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Highly efficient diglycolamide-functionalized dendrimers for the sequestration of tetravalent actinides: Solvent extraction and theoretical studies

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Electronic Supporting Information

S1. Oxidation state adjustment

The oxidation state of Pu was adjusted to its +4 state by the following procedure. To a Pu solution in 1 M HNO_3, a few drops of $NaNO_2$ solution was added followed by slow warming under an infrared lamp inside a well-ventilated fume hood. Subsequently, the aqueous phase was contacted with an equal volume of 0.5 M TTA (2-thenoyltrifluoroacetone)solution (in xylene) in a leak tight Pyrex glass tube. The phases were separated and the aqueous phase was carefully separated to result in the organic extract devoid of any aqueous phase. The organic extract was subsequently contacted with 8 M HNO_3 to back extract the Pu(IV). The aqueous phase was then rinsed with xylene twice to remove traces of dissolved TTA. The aqueous phase was then kept as the Pu(IV) stock which was found to be stable for over 2 months. The valency of Pu(IV) in this stock was checked by a TTA concentration variation experiment, which resulted in a slope value of ca. 4 in the fitted log *D vs* log [TTA] concentration plot. The oxidation state of Np was also checked intermittently in an identical manner and conformed to the +4 state.

S2. Derivation of the extraction equilibrium constant

As mentioned in the main text, the two-phase extraction equilibrium constant (K_{ex}) is given as

$$K_{ex} = \frac{\left[M(NO_3)_b.aL_{(org)}\right]}{\left[M^{+4}_{(aq)}\right]\left[NO_{3\ (aq)}^{-}\right]^b\left[L_{(f,org)}\right]^a} \ldots\ 1$$

Since the extraction of the M(IV) is taken from nitric acid media, one has to take into accountthe nitrate complexation of M(IV) with the NO_3^- ions in the aqueous feed. Various species of M(IV) such as $M(NO_3)^{3+}$, $M(NO_3)_2^{2+}$,$M(NO_3)_3^{+}$, $M(NO_3)_4$etc., can be present in the aqueous phase and the total concentration of M(IV) ($C_{M(IV)}$) is given by equation (2).

$$C_{M(IV)} = \left[M^{4+}_{aq}\right]\left(1 + \sum_{i}^{n}\beta_n\left[NO_3^-\right]^n\right) \quad .. 2$$

Where β_n is the overall concentration stability constant for the complex $M(NO_3)_n^{(4-n)+}$ by equation (3):

$$M^{+4}_{(aq)} + n.NO_{3\ (aq)}^{-} \overset{\beta_n}{\leftrightarrow} M(NO_3)_n^{(4-n)+} \quad .. 3$$

Equation (4) can be easily derived by combining equations (1) and (2):

$$K_{ex} = \frac{K_{Nit}.\left[M(NO_3)_b.aL_{(org)}\right]}{C_{M(IV)}\left[NO_{3\ (aq)}^{-}\right]^b\left[L_{(f,org)}\right]^a} \quad .. 4$$

where

$$K_{Nit} = \left(1 + \sum_{i}^{n} \beta_n [NO_3^-]^n\right) \quad ..5$$

$D_{M(IV)}$, the distribution ratio of the tetravalent actinides in the biphasic system, is given by equation (6). On combining equations(5) and (6) and taking the log on both sides gives equation (7):

$$D_{M(IV)} = \frac{[M(NO_3)_b.aL_{(org)}]}{C_{M(IV)}} \ldots\ 6$$

$$logD_{M(IV)} = logK_{ex}^{'} + a.log[L_{(f,org)}] + b.log[NO_{3\ (aq)}^{-}] \ ..7$$

Where $K_{ex}^{'} = \frac{K_{ex}}{K_{Nit}}$ 8

S3. Solvent extraction studies

S3.1 Time of equilibration

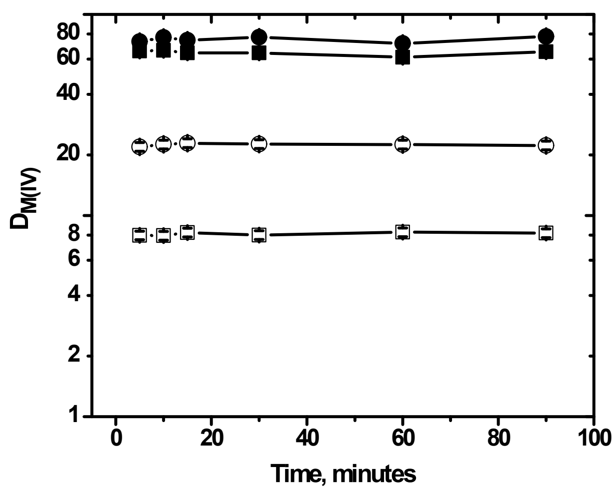

Fig.S1 Extraction of Np(IV) (open symbols) and Pu(IV) (closed symbols) by 0.1 mM $\mathbf{L_I}$ (square) and $\mathbf{L_{II}}$ (circle) dissolved in 5% IDA+ *n*-dodecane as a function of varying time; $[HNO_3]$: 3 M, T: 298 K.

