06546800	H	4.90586800	4.08387900	-1.15488800
H	4.05752300	3.91951000	1.17903900	H	4.02287800	3.81096900	1.09807200
H	3.85330000	1.40156500	3.60308900	H	3.79415000	1.39651300	3.59496000
H	3.92743700	2.91057000	4.52961200	H	3.79392400	2.92480300	4.48794500
H	4.48284500	2.86480100	2.85499800	H	4.39717700	2.86520200	2.83506900
H	2.66742300	4.84463600	2.30076900	H	2.55702100	4.77425900	2.19879600
H	2.20818900	4.79397900	4.00293700	H	2.04039600	4.74662500	3.88228800
H	0.99426200	4.52157500	2.74166000	H	0.87472300	4.42492700	2.59040600
H	0.28808900	2.43400600	3.89504800	H	0.18927800	2.34212700	3.79107800
H	1.54723100	2.72118900	5.11884900	H	1.42009200	2.65967200	5.02763000
H	1.44278200	1.16555300	4.26095000	H	1.36727700	1.09721000	4.19147100
H	2.09857400	-1.28549600	2.45131400	H	2.05163700	-1.17214700	2.52092900
H	3.95587600	-2.89101800	2.99040200	H	3.93065600	-2.74227000	3.06135600
H	4.92682900	-4.21836600	1.06615200	H	4.91234200	-4.07609100	1.15483300
H	4.05807500	-3.91267200	-1.17977900	H	4.02892500	-3.80453900	-1.09813200
H	0.29897600	-2.41014300	-3.90182600	H	0.19299800	-2.34187700	-3.79108800
H	1.56130900	-2.69923600	-5.12197400	H	1.42433400	-2.65737800	-5.02764300
H	1.45968500	-1.14532000	-4.26094900	H	1.36894800	-1.09502100	-4.19145800
H	2.66445500	-4.83355200	-2.30538300	H	2.56475900	-4.77014500	-2.19883700
H	2.21122700	-4.77745900	-4.00907700	H	2.04818200	-4.74333300	-3.88235500
H	0.99391400	-4.50372000	-2.75132900	H	0.88189700	-4.42362800	-2.59052900
H	3.86646700	-1.39151000	-3.59596200	H	3.79632600	-1.39030500	-3.59479700
H	3.93780700	-2.89842700	-4.52606600	H	3.79866200	-2.91852400	-4.48790200
H	4.48906500	-2.85868100	-2.85002300	H	4.40173700	-2.85806100	-2.83499000
H	-2.11004500	-1.27399700	-2.44555200	H	-2.04989600	-1.17526000	-2.52089900
H	-3.96861700	-2.87848600	-2.98676800	H	-3.92640100	-2.74838500	-3.06132700
H	-4.93332900	-4.21444300	-1.06549800	H	-4.90589700	-4.08383700	-1.15482100
H	-4.05753900	-3.91952600	1.17901200	H	-4.02287700	-3.81091900	1.09813300
H	-3.85330600	-1.40157600	3.60309200	H	-3.79434500	-1.39671000	3.59481700
H	-3.92741100	-2.91056600	4.52964200	H	-3.79403800	-2.92501000	4.48778600
H	-4.48284900	-2.86483200	2.85503700	H	-4.39712600	-2.86546200	2.83484600
H	-2.66738400	-4.84466800	2.30082000	H	-2.55674300	-4.77430000	2.19875900
H	-2.20813500	-4.79396000	4.00298100	H	-2.04025100	-4.74662300	3.88229200

H	-0.99422800	-4.52155900	2.74168500
H	-0.28808200	-2.43395900	3.89500700
H	-1.54720000	-2.72113200	5.11883400
H	-1.44279000	-1.16551500	4.26089600
H	-2.09860200	1.28547300	2.45130800
H	-3.95590700	2.89099400	2.99039300
H	-4.92684700	4.21835100	1.06614300
H	-4.05808000	3.91266600	-1.17978500
H	-0.29897400	2.41015100	-3.90182600
H	-1.56130600	2.69925600	-5.12197200
H	-1.45968500	1.14533300	-4.26095900
H	-2.66445000	4.83355200	-2.30536600
H	-2.21121900	4.77747200	-4.00905900
H	-0.99390900	4.50372100	-2.75131100
H	-3.86647000	1.39152600	-3.59597000
H	-3.93780400	2.89845000	-4.52606400
H	-4.48906200	2.85869500	-2.85002000

