Electronic Supplementary Information

Selective Np(V) extraction by unsymmetrical amide-triazine-pyridine ligand enabling simplified actinide separation

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Content

S 1 Experimental Section

S 1.1 Materials

Caution: *In the radioactive experiment, the Np(V) and Pu(IV) feed solution consisted of* ^{237}*Np and* ^{239}*Pu, while the U(VI) feed solution was* ^{238}*U. It should be noted that* ^{237}*Np,* ^{239}*Pu, and* ^{238}*U all have radioactivity and physiological toxicity. Relevant radioactive experiments were carried out in the professional radiochemistry laboratory at Northwest Institute of Nuclear Technology.*

All chemical reagents used in this work are purchased from commercial companies and are analytically pure (AR). The organic synthesis method of Et-Tol-CyMe$_4$-ATP extractant is referred to the previous work.[1]

S 1.2 Solvent Extraction and Stripping

The Et-Tol-CyMe$_4$-ATP extractant was first dissolved in 3-nitrobenzotrifluoride (F-3) to prepare organic phase solutions with concentrations ranging from 1 to 10 mM. The oxidation of Np(V) and Pu(IV) in feed liquid was controlled by $NaNO_2$. The U(VI) feed liquid was prepared by directly dissolving $UO_2(NO_3)_2\cdot 6H_2O$ in dilute nitric acid solution. The aqueous phase for extraction contained trace amounts of Np(V), Pu(IV), and 0.1 mM of U(VI) in nitric acid solutions with concentrations varying from 0.1 to 4.0 M.

For the extraction process, 1 mL each of the aqueous and organic phases was added to a centrifuge tube, and the two phases were thoroughly mixed using a vortex oscillator at 2000 rpm for 30 minutes. After reaching equilibrium, the mixture was subjected to centrifugation at 3000 rpm for 1 minute to separate the phases. To analyze the radioactivity of Np(V) and Pu(IV), 500 μL of the aqueous phase was transferred to a liquid scintillation counting (LSC) vial containing LSC cocktail (Ultimate Gold AB, PerkinElmer). The radioactivity of Np(V) and Pu(IV) in the aqueous phase before and after extraction were measured using an ultra-low level scintillation counter (TriCarb-4910, PerkinElmer). Quantitative analysis of U(VI) concentration in pre- and post-extraction aqueous phases was conducted by ICP-OES (iCAP-PRO, Thermo Scientific). The distribution ratio (*D*), extraction efficiency (*E*), and separation factors (*SF*) for Np(V), Pu(IV), and U(VI) were calculated using Equations S1 to S3. The chemical composition of the extracted complexes was determined by slope analysis with the corresponding calculation equations provided in Equations S5 to S10.

To optimize the stripping process, aqueous solutions of 0.001 M HNO_3, 0.1 M HCl and 0.1 M HF mixture, 0.1 M and 1 M $H_2C_2O_4$ were tested as stripping agents. The acidity of the Np(V) feed solution was 1 M HNO_3, and the concentrations of extractant in the organic phase were 10 mM. The organic and aqueous phases were thoroughly mixed to achieve extraction equilibrium. Subsequently, the extracted organic phase was mixed with fresh stripping agents and subjected to centrifugation. This stripping process was repeated three times with fresh stripping agents, maintaining equal volumes of organic and aqueous phases in each step. The mixing and centrifugation operations are same to the extraction experiments. The stripping efficiency (S%) for both single and total stripping processes was calculated based on measuring the radioactivity of Np(V) in the fresh feed, extracted feed, and stripped aqueous phases with the calculation method outlined in Equation S4.

The distribution ratio (D), the extraction efficiency (E, %) and the stripping efficiency (S, %) were calculated as follows:

$$D = \frac{C_{org.}}{C_{aq.}} \tag{1}$$

$$E(\%) = \frac{C_{org.}}{C_{F.}} \times \frac{V_{org.}}{V_{F.}} \times 100\% \tag{2}$$

$$SF_{A/B} = \frac{D_A}{D_B} \tag{3}$$

$$S(\%) = \frac{C_{str.aq.}}{C_{ext.org.}} \times 100\% \tag{4}$$

The general extraction equilibriums can be described by equation (5). (The subscript (org.) or (aq.) indicate that the substance exists in the organic phase or aqueous phase)

$$M^{m+}_{(aq.)} + mNO^{-}_{3(aq.)} + nL_{(org.)} \rightleftharpoons M(NO_3)_m(L)_{n(org.)} \tag{5}$$

n is the coordination number of ligand to metal ion, the corresponding extraction equilibrium constant, K_{ex}, can be defined as:

$$K_{ex} = \frac{[M(NO_3)_m(L)_n]_{(org.)}}{[M^{m+}]_{(aq.)}[NO^{-}_3]^{m}_{(aq.)}[L]^{n}_{(org.)}} \tag{6}$$