S3.2 Extraction of water and acid

The extraction of water into the organic phase was done by Karl-Fisher titration method while that of nitric acid was done by normal acid base titration using phenolphthaliene indicator. The results are given in Table S1.

Table S1: Water and acid water uptake by 0.1 mM ligands (L_I or L_{II}) in 5% iso-decanol in *n*-dodecane equilibrated with 3M HNO_3. The titration results had about 2% errors.

Sample	Water content (%)	Acidity (M)
5% iso-decanol in *n*-dodecane	0.050	0.029
1×10^{-4} M L_I in 5% iso-decanol in *n*-dodecane	0.053	0.033
1×10^{-4} M L_{II} in 5% iso-decanol in *n*-dodecane	0.053	0.030

S3.3 Determination of K_H value

The acid uptake for the 0.1 mM L-I/II dissolved in 5% Isodecanol + 95 % n-dodecane was found to be comparable to the acid uptake by the 5% Isodecanol + 95 % n-dodecane without any ligand, hence the ligands concentration was increased by 10 times and the acid uptake is evaluated. Even at the lignad concentration (1mM L-I/II) the acid uptake by the system is comparable (within the error limits) acid uptake by the 5% Isodecanol + 95 % n-dodecane without any ligand (Fig. 1)n suggesting the majority of the acid is taken by Isodecanol, which looks logical as the concentration of Isodecanol is >250 time of the ligands concentration under the present system.

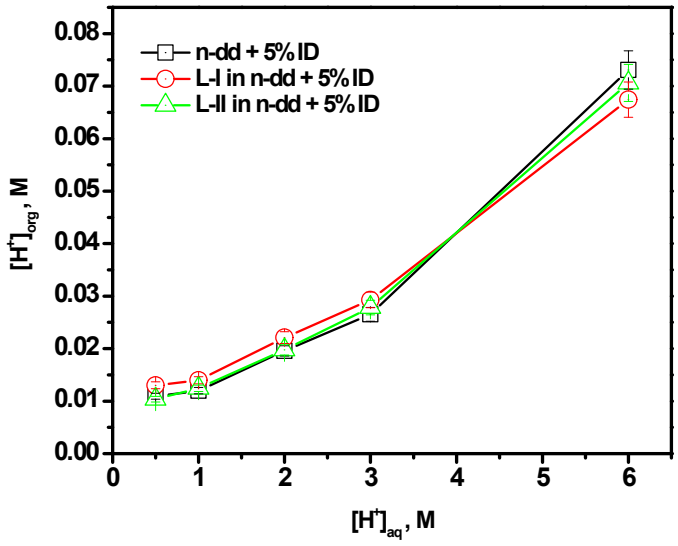

Fig. S2. Acid uptake by the L-I/L-II (1mM) dissolved in 95 % n-dodecane + 5% isodecanol and its comparison with blank 95 % n-dodecane + 5% isodecanol at different acidities.

Although the ligand concentration can be further increased to overcome this issue but it has other limitation such as higher L-I/L-II concentration the system can behave entirely in different manner as compared the one used for the extraction studies, the higher ligand concentration can leads to some micelles/ aggregated formation which may be not true representation of the extraction system beside that the quantity of the synthesized ligands is also is a limiting factor. Considering theses limitation the spectroscopic techniques i.e. FTIR was chosen to get the information about the interaction of HNO_3 with L-I/L-II dissolved in 5% Isodecanol + 95 % n-dodecane. Although the direct quantitative estimation using FTIR is difficult but can be done provided the sample composition does not vary as a function of time or temperature, the thickness of sample should not vary (e.g. due to evaporation of solvent etc) etc. as the present system satisfies the above requirements we have recorded the ATR-FTIR (in Absorbance mode) of the sample before and after acid equilibration and the results were analyzed after subtracting the signal contributed by 5% Isodecanol + 95 % n-dodecane blank using origin 2015. Figure 2 and 3 shows the ATR-FTIR spectra of the present systems in transmittance mode. The C-H scissoring peak at 1465 cm^{-1} was used