[Th(pyNO)₄]⁻

Th	-0.00060800	0.00000200	0.00000400
O	-1.07880700	1.05472500	-1.81573900
O	-1.07954200	-1.05397100	1.81574900
O	0.94808700	-1.10812100	-1.80138200
O	0.94895500	1.10740200	1.80136300
N	-2.00750600	2.06275000	-1.82734500
N	-1.90386300	1.83982800	0.44983800
N	-2.00928400	-2.06101300	1.82743700
N	-1.90526300	-1.83847100	-0.44976600
N	1.80594400	-2.19734000	-1.80400000
N	1.85238400	-1.77210400	0.45582000
N	1.80753100	2.19606000	1.80393300
N	1.85365200	1.77072000	-0.45587500
C	-2.47968100	2.45800300	-0.62188800
C	-2.30095200	2.16591600	1.69404100
C	-3.27604200	3.10594300	1.97287800
C	-3.88146000	3.74383100	0.88043600
C	-3.50093900	3.43266600	-0.41077100
C	-2.39487600	2.57369500	-3.17253100
C	-3.87276200	2.24150900	-3.47101300
C	-2.10728300	4.08658300	-3.27994900
C	-1.53014300	1.86618900	-4.22858500
C	-2.48152000	-2.45619800	0.62198600
C	-2.30253900	-2.16435900	-1.69395300

H	-0.87450900	-4.42480100	2.59050200
H	-0.18937600	-2.34193500	3.79127200
H	-1.42027100	-2.65962100	5.02770700
H	-1.36754100	-1.09714500	4.19156900
H	-2.05160600	1.17216400	2.52093900
H	-3.93062900	2.74228000	3.06137300
H	-4.91233700	4.07608700	1.15485100
H	-4.02893400	3.80453100	-1.09811800
H	-0.19305300	2.34171200	-3.79114800
H	-1.42441200	2.65728500	-5.02766400
H	-1.36911700	1.09493900	-4.19145000
H	-2.56456200	4.77020400	-2.19886800
H	-2.04804900	4.74330700	-3.88240300
H	-0.88174300	4.42354200	-2.59061200
H	-3.79644600	1.39042200	-3.59470200
H	-3.79870600	2.91862700	-4.48783000
H	-4.40171400	2.85823500	-2.83489100

[Th(pyNO)₄]⁰

Th	-0.00000100	0.00000400	0.00000300
O	0.98784400	1.15702700	1.74592500
O	0.98965900	-1.15546500	-1.74593300
O	-0.98784000	-1.15702100	1.74592800
O	-0.98966700	1.15547300	-1.74592900
N	2.00309600	2.07903200	1.76399200
N	1.99089200	1.71111800	-0.49890900
N	2.00628700	-2.07595000	-1.76398400
N	1.99365700	-1.70789200	0.49888700
N	-2.00308900	-2.07903000	1.76399500
N	-1.99089500	-1.71111000	-0.49890500
N	-2.00629800	2.07595400	-1.76397700
N	-1.99365600	1.70790000	0.49889400
C	2.53655200	2.37940600	0.55769600
C	2.46095900	1.93610700	-1.73879100
C	3.47762300	2.82023800	-2.03047300
C	4.04620500	3.51650100	-0.95028900
C	3.59459600	3.31012000	0.33140400
C	2.32559500	2.68133800	3.09462100
C	3.78412300	2.36478400	3.48427800
C	2.04521100	4.19811800	3.08162600
C	1.40854400	2.04454300	4.15060100
C	2.54031900	-2.37537300	-0.55771100
C	2.46415700	-1.93206600	1.73875300