The distribution ratio of metal ion, D_M, can be represented as:

$$D_M = \frac{[M(NO_3)_m(L)_n]_{(org.)}}{[M^{m+}]_{(aq.)}} \tag{7}$$

By substituting equation (7) into equation (6), and transforming equation (7) into the log form, equations (8), (9), and (10) are obtained:

$$LogD_M = logK_{ex} + nlog[L]_{(org.)} + mlog[NO_3]_{(aq.)} \tag{8}$$

$$LogD_M = nlog[L]_{(org.)} + C_1 \ \ (C_1 = logK_{ex} + mlog[NO_3]_{(aq.)}) \tag{9}$$

$$LogD_M = mlog[N\ \ _3]_{(aq.)} + C_2\ (C_2 = logK_{ex} + nlog[L]_{(org.)}) \quad (10)$$

C is the constant when the corresponding condition is controlled. Based on above analysis, C_1 and C_2 are the constants when the corresponding condition is controlled. Based on above analysis, keeping the concentration of nitric acid constant, the slope of log-log plot regarding *D* vs. initial [L] present the number of extractant molecules coordinated to metal ion in the organic phase.

S 1.3 UV-Vis-NIR Spectroscopy

First, dilute the Np(V) reserve solution with a concentration of 10 mM using dilute nitric acid as the aqueous phase solution. The concentration of Np(V) in the feed liquid is 0.1 mM, and the acidity of the solution is 1.06 M HNO_3. The organic phase is an F-3 solution containing Et-Tol-CyMe$_4$-ATP with concentration of 10 mM. The extraction method is the same as that in section S1.2. Then, 0.5 mL of the feed liquid and the organic phase before and after extraction were respectively added to the microvolume cuvettes with screw caps (Yixing Purshee Optical Elements Co., Ltd.) with a slit width of 2 μm. The absorption spectra in the range of 900-1200 nm were determined by using a UV-Vis-NIR spectrometer (lambda 1050+, PerkinElmer).

S 1.4 DFT Calculations

All calculations were performed using Gaussian 16 with the PBE0 functional.[2, 3] The 6-311G* basis set was used for O, N, C, and H atoms, while the Stuttgart relativistic pseudopotential (ECP60MWB) and its associated valence basis set were employed for Np.[4] Frequency analyses confirmed all optimized geometries as global minima (no imaginary frequencies). Wavefunction files generated by Gaussian 16 were processed using Multiwfn 3.8 to compute electrostatic potentials (ESP), Wiberg bond orders, and perform energy decomposition analysis (EDA).[5-7] Gibbs free energies were derived via a literature-reported thermodynamic,[8] incorporating zero-point energy (ZPE) corrections. Solvation effects were included using the IEFPCM solvation model to obtain solvation free energies.[9]