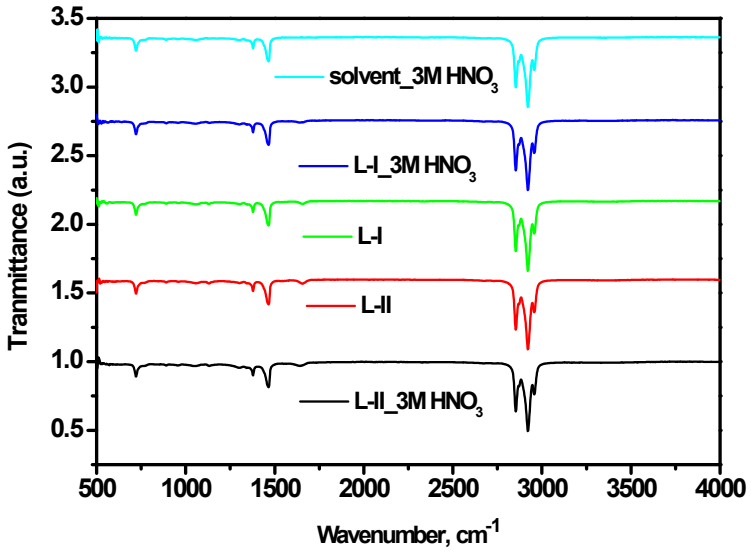

Fig. S3. The ATR-FTIR spectra of L-I/II dissolved in 5% Isodecanol + 95 % n-dodecane before and after acid equilibration, [Ligand] ~ 10 mM, [HNO_3] : 3M

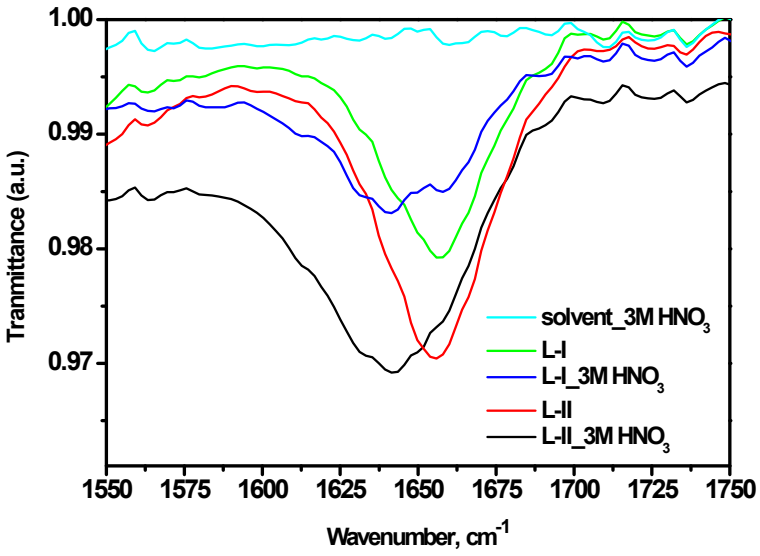

Fig. S4. The ATR-FTIR spectra of L-I/II dissolved in 5% Isodecanol + 95 % n-dodecane before and after acid equilibration in the 1650 -1750 cm^{-1} region, [Ligand] ~ 10 mM, [HNO_3] : 3M

as internal standard as this peak is not affected by the HNO_3 coordination of either ligand or solvent. All the peak are normalized by the peak area of 1465 cm^{-1} peak and the peak area in region 1550 -1750 cm^{-1} was analyzed for the quantitative estimation. For the quantitative analysis, The peak area of the L-I/L-II in 5% Isodecanol + 95 % n-dodecane were fitted using in build Gaussian function of Origin 2015 and area under peak, peak centre and peak width were noted. The peak area after the acid equilibration was fitted into two peaks assuming free and acid-bound L-I/L-II in the same region. Since the peak fitting parameters for the free ligands (mainly free C=O groups) is known from the peak fitting of the L-I/L-II in 5% Isodecanol + 95 % n-dodecane before acid equilibration and fixed for initial fitting runs. The peak parameters for the peak at lower wavelength due to HNO_3-L-I/L-II is kept free as the transition integral moment and other peak parameters can change after HNO_3 coordination to L-I/L-II. The area under the peak at 1655 cm^{-1} was compared before and after acid equilibration to get free and acid bound L-I/L-II. The K_H values obtained using this found to be 0.27 (±0.05) and 0.32 (±0.06) for L-I and L-II, respectively and the obtained K_H values were used for the calculation of L_{free} in the organic phase at 3M HNO_3 for ligands variation experiments.