C	-3.27820900	-3.10378900	-1.97277500	C	3.48224800	-2.81455700	2.03042200
C	-3.88397200	-3.74132300	-0.88031500	C	4.05189300	-3.50995500	0.95023900
C	-3.50328200	-3.43034400	0.41087900	C	3.59988000	-3.30436200	-0.33143700
C	-2.39656600	-2.57203000	3.17262500	C	2.32975500	-2.67773800	-3.09460500
C	-1.53163500	-1.86469500	4.22862400	C	1.41159200	-2.04250500	-4.15056200
C	-2.10920000	-4.08497400	3.27988100	C	2.05191100	-4.19498700	-3.08156000
C	-3.87435600	-2.23961800	3.47133800	C	3.78774600	-2.35876500	-3.48429800
C	2.42038000	-2.43443200	-0.59722700	C	-2.53655000	-2.37940000	0.55770100
C	2.32250500	-2.01783600	1.71298000	C	-2.46097100	-1.93609700	-1.73878400
C	3.36327700	-2.88396800	1.98625200	C	-3.47763800	-2.82022600	-2.03046100
C	3.97976200	-3.53258200	0.91051000	C	-4.04621800	-3.51648700	-0.95027400
C	3.51646500	-3.30017900	-0.39050700	C	-3.59460100	-3.31010900	0.33141600
C	2.34138500	-2.53431200	-3.15243200	C	-2.32558400	-2.68134700	3.09461900
C	3.71029200	-1.86442600	-3.39301900	C	-3.78413700	-2.36486000	3.48423700
C	2.40571400	-4.06563400	-3.33958100	C	-2.04513400	-4.19811500	3.08163000
C	1.34772900	-2.00912600	-4.20416500	C	-1.40858300	-2.04450900	4.15061800
C	2.42214800	2.43266100	0.59715100	C	-2.54032200	2.37538300	-0.55770200
C	2.32395600	2.01607300	-1.71304600	C	-2.46414800	1.93207700	1.73876300
C	3.36537000	2.88142500	-1.98633900	C	-3.48223300	2.81457200	2.03043900
C	3.98234700	3.52960500	-0.91061800	C	-4.05187800	3.50997600	0.95026000
C	3.51888000	3.29757100	0.39041000	C	-3.59987400	3.30438100	-0.33141900
C	2.34321300	2.53271200	3.15234300	C	-2.32976700	2.67773400	-3.09460200
C	1.34915800	2.00834300	4.20411200	C	-1.41155500	2.04253600	-4.15053700
C	2.40869400	4.06399700	3.33939800	C	-2.05198200	4.19499200	-3.08155200
C	3.71162200	1.86182300	3.39296700	C	-3.78773500	2.35869800	-3.48433400
H	-1.78690600	1.62767100	2.48323400	H	1.97504900	1.35628500	-2.51693400
H	-3.55444300	3.33100200	2.99606800	H	3.81771000	2.96402500	-3.04851000
H	-4.65985300	4.48590300	1.03809600	H	4.85180300	4.22502900	-1.11877000
H	-3.98638300	3.92482100	-1.23841100	H	4.04707200	3.85136900	1.14638200
H	-4.02737300	1.16179900	-3.40934800	H	3.94027400	1.28384800	3.50205600
H	-4.13891700	2.56872200	-4.48141700	H	3.99728800	2.75614200	4.48297900
H	-4.56639700	2.71345800	-2.77502200	H	4.51787200	2.79207000	2.80153700
H	-2.67383400	4.68703500	-2.56929100	H	2.66167800	4.74608800	2.36963700
H	-2.35040700	4.44345300	-4.28592400	H	2.23206500	4.62106900	4.07269500
H	-1.04668800	4.27347200	-3.09782100	H	0.99932200	4.38204400	2.82586800
H	-0.47050100	2.05204200	-4.06115600	H	0.35845700	2.23472400	3.93492100
H	-1.80644300	2.25115200	-5.21561400	H	1.65098800	2.47980700	5.12392200
H	-1.68144200	0.78868300	-4.21362600	H	1.54720500	0.96593200	4.20695900
H	-1.78813000	-1.62648600	-2.48316400	H	1.97737500	-1.35297200	2.51689300
H	-3.55673500	-3.32871700	-2.99595900	H	3.82262300	-2.95774800	3.04844700
H	-4.66274700	-4.48299800	-1.03796100	H	4.85864700	-4.21716900	1.11870600
H	-3.98893100	-3.92229000	1.23852300	H	4.05319200	-3.84490300	-1.14642100
H	-0.47204400	-2.05078700	4.06117600	H	0.36183400	-2.23443100	-3.93482200
H	-1.80800700	-2.24955200	5.21567400	H	1.65470900	-2.47740300	-5.12387700
H	-1.68269600	-0.78715000	4.21363300	H	1.54845200	-0.96366700	-4.20696700
H	-2.67593500	-4.68523800	2.56920400	H	2.66931700	-4.74190800	-2.36957900

H	-2.35227000	-4.44192300	4.28584200
H	-1.04865600	-4.27201600	3.09761100
H	-4.02879400	-1.15987700	3.40980000
H	-4.14040000	-2.56688000	4.48175500
H	-4.56820000	-2.71137700	2.77543400
H	1.82113800	-1.46317900	2.49789300
H	3.69153800	-3.03700300	3.00946000
H	4.81829300	-4.20442500	1.06883500
H	4.01323300	-3.78072900	-1.21750200
H	3.62055900	-0.78383300	-3.25853000
H	4.06259700	-2.05728200	-4.41226400
H	4.47288800	-2.22048900	-2.69857900
H	3.11169100	-4.56415000	-2.67915800
H	2.69780800	-4.29711400	-4.36892000
H	1.42026700	-4.50065100	-3.15742500
H	0.35302600	-2.42817400	-4.04424300
H	1.69734000	-2.30848200	-5.19772000
H	1.26071700	-0.92627600	-4.16763100
H	1.82217300	1.46177100	-2.49794400
H	3.69373500	3.03419200	-3.00955400
H	4.82138200	4.20081500	-1.06896200
H	4.01602000	3.77775400	1.21739600
H	0.35476600	2.42811000	4.04414100
H	1.69897500	2.30752700	5.19764700
H	1.26135400	0.92555500	4.16766700
H	3.11506900	4.56194100	2.67897100
H	2.70092800	4.29531500	4.36873400
H	1.42358100	4.49974700	3.15718500
H	3.62108400	0.78128900	3.25853800
H	4.06407800	2.05447400	4.41219800
H	4.47447400	2.21728200	2.69849700