S 2 Results and Discussion

S 2.1 Solvent Extraction and Stripping

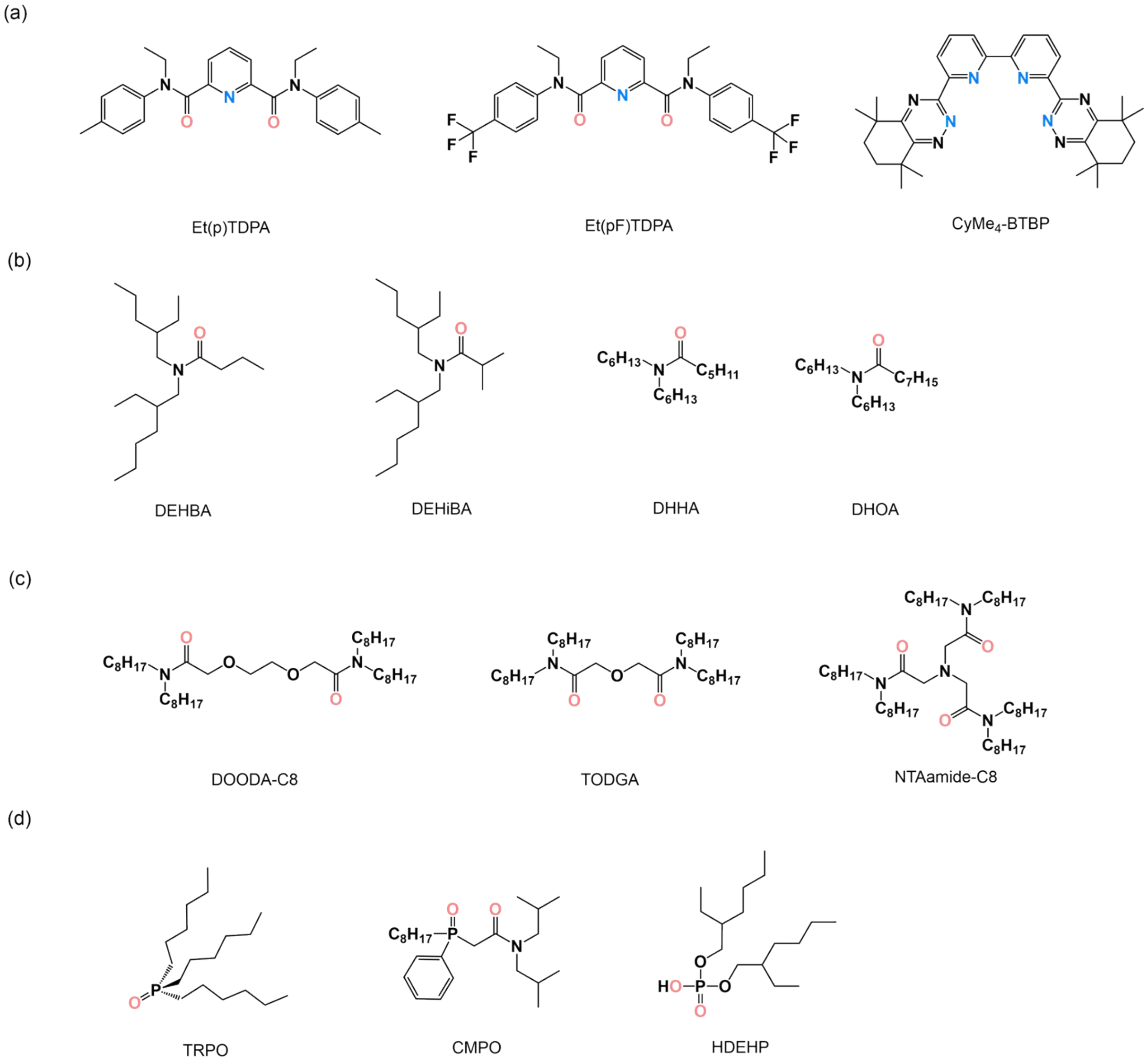

Figure S1. The chemical structures of different types of extractants for Np(V) extraction reported in the literature**:** **(a)** heterocyclic skeleton derived chelating extractants, **(b)** monoamide extractants, **(c)** diamide extractants, and **(d)** organophosphorus extractants.

Table S1. Extraction data of Np(V) by different types of extractants reported in the literature

Extractants	Organic solvent	Concentration	Distribution ratio (1 M)	Distribution ratio (3 M)	References
Et-Tol-$CyMe_4$-ATP	F-3	0.01 M	100.18	36.73	This work.
Et(p)TDPA	FS-13	0.01 M	0.02	1.26	[9]
Et(pFPh)DPA	F-3	0.2 M	0.35	2.00	[11]
$CyMe_4$-BTBP	cyclohexanone	0.01 M	0.32	0.53 (4 M)	[12, 13]
DEHBA	Exxsol D60	1 M	0.025	0.07	[14, 15]
DEHiBA			0.015	0.05	
DHHA			0.06	0.13	
DHOA			0.09	0.15	
DOODA-C8	*n*-dodecane	0.1 M	0.005	0.2	[16, 17]
TODGA			0.01	0.1	
NTAamide-C8			0.1	0.15	
TRPO	kerosene	30%	0.15	0.4	[18]
CMPO	decalin	0.22 M	0.30	0.45	[18]
HDEHP	kerosene	1 M	0.07	0.3	[20]