Table S2: Slope and R^2 value for the linear fit of ligand, nitrate and temperature variation studies

Ligand Variation				
Ligand	**Np(IV)**		**Pu(IV)**	
	slope	**R^2**	**slope**	**R^2**
L_I	1.19 ± 0.01	0.999	1.35 ± 0.06	0.992
L_{II}	0.98 ± 0.02	0.998	1.31 ± 0.07	0.987
Nitrate Variation				
Ligand	**Np(IV)**		**Pu(IV)**	
	slope	**R^2**	**slope**	**R^2**
L_I	3.77 ± 0.47	0.962	3.73 ± 0.10	0.976
L_{II}	3.74 ± 0.36	0.940	3.58 ± 0.28	0.997
Temperature Variation				
Ligand	**Np(IV)**		**Pu(IV)**	
	slope	**R^2**	**slope**	**R^2**
L_I	979.70 ± 67.56	0.986	692.17 ± 15.35	0.998
L_{II}	1072.48 ± 104.03	0.972	589.73 ± 43.91	0.984

S5. DFT studies

The optimized structures for Pu(IV) complexes are given below.

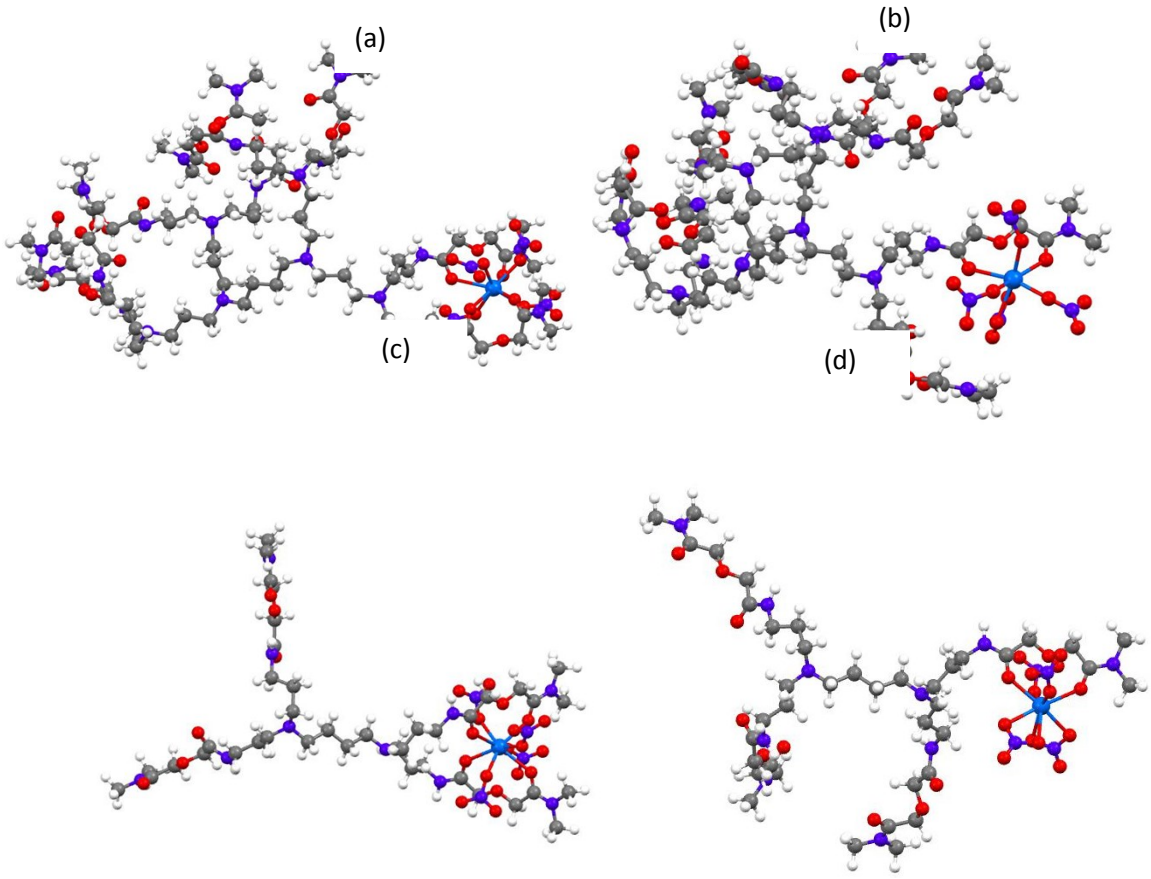

Figure S5. Optimized structure of complexes of $\mathbf{L_I}$ and $\mathbf{L_{II}}$ with Pu^{4+} at the B3LYP/SVP level of theory. (a) Pu^{4+} ion is coordinated to $\mathbf{L_I}$ with two DGA units and four monodentate nitrate ions (b) Pu^{4+} ion is coordinated to $\mathbf{L_I}$ with one DGA unit and two monodentate and two bidentate nitrate ions. (c) Pu^{4+} ion is coordinated to $\mathbf{L_{II}}$ with two DGA units and four monodentate nitrate ions (d) Pu^{4+} ion is coordinated to $\mathbf{L_{II}}$ with one DGA unit and three monodentate and one bidentate nitrate ions. Grey: C , Deep blue: N, Red: O, White: H and Light blue : Pu.

Table S3: Calculated structural parameters for the Pu^{4+} ion complexes with $\mathbf{L_I}$ and $\mathbf{L_{II}}$ in Å at B3LYP level of theory using SVP basis set.

System			
$\mathbf{L_I}$	Pu-O (Å)	Pu-O (Å)	Pu-O (Å)
Four nitrate ions as monodentate	O of C=O	Ether O	O of NO3
	2.446, 2.426, 2.445, 2.382	2.877, 2.892	2.301, 2.330, 2.360, 2.395
Two nitrate ions as monodentate and two as bidentate	2.394, 2.381	2.774	2.229, 2.288, 2.389, 2.419, 2.391, 2.421
$\mathbf{L_{II}}$			
Four nitrate ions as monodentate	O of C=O	Ether O	O of NO3
	2.382, 2.457, 2.498, 2.557	2.673, 3.317	2.249, 2.262, 2.310, 2.348
Three nitrate ions as monodentate and one as bidentate	2.356, 2.382	2.686	2.171, 2.208, 2.257 2.412, 2.450