[U(pyNO)₄]⁻

O	-0.40423000	1.54950900	1.71252700
O	1.59392100	-0.14897100	-1.71229600
O	0.40423000	-1.54950900	1.71252700
O	-1.59392100	0.14897100	-1.71229600
N	-0.21984300	2.91458000	1.69785200
N	0.20246500	2.58105700	-0.53438700
N	2.91184600	0.25155700	-1.69793300
N	2.51521300	0.61659800	0.53411600
N	0.21984300	-2.91458000	1.69785200
N	-0.20246500	-2.58105700	-0.53438700

H	2.23944700	-4.61764100	-4.07262600
H	1.00634000	-4.38066200	-2.82576700
H	3.94210500	-1.27757200	-3.50208400
H	4.00154000	-2.74977300	-4.48300200
H	4.52221600	-2.78483500	-2.80156700
H	-1.97506500	-1.35627500	-2.51692900
H	-3.81773200	-2.96401100	-3.04849600
H	-4.85182000	-4.22501100	-1.11875000
H	-4.04707500	-3.85135300	1.14639900
H	-3.94033600	-1.28393100	3.50201700
H	-3.99731300	-2.75623400	4.48293000
H	-4.51784700	-2.79217400	2.80147000
H	-2.66156200	-4.74611200	2.36962700
H	-2.23199000	-4.62107300	4.07269500
H	-0.99923200	-4.38199500	2.82589300
H	-0.35848400	-2.23464100	3.93495900
H	-1.65102700	-2.47978500	5.12393300
H	-1.54729500	-0.96590400	4.20697300
H	-1.97736400	1.35298000	2.51690000
H	-3.82260100	2.95776400	3.04846600
H	-4.85862500	4.21719600	1.11873300
H	-4.05318400	3.84493100	-1.14639800
H	-0.36181000	2.23450600	-3.93477400
H	-1.65466900	2.47742200	-5.12385900
H	-1.54837000	0.96369300	-4.20694200
H	-2.66942300	4.74189100	-2.36958400
H	-2.23951300	4.61764000	-4.07262200
H	-1.00642300	4.38070800	-2.82573800
H	-3.94204800	1.27749900	-3.50212100
H	-4.00151700	2.74969300	-4.48304600
H	-4.52224300	2.78473900	-2.80162700

[U(pyNO)₄]⁰

O	-0.28242200	1.54710200	1.60830500
O	1.57351900	-0.04310000	-1.60854000
O	0.28242200	-1.54710200	1.60830500
O	-1.57351900	0.04310000	-1.60854000
N	-0.16816200	2.91615500	1.59155300
N	0.12469500	2.53660100	-0.64825400
N	2.90930100	0.27756300	-1.59141900
N	2.48738300	0.51331900	0.64752700
N	0.16816200	-2.91615500	1.59155300
N	-0.12469500	-2.53660100	-0.64825400