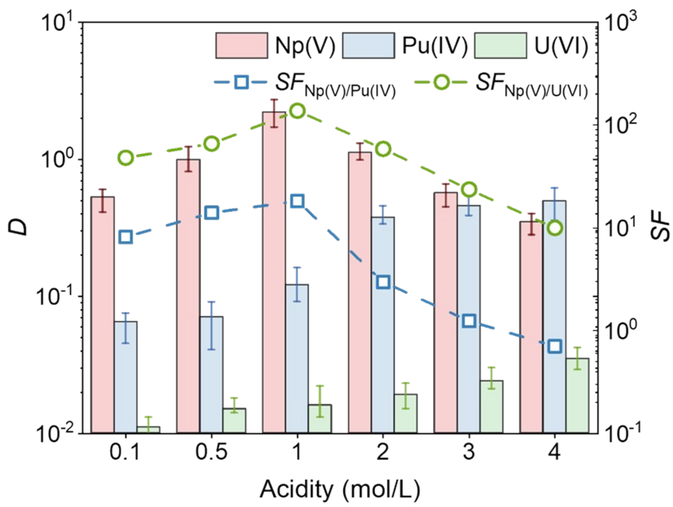

Figure S2. The influence of acidity in aqueous solution on the extraction and separation of U(VI), Np(V) and Pu(IV) in n-octanol as organic phase ($[HNO_3]$ = 0.1-4.0 M, [L] = 10 mM)

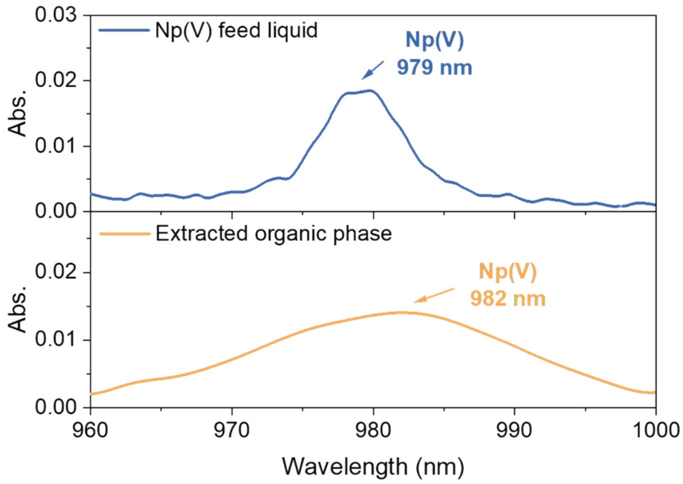

Figure S3. Absorption spectra of Np(V) in the aqueous phase and organic phase before and after extraction ($[HNO_3]$ = 4.0 M, [Np(V)] = 0.1 mM, [L] = 10 mM).

Table S2. The stability constants of complex formed between fluoride ions and actinide ions

Actinide ion	I medium (M)	T, K	log β_1	log β_2	log β_3	Ref
U(VI)	0.2 M $HClO_4$		4.50±0.08	7.48±0.09	10.44±0.10	
Np(V)	1 M $HClO_4$	298	3.95	7.43	10.47	[20]
Pu(IV)			4.66	7.21	/	

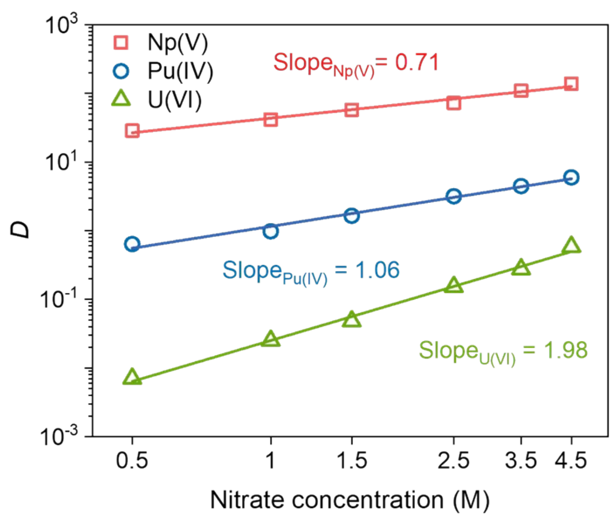

Figure S4. The influence of nitrate concentration on the extraction of U(VI), Np(V) and Pu(IV) ($[NO_3^-]$ = 0.5-4.5 M, [L] = 10 mM).

S 2.2 DFT Calculations

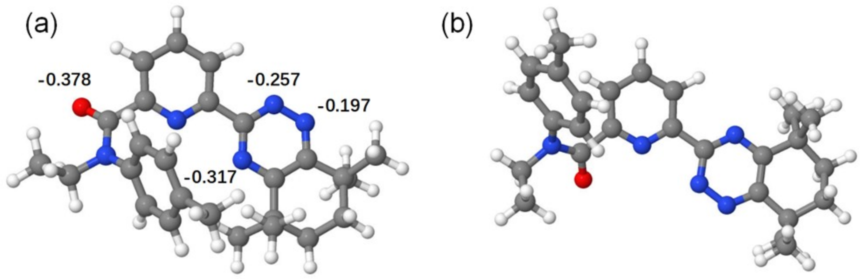

Figure S5. The geometries of free and coordinated L and the corresponding Mulliken charge of atoms (a. u.).