Table S4: Calculated charge and orbital population using NBO analysis in gas phase at B3LYP/SVP level of theory.

System	charge	s	p	d	f
$\mathbf{L_I}$					
Four nitrate ions as monodentate	1.675	4.19	11.97	11.10	5.04
Two nitrate ions as monodentate and two as bidentate	1.690	4.18	11.97	11.03	5.09
$\mathbf{L_{II}}$					
Four nitrate ions as monodentate	1.687	4.19	11.96	11.09	5.04
Three nitrate ions as monodentate and one as bidentate	1.817	4.17	11.96	10.99	5.04

Optimized coordinates

$[L_I\text{-}Np(NO_3)_4]$ (all nitrate monodentate)

C	-3.9623261	-1.2637697	-2.3083313
H	-4.5719723	-2.1284507	-2.6186692
H	-4.6008339	-0.3641360	-2.3077771
H	-3.1374292	-1.1267026	-3.0191373
C	-1.5500233	-1.7877101	0.6226673
H	-1.9105797	-1.0582149	1.3708523
H	-1.8588914	-2.8105708	0.9008343
C	0.6409923	-1.9892882	1.6106925
H	0.4469569	-1.2708631	2.4279430
H	0.4836278	-3.0257496	1.9631159
C	4.4683248	-1.9359978	1.6563250
C	5.0017988	-3.1937539	0.9643626
H	5.0366662	-1.7047038	2.5714612
H	4.5603270	-1.0723902	0.9800817
C	6.4093395	-2.9763034	0.3739023
H	5.0017261	-4.0403117	1.6735231
H	4.2962447	-3.4556018	0.1606464
H	6.3827720	-2.0854073	-0.2771444
H	7.1153925	-2.7229276	1.1828746
C	7.5294718	-5.1524507	0.4746172
C	8.9619870	-4.8613249	0.9408862
H	7.5343768	-6.0939747	-0.0990086
H	6.8905451	-5.3575625	1.3623063
C	9.4756605	-5.8774128	1.9644184
H	9.6189012	-4.8351864	0.0530805
H	9.0094555	-3.8478125	1.3776783
C	10.9473617	-5.6731935	2.3376874
H	8.8526335	-5.8171144	2.8746308
H	9.3535841	-6.9083466	1.5869195
H	11.5578870	-5.8420774	1.4359256
H	11.1121515	-4.6048275	2.6159361
C	12.8286312	-6.9138057	3.3081073
C	13.1640764	-7.9220796	2.2036300
H	13.4682735	-6.0064289	3.1875043
H	13.1255082	-7.3599664	4.2703036
C	14.6514491	-8.2961840	2.1963808
H	12.5549938	-8.8297230	2.3467406
H	12.8883954	-7.5123059	1.2151220
H	15.2723504	-7.3857920	2.1098289
H	14.9271160	-8.7914178	3.1395422
C	15.6450930	-11.3483087	0.1137053
H	14.9149148	-12.1850893	0.1086001
H	15.4734832	-10.7584082	-0.8135524
C	17.2598156	-12.7705028	-0.7965511
H	17.0990609	-12.3662158	-1.8211425
H	16.5981035	-13.6582826	-0.7027633
C	20.5203782	-14.6858849	-1.3633404