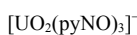
N	-2.91184600	-0.25155700	-1.69793300
N	-2.51521300	-0.61659800	0.53411600
C	-0.01275000	3.47454000	0.47648400
C	0.45397900	3.03623700	-1.77135600
C	0.49785900	4.37624500	-2.11566200
C	0.25732400	5.30432600	-1.09285600
C	0.00000000	4.87122700	0.19372000
C	-0.65031700	3.61661500	2.94013300
C	0.43563500	4.61076200	3.40451200
C	-2.01801000	4.30359400	2.73816900
C	-0.80619400	2.56871500	4.05586400
C	3.43154500	0.54615500	-0.47675100
C	2.92439900	0.93911600	1.77068400
C	4.24012900	1.19726300	2.11462600
C	5.19471700	1.10685600	1.09192600
C	4.80829000	0.78207600	-0.19422200
C	3.67373900	-0.06234300	-2.93989500
C	2.66419800	-0.38352900	-4.05561500
C	4.56957100	-1.30313600	-2.73695000
C	4.48247100	1.16775600	-3.40482200
C	0.01275000	-3.47454000	0.47648400
C	-0.45397900	-3.03623700	-1.77135600
C	-0.49785900	-4.37624500	-2.11566200
C	-0.25732400	-5.30432600	-1.09285600
C	0.00000000	-4.87122700	0.19372000
C	0.65031700	-3.61661500	2.94013300
C	-0.43563500	-4.61076200	3.40451200
C	2.01801000	-4.30359400	2.73816900
C	0.80619400	-2.56871500	4.05586400
C	-3.43154500	-0.54615500	-0.47675100
C	-2.92439900	-0.93911600	1.77068400
C	-4.24012900	-1.19726300	2.11462600
C	-5.19471700	-1.10685600	1.09192600
C	-4.80829000	-0.78207600	-0.19422200
C	-3.67373900	0.06234300	-2.93989500
C	-2.66419800	0.38352900	-4.05561500
C	-4.56957100	1.30313600	-2.73695000
C	-4.48247100	-1.16775600	-3.40482200
H	0.62820400	2.25624300	-2.50642300
H	0.70511200	4.68273200	-3.13483300
H	0.26374100	6.37123000	-1.30155500
H	-0.19914200	5.60119000	0.96221600
H	1.38066700	4.08256700	3.55023100
H	0.14365800	5.06094800	4.35885700
H	0.62056500	5.42164000	2.70219800
H	-1.99073300	5.08449900	1.97716300

N	-2.90930100	-0.27756300	-1.59141900
N	-2.48738300	-0.51331900	0.64752700
C	-0.02249500	3.44928600	0.35096900
C	0.31392600	2.96150000	-1.90842200
C	0.35530800	4.29093600	-2.27582900
C	0.18799100	5.24078300	-1.25615000
C	0.00000000	4.84042100	0.04682500
C	-0.57515000	3.61848600	2.84883900
C	0.52806100	4.60376500	3.28569200
C	-1.93683400	4.31796700	2.66417500
C	-0.72204300	2.56918700	3.96224000
C	3.41246800	0.50753100	-0.35110600
C	2.87723800	0.76749100	1.90757900
C	4.18407000	1.01461300	2.27534800
C	5.14872000	0.99657300	1.25596200
C	4.78291400	0.74750300	-0.04695100
C	3.66671300	-0.02076400	-2.84719800
C	2.65360200	-0.33825900	-3.95852300
C	4.57244800	-1.25399100	-2.65606300
C	4.46540100	1.22168100	-3.29089300
C	0.02249500	-3.44928600	0.35096900
C	-0.31392600	-2.96150000	-1.90842200
C	-0.35530800	-4.29093600	-2.27582900
C	-0.18799100	-5.24078300	-1.25615000
C	0.00000000	-4.84042100	0.04682500
C	0.57515000	-3.61848600	2.84883900
C	-0.52806100	-4.60376500	3.28569200
C	1.93683400	-4.31796700	2.66417500
C	0.72204300	-2.56918700	3.96224000
C	-3.41246800	-0.50753100	-0.35110600
C	-2.87723800	-0.76749100	1.90757900
C	-4.18407000	-1.01461300	2.27534800
C	-5.14872000	-0.99657300	1.25596200
C	-4.78291400	-0.74750300	-0.04695100
C	-3.66671300	0.02076400	-2.84719800
C	-2.65360200	0.33825900	-3.95852300
C	-4.57244800	1.25399100	-2.65606300
C	-4.46540100	-1.22168100	-3.29089300
H	0.43635800	2.16793600	-2.63760800
H	0.50806000	4.57914600	-3.30859300
H	0.20345500	6.30184900	-1.48676100
H	-0.13009300	5.58357100	0.81666300
H	1.47490900	4.07404700	3.41075300
H	0.26050200	5.05589600	4.24471800
H	0.69645200	5.41585400	2.58000600
H	-1.91478700	5.09868500	1.90320900