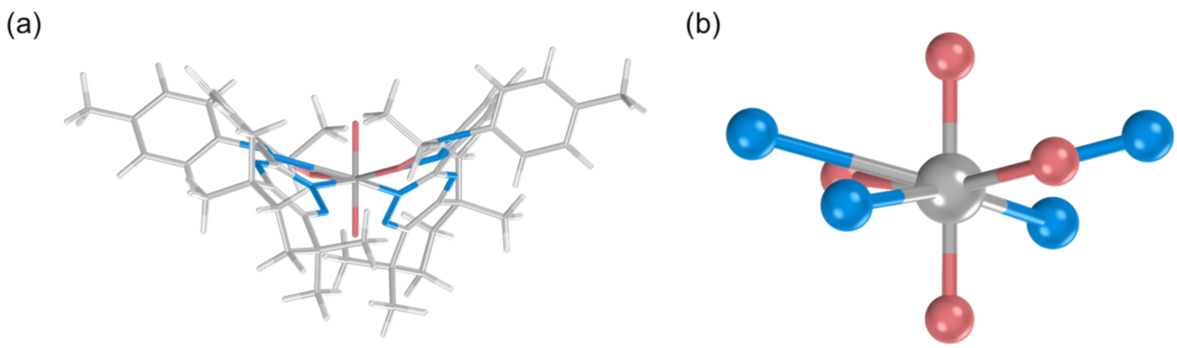

Figure S6. (a) The radial view of $[NpO_2(L)_2]^+$ complex and **(b)** The coordination mode of Np(V) in $[NpO_2(L)_2]^+$ complex.

Table S3. Summary of experimental and computed Np-O and Np-N bond lengths for representative 1:2 actinyl-ligand Complexes.

	An-O	An-N	Ref
$UO_2Cl_2(phen)_2$	-	2.678(3)	
Np-phen$_2$	-	2.651(3)	
Np-phen$_2$-$P2_1/n$	-	2.633(8)	22
PuO_2^+-phen$_2$	-	2.618(4)	
PuO_2^+-phen$_2$·MeCN	-	2.634(4)	
$NpO_2(DPA)_2^{3-}$	2.563(5)	2.671(6)	23
$NpO_2(ODA)_2^{3-}$	2.543	2.577	24
$[NpO_2(L)(NO_3)]$	2.552	2.632	This work
$[NpO_2(L)_2]^+$	2.510	2.703	This work

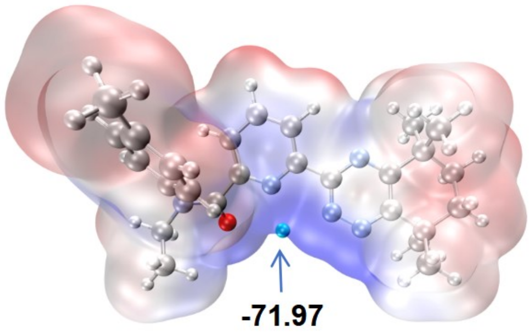

Figure S7. The ESP diagrams and the most negative ESP values of coordinated L (a.u.).

Table S4. The calculated properties at BCPs of Np-N/O bonds for the 1:1 and 1:2 type complexes(a.u.).

	$[NpO_2(L)(NO_3)]$				$[NpO_2(L)_2]^+$		
Bond	ρ(r)	G(r)	V(r)	Bond	ρ(r)	G(r)	V(r)
Np-$N_{trizane}$	0.0430	0.0387	-0.0409	Np-N_{tri}	0.0394	0.0342	-0.0357
Np-N_{pyr}	0.0415	0.0381	-0.0399	Np-N_{pyr}	0.0329	0.0282	-0.0289
Np-O_{ami}	0.0402	0.0418	-0.0411	Np-O_{ami}	0.0452	0.0472	-0.0469

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Appendix

Cartesian coordinates of PBE0 optimized geometries of L and $[NpO_2(L)(NO_3)]$.