H	21.0775566	-14.5914376	-2.3125244
H	21.0260386	-14.1022453	-0.5851046
H	20.5187087	-15.7525861	-1.0718050
N	-3.4298098	-1.5035822	-0.9678590
N	19.1653788	-14.1832996	-1.5083295
C	-4.3889894	-1.9063631	0.0477036
H	-5.2824658	-1.2659127	-0.0220841
H	-4.7039039	-2.9556630	-0.0932393
H	-3.9805095	-1.7928587	1.0588550
C	18.3362232	-14.8707600	-2.4775721
H	18.8901107	-14.9927050	-3.4246855
H	18.0413608	-15.8813824	-2.1333320
H	17.4230403	-14.3089636	-2.7081429
C	18.7299590	-13.1970338	-0.6467692
C	-2.1077218	-1.4300300	-0.7549554
O	-1.3275416	-1.0796062	-1.6526875
O	19.4519088	-12.6808434	0.1815236
O	-0.1534529	-1.7091271	0.4882250
O	16.9619687	-11.8199725	0.1770554
C	15.3605769	-10.5218773	1.3748016
C	2.0813286	-1.8355675	1.1340715
O	2.3331507	-1.5320073	-0.0383365
O	15.4274008	-11.0142095	2.4838308
N	3.0562443	-2.0414856	2.0264493
H	2.8078151	-2.3329529	2.9650164
N	15.0083364	-9.2224899	1.1361916
H	15.0102695	-8.8854658	0.1811379
N	6.9717149	-4.0999689	-0.3716686
N	11.4129300	-6.5703496	3.3891928
C	10.9446305	-6.2094599	4.7308018
C	10.0580438	-7.2636677	5.4072170
H	11.8093950	-5.9893467	5.3884095
H	10.3756613	-5.2638653	4.6782826
C	10.7495265	-8.6130511	5.6332608
H	9.7218992	-6.8604937	6.3807848
H	9.1525115	-7.4302535	4.7998277
H	10.9791886	-9.0797328	4.6647104
H	11.7034611	-8.4628232	6.1716851
C	8.5003621	-11.4639225	6.7951516
H	7.4814940	-11.5915777	6.3783198
H	8.9691476	-12.4689535	6.8240153
C	7.9430438	-11.6028230	9.1047962
H	8.4333316	-12.5964177	9.1884434
H	6.8601718	-11.7927689	8.9458259
C	7.8803288	-10.6907036	12.8238413
H	8.5297502	-11.2886536	13.4893243
H	8.3631696	-9.7272438	12.6225224
H	6.9214653	-10.5192545	13.3442187
N	7.6611971	-11.3729921	11.5596872
C	7.0322944	-12.6764022	11.6475790
H	7.6967224	-13.4200324	12.1282120
H	6.1119234	-12.6134675	12.2542388