H	-2.36268600	4.75784300	3.67328600	H	-2.25482300	4.77993100	3.60317400
H	-2.75583600	3.56071900	2.42671500	H	-2.69460400	3.58751200	2.37171400
H	-1.57531700	1.84035700	3.81120800	H	-1.50331800	1.84754300	3.73275600
H	-1.07907400	3.08503500	4.98251400	H	-0.98123300	3.08526700	4.89061700
H	0.12298600	2.02294100	4.21963600	H	0.20630000	2.02028400	4.12044700
H	2.12673200	0.98688900	2.50588600	H	2.07376600	0.76668700	2.63615700
H	4.50956300	1.45202700	3.13349500	H	4.44467500	1.21106100	3.30806200
H	6.24689800	1.28385000	1.30043000	H	6.19427900	1.17783900	1.48667100
H	5.56066500	0.70086800	-0.96258700	H	5.53735200	0.73552700	-0.81676700
H	2.06765000	-1.25877500	-3.81069700	H	2.06455800	-1.22241200	-3.72354100
H	3.21745700	-0.57095300	-4.98216700	H	3.20412500	-0.51841300	-4.88582100
H	1.97743400	0.44683800	-4.21969000	H	1.96485000	0.49064600	-4.12161900
H	5.33635100	-1.15126500	-1.97621900	H	5.34058300	-1.10505900	-1.89665700
H	5.07268800	-1.57204600	-3.67190900	H	5.07804500	-1.50021700	-3.59413400
H	3.95357800	-2.14944100	-2.42455700	H	3.97093200	-2.11593500	-2.35848800
H	3.81057600	2.01648600	-3.55158300	H	3.79247900	2.07173000	-3.42261300
H	4.97384200	0.95041600	-4.35876700	H	4.95622500	1.02317200	-4.24769200
H	5.25322100	1.48014600	-2.70244700	H	5.23895500	1.52110100	-2.58529800
H	-0.62820400	-2.25624300	-2.50642300	H	-0.43635800	-2.16793600	-2.63760800
H	-0.70511200	-4.68273200	-3.13483300	H	-0.50806000	-4.57914600	-3.30859300
H	-0.26374100	-6.37123000	-1.30155500	H	-0.20345500	-6.30184900	-1.48676100
H	0.19914200	-5.60119000	0.96221600	H	0.13009300	-5.58357100	0.81666300
H	-1.38066700	-4.08256700	3.55023100	H	-1.47490900	-4.07404700	3.41075300
H	-0.14365800	-5.06094800	4.35885700	H	-0.26050200	-5.05589600	4.24471800
H	-0.62056500	-5.42164000	2.70219800	H	-0.69645200	-5.41585400	2.58000600
H	1.99073300	-5.08449900	1.97716300	H	1.91478700	-5.09868500	1.90320900
H	2.36268600	-4.75784300	3.67328600	H	2.25482300	-4.77993100	3.60317400
H	2.75583600	-3.56071900	2.42671500	H	2.69460400	-3.58751200	2.37171400
H	1.57531700	-1.84035700	3.81120800	H	1.50331800	-1.84754300	3.73275600
H	1.07907400	-3.08503500	4.98251400	H	0.98123300	-3.08526700	4.89061700
H	-0.12298600	-2.02294100	4.21963600	H	-0.20630000	-2.02028400	4.12044700
H	-2.12673200	-0.98688900	2.50588600	H	-2.07376600	-0.76668700	2.63615700
H	-4.50956300	-1.45202700	3.13349500	H	-4.44467500	-1.21106100	3.30806200
H	-6.24689800	-1.28385000	1.30043000	H	-6.19427900	-1.17783900	1.48667100
H	-5.56066500	-0.70086800	-0.96258700	H	-5.53735200	-0.73552700	-0.81676700
H	-2.06765000	1.25877500	-3.81069700	H	-2.06455800	1.22241200	-3.72354100
H	-3.21745700	0.57095300	-4.98216700	H	-3.20412500	0.51841300	-4.88582100
H	-1.97743400	-0.44683800	-4.21969000	H	-1.96485000	-0.49064600	-4.12161900
H	-5.33635100	1.15126500	-1.97621900	H	-5.34058300	1.10505900	-1.89665700
H	-5.07268800	1.57204600	-3.67190900	H	-5.07804500	1.50021700	-3.59413400
H	-3.95357800	2.14944100	-2.42455700	H	-3.97093200	2.11593500	-2.35848800
H	-3.81057600	-2.01648600	-3.55158300	H	-3.79247900	-2.07173000	-3.42261300
H	-4.97384200	-0.95041600	-4.35876700	H	-4.95622500	-1.02317200	-4.24769200
H	-5.25322100	-1.48014600	-2.70244700	H	-5.23895500	-1.52110100	-2.58529800
U	0.00000000	0.00000000	0.00026700	U	0.00000000	0.00000000	-0.00113700