L				$[NpO_2(L)(NO_3)]$			
N	-3.17499800	-2.00351700	0.49233800	N	2.88285900	-0.42041100	0.42412800
N	-1.93616100	-2.42207700	0.59803300	N	1.76561400	0.08397300	-0.03530700
C	-3.43122300	-0.78578500	0.02203500	C	3.98825300	0.31433800	0.42516100
C	-0.95164900	-1.60247300	0.22385400	C	1.75192000	1.33789600	-0.48830800
C	-4.89344800	-0.41102700	-0.10735400	C	5.23440700	-0.36108700	0.95243200
C	-2.36979200	0.05600200	-0.35977600	C	3.95836000	1.63127800	-0.08565800
N	-1.12249300	-0.36947700	-0.24562400	N	2.81329800	2.13447800	-0.52482300
C	0.42683600	-2.14061200	0.34929900	C	0.44321900	1.84140300	-0.94676600
C	-5.46060600	-1.17042500	-1.31422800	C	5.69062200	-1.37607400	-0.10553800
C	-5.65885400	-0.83133000	1.14728200	C	4.91687100	-1.10445600	2.25083700
C	-5.02925700	1.10386500	-0.30535000	C	6.31944800	0.69072800	1.21136900
C	-2.57525100	1.47134900	-0.85492600	C	5.17459300	2.52811600	-0.12572300
N	1.41514100	-1.42206700	-0.17936100	N	-0.52356400	0.92940400	-1.00118900
C	0.63749500	-3.36096700	0.99556500	C	0.21689200	3.17686900	-1.26293500
H	-4.96027500	-0.89553500	-2.24676600	H	5.94551300	-0.89986500	-1.05610500
H	-6.52851100	-0.95879700	-1.42600200	H	6.57272200	-1.91474500	0.25242700
H	-5.33473500	-2.24651200	-1.17408900	H	4.89883000	-2.10289500	-0.29980600
H	-5.59423000	-1.90826400	1.30448200	H	4.16799100	-1.88071800	2.09171900
H	-6.71252400	-0.55206200	1.05017700	H	5.82695500	-1.57327200	2.63589400
H	-5.25836100	-0.33608700	2.03694600	H	4.53933500	-0.42078200	3.01702000
H	-6.05229300	1.32414200	-0.62874100	H	7.27242400	0.17630800	1.37049400
H	-4.90687200	1.60227600	0.66323500	H	6.09785800	1.21028700	2.15090500
C	-4.02818800	1.66610700	-1.30012100	C	6.44706200	1.69775800	0.08183400
C	-1.62603000	1.75450000	-2.01802900	C	5.24366300	3.24854800	-1.47243800
C	-2.22318500	2.40349300	0.31266400	C	5.00958500	3.56894100	0.99150300
C	2.64872300	-1.90735600	-0.10154000	C	-1.76685100	1.29758300	-1.28620500
C	1.92949100	-3.85538800	1.07048800	C	-1.07277500	3.55566200	-1.60913500
H	-0.20906100	-3.89366700	1.40934300	H	1.03734800	3.88286100	-1.22826900
H	-4.20763900	2.73514500	-1.45794100	H	7.28113900	2.38125100	0.27130600
H	-4.16807500	1.18972000	-2.27767600	H	6.68988300	1.17837300	-0.85215200
H	-0.59010300	1.59782900	-1.71648500	H	4.36452600	3.87361000	-1.63392900
H	-1.74918100	2.78869600	-2.35446200	H	6.13260800	3.88488900	-1.50253500
H	-1.83484300	1.09603500	-2.86651600	H	5.31065600	2.53652400	-2.29991900
H	-1.19702600	2.22000700	0.63588200	H	4.08973600	4.14045200	0.84708100
H	-2.88010800	2.25570500	1.17398800	H	4.96661900	3.11042600	1.98257700
H	-2.30729300	3.44840000	-0.00294000	H	5.85299500	4.26510800	0.97585300
C	3.77859500	-1.16882500	-0.76742700	C	-2.70112500	0.11410800	-1.29985300
C	2.95963500	-3.12620700	0.49855800	C	-2.09211000	2.61256600	-1.60154500
H	2.12800000	-4.80312100	1.56070900	H	-1.28824300	4.58690400	-1.86767600
O	4.71743300	-1.80703900	-1.21605900	O	-2.24993800	-0.95546200	-1.71552300
N	3.69859700	0.18891400	-0.88893900	N	-3.96335000	0.25927500	-0.86752700