H	6.7477715	-13.0615057	10.6615542
C	8.1543383	-10.8076930	10.4070897
O	8.7310428	-9.7362094	10.3888789
O	8.4852533	-10.8581748	8.0621548
C	9.3057646	-10.6094205	5.8092758
N	9.9358525	-9.5528918	6.3793218
H	9.7669422	-9.4072662	7.3719718
C	6.1575894	-4.5820378	-1.4819570
C	5.8343908	-3.5005932	-2.5179382
H	6.7220143	-5.3917665	-1.9760310
H	5.2012981	-5.0451651	-1.1442537
C	4.9002319	-4.0271410	-3.6132470
H	5.3338813	-2.6426361	-2.0458354
H	6.7715961	-3.1163098	-2.9562460
H	5.3890488	-4.8031311	-4.2241606
H	4.0083546	-4.4789927	-3.1534914
C	3.0280040	-1.0978264	-5.2118496
H	3.9288064	-0.6233320	-5.6435711
H	2.4294305	-1.5805480	-6.0071344
C	1.8190922	0.9783398	-5.2016820
H	1.3124958	0.7061462	-6.1473001
H	2.6736127	1.6465089	-5.4045646
C	-0.4717937	3.5970949	-3.5981154
H	-0.0245001	4.5628494	-3.3118189
H	-1.4541379	3.7833495	-4.0640099
H	-0.6019171	2.9781038	-2.7032206
N	0.4140275	2.9095583	-4.5342436
C	0.8849750	3.6840982	-5.6725834
H	0.0495766	4.2788790	-6.0733619
H	1.6957415	4.3744776	-5.3806392
H	1.2429770	3.0365070	-6.4820153
C	0.8150424	1.6570469	-4.2709575
O	0.3744067	1.0231767	-3.2986361
O	2.2459422	-0.1668968	-4.5133418
C	3.4351305	-2.1481749	-4.1884946
O	2.8285050	-2.2555562	-3.1159186
N	4.4308191	-2.9808383	-4.5210712
H	4.9689649	-2.7793330	-5.3562648
N	0.2415600	-4.0369321	-0.8608482
O	0.9920082	-4.5211765	-0.0180444
O	0.7590718	-3.2269731	-1.7395901
O	-0.9575053	-4.2835209	-0.9286118
N	0.1485618	0.9963738	0.6179366
O	1.0087755	0.9681834	1.4928846
O	0.5144004	0.8183171	-0.6178869
O	-1.0424798	1.1965617	0.8405047
N	3.8751226	0.8342908	-2.6962624
O	3.7041625	1.9789890	-3.1028595
O	4.8503990	0.1469460	-2.9908409
O	2.9825713	0.3281300	-1.8981044
Np	1.0428673	-0.9485934	-2.0377798
N	-0.5718828	-1.2842543	-5.0579048

O	0.0374607	-1.3895880	-6.1264327
O	-0.0004095	-1.7446279	-3.9863887
O	-1.6853233	-0.7835356	-4.9695781
O	9.3566997	-10.9166953	4.6294002

$[L_I\text{-}Np(NO_3)_4]$ (two monodentate and two bidentate nitrate)

C	-4.6545520	0.5640591	-3.1489483
H	-5.2661304	-0.1618764	-3.7081343
H	-5.1894555	1.5277826	-3.1154192
H	-3.6921317	0.6980623	-3.6546128
C	-2.9446551	-0.5792935	0.0849532
H	-3.4042651	0.0880029	0.8347225
H	-3.3694113	-1.5962331	0.1640285
C	-1.0817454	-0.9936607	1.5322895
H	-1.4308232	-0.2760550	2.2993822
H	-1.4156630	-2.0132332	1.7943882
C	2.6306829	-1.5366772	2.3395736
C	3.2148175	-2.7366569	1.5824995
H	2.9994550	-1.4967428	3.3769388
H	2.9306132	-0.6007424	1.8463041
C	4.6822415	-2.4720580	1.1708118
H	3.1464082	-3.6476375	2.2033888
H	2.6042557	-2.9180318	0.6831910
H	4.6909776	-1.6037876	0.4860356
H	5.2595432	-2.1575630	2.0588000
C	5.9583487	-4.5604992	1.4508144
C	7.3911011	-4.2079384	1.8753536
H	5.9685373	-5.5444549	0.9538591
H	5.3283366	-4.7003335	2.3563130
C	8.0534836	-5.2456752	2.7845841
H	7.9909305	-4.0733517	0.9583466
H	7.3871733	-3.2225184	2.3763262
C	9.4935387	-4.8675069	3.1476333
H	7.4525895	-5.3752648	3.7037842
H	8.0713439	-6.2336771	2.2911241
H	10.0562523	-4.7530853	2.2085754
H	9.5037365	-3.8600806	3.6262793
C	11.6277794	-5.8771865	3.7730502
C	12.0601378	-6.5107044	2.4468034
H	12.0616769	-4.8509445	3.8522996
H	12.0849444	-6.4532787	4.5920734
C	13.5864210	-6.5443141	2.2895805
H	11.6609277	-7.5362678	2.3845650
H	11.6286882	-5.9513752	1.5983375
H	14.0090528	-5.5411844	2.4799230
H	14.0242356	-7.2358831	3.0251186
C	14.9001821	-8.5430990	-0.6927514
H	14.7317397	-7.6657822	-1.3545350
H	15.9998052	-8.6837214	-0.6153213
C	14.9163035	-10.2361420	-2.3041287