O	0.24494700	1.51403600	-1.52388800
O	-1.53275300	-0.06705300	1.52556800
O	-0.24494700	-1.51403200	-1.52389100
O	1.53275600	0.06705000	1.52556600
N	0.12304200	2.88043100	-1.53239100
N	-0.17461700	2.46239600	0.69939600
N	-2.87592200	0.21180200	1.53254700
N	-2.42477200	0.45741800	-0.69898800
N	-0.12304400	-2.88042700	-1.53239600
N	0.17462000	-2.46239600	0.69939000
N	2.87592400	-0.21180500	1.53254400
N	2.42477300	-0.45741600	-0.69899200
C	-0.03285000	3.39528700	-0.27890800
C	-0.37729100	2.86490900	1.97124400
C	-0.43435800	4.18692800	2.35008000
C	-0.27701800	5.15549300	1.34645200
C	-0.07817800	4.77650400	0.03838900
C	0.57986200	3.58031800	-2.78408900
C	-0.50496700	4.57146800	-3.24644600
C	1.93589200	4.27054400	-2.54721900
C	0.75297100	2.52600300	-3.88750500
C	-3.36852700	0.42464900	0.27861500
C	-2.80009100	0.70488800	-1.97121400
C	-4.10637100	0.91399900	-2.35118800
C	-5.08748500	0.86918300	-1.34843100
C	-4.73513700	0.62812800	-0.04004200
C	-3.62476100	-0.15543600	2.78532100
C	-2.59826800	-0.44436600	3.89066700
C	-4.46710700	-1.42348600	2.55325500
C	-4.48414600	1.03877200	3.24195300
C	0.03285000	-3.39528500	-0.27891500
C	0.37729600	-2.86491300	1.97123700
C	0.43436300	-4.18693300	2.35006900
C	0.27702200	-5.15549500	1.34643800
C	0.07818000	-4.77650300	0.03837700
C	-0.57986600	-3.58031600	-2.78409300
C	0.50495000	-4.57148900	-3.24642900
C	-1.93590900	-4.27051900	-2.54722600



U	0.14796300	-0.18536400	0.01576000
O	-1.95198100	-0.68683400	0.84726400
O	0.69501200	2.07933400	-0.06322000
O	1.91203100	-1.51440000	-0.75400900
O	-0.54110200	-0.03958700	-1.63928100
O	0.78055200	-0.35539100	1.69056100
N	-0.72608200	-2.68422100	-0.15642000
N	-2.73614200	-1.70380300	0.35706600
N	-2.68917500	3.21256300	-0.16506300
N	-0.56830800	2.37398800	0.45238600
N	4.53810300	0.54696300	0.50380600
N	2.73801800	-0.38818700	-0.71043400
C	-2.07346900	-2.83288100	0.00553900
C	-2.66395600	-4.11540100	-0.19866900
H	-3.71561800	-4.28033400	-0.02746300
C	-1.86941300	-5.17204200	-0.58577400
H	-2.32439100	-6.14887400	-0.73113700
C	-0.49226800	-4.99593800	-0.77287700
H	0.15618700	-5.80623900	-1.08475200
C	0.01707800	-3.72913500	-0.53693300
H	1.07155000	-3.50616800	-0.66620900
C	-4.18811400	-1.56509100	0.66430400
C	-5.03769400	-1.96053700	-0.56091500
H	-4.76236800	-1.33842800	-1.41509800
H	-6.09654700	-1.79161600	-0.34171900
H	-4.92795400	-3.00090300	-0.86220900
C	-4.47170600	-0.08009700	0.94707300
H	-3.94944900	0.26407700	1.83607100
H	-5.54969100	0.04636100	1.09344100
H	-4.15093600	0.55120700	0.11947800
C	-4.55926500	-2.37912300	1.92174300
H	-4.43513200	-3.45473300	1.78400500
H	-5.60110700	-2.19576900	2.20424400
H	-3.92069000	-2.07237000	2.75316900
C	-1.44208800	2.89783000	-0.53759900
C	-1.00167900	3.04764200	-1.86723900
H	0.01162800	2.77765900	-2.11699000
C	-1.89532100	3.52236700	-2.80958700