H	3.98506200	-3.47458900	0.48918200	H	-3.11430000	2.88931300	-1.82720300
C	4.77421600	0.84230400	-1.63596900	C	-4.83979900	-0.92266500	-0.89411000
C	2.89626200	1.01793600	-0.06160000	C	-4.31646100	1.32223000	0.01583100
C	5.97118800	1.16445400	-0.75933500	C	-4.70888400	-1.76829400	0.35880700
H	4.36332200	1.75120400	-2.08107300	H	-5.86057900	-0.55277500	-1.02125600
H	5.06161200	0.16824300	-2.44271400	H	-4.57012700	-1.49712200	-1.77999100
C	2.13472700	2.03285900	-0.62753400	C	-5.38918000	2.15442900	-0.28356800
C	2.92042100	0.88368600	1.32462700	C	-3.59356400	1.50568000	1.19125200
H	6.74397200	1.67826000	-1.33772500	H	-5.40213100	-2.61141200	0.30517200
H	6.40159800	0.24496600	-0.35775600	H	-3.70042300	-2.17161300	0.46205100
H	5.68514300	1.81211000	0.07407700	H	-4.94979800	-1.18880000	1.25380900
H	2.09756500	2.13371000	-1.70731000	H	-5.94834100	2.00199600	-1.20193600
C	1.40826500	2.89489800	0.18032800	C	-5.72048400	3.18566900	0.58286800
C	2.16606600	1.72908800	2.12210000	C	-3.93061500	2.54907300	2.04170400
H	3.53320300	0.10887500	1.77466200	H	-2.77849600	0.82439100	1.42649300
H	0.81991700	3.68387800	-0.28016800	H	-6.55533700	3.83764600	0.34126200
C	1.40169900	2.75566400	1.56691200	C	-4.99522300	3.40367100	1.75594900
H	2.18829000	1.60177800	3.20132200	H	-3.35961200	2.69139900	2.95485100
C	0.59861500	3.67342900	2.44088100	C	-5.37765200	4.50209500	2.70284000
H	-0.16809800	3.12425800	2.99686600	H	-4.51211500	4.87715500	3.25351200
H	0.09253500	4.44333800	1.85464900	H	-5.83666300	5.34407400	2.17945800
H	1.23043600	4.17851800	3.17776000	H	-6.10249600	4.14422800	3.44178800
				Np	-0.24009000	-1.59185300	-0.27687800
				O	0.66828600	-2.19549600	-1.65254800
				O	-1.13663200	-0.90930500	1.09339500
				N	-0.88598900	-4.21519600	0.81344400
				O	-1.16870000	-5.26986000	1.31603500
				O	0.21009600	-3.62364700	1.06111100
				O	-1.66102000	-3.62346200	0.00278300

Cartesian coordinates of PBE0 optimized geometries of $[NpO_2(L)_2]^+$.

$[NpO_2(L)_2]^+$							
N	-1.54768500	-2.89814800	-1.47982500	C	-4.59537000	4.21200600	0.32429300
N	-1.79719900	-1.93711000	-0.62330600	C	-4.96208000	5.68119600	2.64549400
C	-2.42259400	-3.88332700	-1.64274800	H	-2.86790800	5.34927000	3.00933800
C	-2.96185400	-1.95036900	0.02595900	C	-5.85089600	4.70436500	0.64966500
C	-3.52114600	-3.99375100	-0.76284700	H	-4.44370900	3.64970700	-0.59181300
N	-3.79904400	-2.97891000	0.04214600	C	-6.05810300	5.44695800	1.81220600
C	-3.31625000	-0.72417000	0.76124100	H	-5.09697300	6.25801000	3.55585700
N	-2.62218100	0.36337700	0.43351600	H	-6.68423000	4.51775200	-0.02133700
C	-4.31798600	-0.71685800	1.72751200	C	7.40770900	-6.01122600	2.13911100
C	-2.90295900	1.51928900	1.03597600	H	7.51145600	-7.02485000	1.73807100
C	-4.57041500	0.47043500	2.39214900	H	8.21103200	-5.40860400	1.71055700
H	-4.85505100	-1.63097800	1.94740700	H	7.56819100	-6.07195300	3.21769300