C	-0.75295000	-2.52601100	-3.88752300	H	-1.57527400	3.64273200	-3.84099000
C	3.36852900	-0.42464800	0.27861100	C	-3.20183500	3.84045500	-2.43022100
C	2.80009100	-0.70488300	-1.97121800	H	-3.93399100	4.20537500	-3.14316300
C	4.10637000	-0.91399200	-2.35119500	C	-3.53405000	3.66645300	-1.09350200
C	5.08748600	-0.86917500	-1.34843900	H	-4.53645300	3.90225100	-0.73809400
C	4.73513900	-0.62812400	-0.04004900	C	-0.51582700	3.10346000	1.80100100
C	3.62476300	0.15543300	2.78531900	C	-1.68940800	2.63230700	2.67308800
C	2.59826600	0.44439900	3.89065100	H	-2.64470700	2.88020500	2.21610900
C	4.46713800	1.42346300	2.55324300	H	-1.62869900	3.10952000	3.65816300
C	4.48411800	-1.03878700	3.24197500	H	-1.64327600	1.55017500	2.81107600
H	-0.49415800	2.06339900	2.69042400	C	-0.55600400	4.62791500	1.58228500
H	-0.59502000	4.45977100	3.38521600	H	0.23372600	4.93122100	0.88898100
H	-0.31082600	6.21116600	1.59398100	H	-0.38453600	5.14218500	2.53318300
H	0.03931500	5.52789000	-0.72494300	H	-1.51523600	4.96285100	1.18733600
H	-1.45493700	4.05409900	-3.39508300	C	0.80182700	2.75610600	2.50667700
H	-0.20835400	5.01699300	-4.19867000	H	1.66262400	3.08382500	1.92629600
H	-0.67823900	5.39043800	-2.55005500	H	0.90075000	1.68657100	2.67887200
H	1.88936800	5.05441600	-1.79078100	H	0.81089700	3.26754400	3.47532300
H	2.28558300	4.73118100	-3.47415800	C	3.65199600	-0.44685000	0.37824200
H	2.68447200	3.54061000	-2.23064200	C	3.59101900	-1.50981700	1.30043100
H	1.52990700	1.80423300	-3.64078000	H	2.85577200	-2.28563300	1.16248200
H	1.03997000	3.03799900	-4.80810400	C	4.46771400	-1.50706100	2.36996500
H	-0.17348500	1.98286200	-4.07732800	H	4.43240300	-2.31550200	3.09516700
H	-1.98967600	0.72828800	-2.68951800	C	5.38519700	-0.46391200	2.51444400
H	-4.35800200	1.10510300	-3.38652600	H	6.08019600	-0.42160900	3.34674100
H	-6.13205100	1.02405400	-1.59695100	C	5.37072300	0.53091400	1.54648300
H	-5.49572200	0.59736600	0.72254100	H	6.06555100	1.36796100	1.60309700
H	-1.97074100	-1.30036800	3.64795300	C	3.29822800	0.00406700	-2.07987600
H	-3.14049300	-0.66641400	4.81190500	C	2.29200000	-0.40536700	-3.16353500
H	-1.95203500	0.41408100	4.07724500	H	2.13230300	-1.48228200	-3.17280600
H	-5.23923700	-1.28998600	1.79505000	H	1.32271000	0.07056200	-3.02580100
H	-4.96641500	-1.71315200	3.48087200	H	2.69457100	-0.09854100	-4.13452800
H	-3.82838800	-2.25303700	2.24135000	C	3.49039400	1.52881300	-2.13525100
H	-3.86049800	1.92313300	3.38753100	H	4.27452500	1.85602400	-1.45748400
H	-4.96171300	0.79959600	4.19480300	H	3.75193400	1.82562600	-3.15763300
H	-5.27708700	1.30293200	2.54393900	H	2.56721200	2.03583000	-1.84756100
H	0.49416400	-2.06340500	2.69041900	C	4.62006800	-0.74152000	-2.34270100
H	0.59502700	-4.45977900	3.38520400	H	4.95503200	-0.55744100	-3.36850800
H	0.31083100	-6.21117000	1.59396500	H	5.41258400	-0.41818700	-1.66741300
H	-0.03931400	-5.52788700	-0.72495700	H	4.47545300	-1.81910100	-2.22303900
H	1.45493000	-4.05413800	-3.39506500				
H	0.20833800	-5.01702200	-4.19865000				
H	0.67820200	-5.39045300	-2.55002500				
H	-1.88940200	-5.05438400	-1.79078000				
H	-2.28559900	-4.73116000	-3.47416300				
H	-2.68447900	-3.54056900	-2.23066200				

H	-1.52987800	-1.80422700	-3.64081400
H	-1.03994700	-3.03801300	-4.80811900
H	0.17351600	-1.98288400	-4.07734400
H	1.98967400	-0.72828200	-2.68952100
H	4.35800000	-1.10509300	-3.38653300
H	6.13205200	-1.02404300	-1.59696100
H	5.49572500	-0.59736000	0.72253200
H	1.97075900	1.30041100	3.64792100
H	3.14048800	0.66644800	4.81189100
H	1.95201500	-0.41403200	4.07723500
H	5.23927000	1.28993600	1.79504500
H	4.96644500	1.71313000	3.48085900
H	3.82843900	2.25302300	2.24132200
H	3.86045000	-1.92313300	3.38755800
H	4.96168000	-0.79960900	4.19482800
H	5.27706100	-1.30297300	2.54397400
U	0.00000100	0.00000000	0.00091700