C	-1.98795400	2.62134500	0.57885500	C	-7.40770900	6.01122600	2.13911100
C	-3.85873200	1.61095800	2.04455500	H	-7.51145600	7.02485000	1.73807100
H	-5.31699000	0.51489700	3.17754000	H	-8.21103200	5.40860400	1.71055700
O	-0.96146400	2.30431500	-0.02338900	H	-7.56819100	6.07195300	3.21769300
N	-2.23460400	3.91776500	0.86133300	C	4.40020900	5.21901800	-0.68640200
H	-4.04702200	2.54580500	2.55360400	C	3.80043400	6.33354500	-1.55264700
Np	0.00000000	0.00000000	-0.28228600	H	4.54686100	7.12436100	-1.67447800
O	0.00000000	0.00000000	1.47728400	H	2.95957300	6.79228000	-1.01821600
O	0.00000000	0.00000000	-2.02505600	C	3.33240800	5.82395700	-2.90489700
N	1.54768500	2.89814800	-1.47982500	H	4.16526100	5.33601800	-3.42372000
N	1.79719900	1.93711000	-0.62330600	H	3.02749100	6.65651300	-3.54596700
C	2.42259400	3.88332700	-1.64274800	C	2.16218100	4.83826000	-2.78828000
C	2.96185400	1.95036900	0.02595900	C	-3.80043400	-6.33354500	-1.55264700
C	3.52114600	3.99375100	-0.76284700	H	-2.95957300	-6.79228000	-1.01821600
N	3.79904400	2.97891000	0.04214600	H	-4.54686100	-7.12436100	-1.67447800
C	3.31625000	0.72417000	0.76124100	C	-3.33240800	-5.82395700	-2.90489700
N	2.62218100	-0.36337700	0.43351600	H	-4.16526100	-5.33601800	-3.42372000
C	4.31798600	0.71685800	1.72751200	H	-3.02749100	-6.65651300	-3.54596700
C	2.90295900	-1.51928900	1.03597600	C	-2.16218100	-4.83826000	-2.78828000
C	4.57041500	-0.47043500	2.39214900	C	-4.40020900	-5.21901800	-0.68640200
H	4.85505100	1.63097800	1.94740700	C	-0.84513700	-5.58115500	-2.54757300
C	1.98795400	-2.62134500	0.57885500	H	-0.63843300	-6.25101200	-3.38663900
C	3.85873200	-1.61095800	2.04455500	H	-0.02178200	-4.86874700	-2.47024500
H	5.31699000	-0.51489700	3.17754000	H	-0.86949500	-6.18265500	-1.63434600
O	0.96146400	-2.30431500	-0.02338900	C	2.03871100	4.02206700	-4.07880500
N	2.23460400	-3.91776500	0.86133300	H	1.20843600	3.31617800	-4.01803000
H	4.04702200	-2.54580500	2.55360400	H	1.86732500	4.69225100	-4.92600200
C	-1.16327500	4.87352100	0.54173500	H	2.95265300	3.45504200	-4.27843500
H	-0.82024200	4.65692300	-0.47071000	C	-2.03871100	-4.02206700	-4.07880500
H	-1.61946700	5.86394100	0.54081300	H	-1.20843600	-3.31617800	-4.01803000
C	0.00000000	4.80191400	1.51332600	H	-1.86732500	-4.69225100	-4.92600200
H	0.44329800	3.80472500	1.51717100	H	-2.95265300	-3.45504200	-4.27843500
H	0.77332700	5.51633900	1.21691100	C	0.84513700	5.58115500	-2.54757300
H	-0.30913200	5.04758100	2.53225300	H	0.02178200	4.86874700	-2.47024500
C	1.16327500	-4.87352100	0.54173500	H	0.86949500	6.18265500	-1.63434600
H	1.61946700	-5.86394100	0.54081300	H	0.63843300	6.25101200	-3.38663900
H	0.82024200	-4.65692300	-0.47071000	C	4.48582900	5.67832000	0.77097500
C	0.00000000	-4.80191400	1.51332600	H	4.92880900	4.90677500	1.40302500
H	-0.77332700	-5.51633900	1.21691100	H	5.10513500	6.57679100	0.83890200
H	0.30913200	-5.04758100	2.53225300	H	3.49669300	5.92119700	1.17099000
H	-0.44329800	-3.80472500	1.51717100	C	-5.80398800	-4.83606200	-1.17323600
C	3.52150900	-4.43378200	1.17968000	H	-6.47407000	-5.69517100	-1.08186400
C	3.70517800	-5.18149000	2.33926700	H	-6.20671400	-4.01934400	-0.57067000
C	4.59537000	-4.21200600	0.32429300	H	-5.80698200	-4.51465100	-2.21760500

C	4.96208000	-5.68119600	2.64549400	C	5.80398800	4.83606200	-1.17323600
H	2.86790800	-5.34927000	3.00933800	H	6.20671400	4.01934400	-0.57067000
C	5.85089600	-4.70436500	0.64966500	H	5.80698200	4.51465100	-2.21760500
H	4.44370900	-3.64970700	-0.59181300	H	6.47407000	5.69517100	-1.08186400
C	6.05810300	-5.44695800	1.81220600	C	-4.48582900	-5.67832000	0.77097500
H	5.09697300	-6.25801000	3.55585700	H	-4.92880900	-4.90677500	1.40302500
H	6.68423000	-4.51775200	-0.02133700	H	-5.10513500	-6.57679100	0.83890200
C	-3.52150900	4.43378200	1.17968000	H	-3.49669300	-5.92119700	1.17099000
C	-3.70517800	5.18149000	2.33926700				