H	15.9398187	-10.5734586	-2.0362574
H	15.0326032	-9.4917163	-3.1236301
C	13.9411271	-13.3243885	-4.3411100
H	14.5277051	-14.2496213	-4.1932547
H	12.9914606	-13.4075639	-3.7992346
H	13.7360830	-13.2199139	-5.4224800
N	-4.4277541	0.0648067	-1.7929755
N	14.6608874	-12.1698389	-3.8350824
C	-5.6189852	-0.3243603	-1.0524460
H	-6.3370666	0.5120980	-1.0378451
H	-6.1060019	-1.1899387	-1.5325289
H	-5.3871745	-0.5865775	-0.0143555
C	15.9625253	-11.9354264	-4.4247505
H	16.6733943	-12.7476491	-4.1788093
H	15.8834957	-11.8889467	-5.5264414
H	16.4015451	-10.9895587	-4.0884395
C	14.0862599	-11.4204716	-2.8277012
C	-3.1808605	-0.0173757	-1.3125390
O	-2.2012860	0.3569932	-1.9818835
O	12.9851747	-11.6623108	-2.3770880
O	-1.5478403	-0.6180653	0.2565380
O	14.2733000	-9.6864331	-1.1976999
C	14.3996469	-8.2866362	0.7352239
C	0.4370910	-0.9384843	1.4392657
O	0.9629601	-0.3074235	0.5072102
O	14.4057064	-9.1586425	1.5799971
N	1.1639206	-1.5262704	2.3877125
H	0.6901258	-2.1092031	3.0698626
N	14.0312875	-6.9921914	0.9811317
H	13.9390685	-6.3562421	0.1977659
N	5.3852345	-3.5737012	0.5436858
N	10.1793800	-5.8574191	3.9762636
C	9.7759437	-5.8079009	5.3819966
C	9.4823623	-7.1699270	6.0276317
H	10.5248571	-5.2599404	5.9957265
H	8.8517178	-5.2138057	5.4535507
C	10.6982136	-8.0548323	6.2983335
H	8.9749387	-6.9724986	6.9927621
H	8.7650143	-7.7171202	5.3928088
H	11.1875085	-8.3741244	5.3659655
H	11.4582929	-7.4875528	6.8718557
C	10.5362416	-11.5536461	7.8320980
H	9.5585955	-11.3027736	8.3002174
H	10.3485652	-12.3731265	7.1065390
C	11.1932095	-13.1513265	9.4050335
H	11.1651124	-13.9712337	8.6555402
H	10.1941016	-13.1386769	9.8953155
C	13.1863239	-15.0157066	12.0867049
H	13.7379093	-15.9203470	11.7704887
H	13.8892857	-14.1793306	12.1783747
H	12.7308450	-15.2203179	13.0725958
N	12.1704300	-14.6602002	11.1118260

C	11.1626005	-15.6699044	10.8602541
H	11.5975352	-16.5710077	10.3866430
H	10.6941633	-15.9894962	11.8089713
H	10.3633579	-15.2987826	10.2088691
C	12.2700202	-13.4455287	10.4637287
O	13.1468514	-12.6416483	10.7062215
O	11.4777914	-11.9312256	8.7968592
C	11.1025996	-10.3764121	7.0269955
N	10.3146517	-9.2599369	7.0149698
H	9.5409321	-9.2012109	7.6668819
C	4.8224717	-4.0571900	-0.7084369
C	5.8593630	-4.6718438	-1.6556606
H	4.0006182	-4.7954747	-0.5524503
H	4.3562394	-3.1947193	-1.2154101
C	5.2472992	-5.0572568	-3.0098073
H	6.6804436	-3.9540038	-1.8147000
H	6.3054898	-5.5724597	-1.1972870
H	4.3184325	-5.6345530	-2.8555202
H	4.9797298	-4.1483838	-3.5700519
C	7.8361500	-6.2628935	-5.5396551
H	8.7702766	-6.3764304	-4.9589571
H	7.3425869	-7.2579775	-5.5811721
C	8.6428256	-6.7054311	-7.7251807
H	8.5568438	-6.2515248	-8.7265478
H	8.0561092	-7.6506712	-7.7430035
C	12.1565675	-8.2051010	-8.1095096
H	12.2661170	-9.2983225	-7.9852478
H	12.7921386	-7.8915080	-8.9572136
H	12.4946074	-7.7024186	-7.1957176
N	10.7693747	-7.8463690	-8.3479239
C	10.1665171	-8.4275156	-9.5312971
H	10.7500134	-8.1677750	-10.4333655
H	10.1370552	-9.5315186	-9.4625008
H	9.1414124	-8.0738796	-9.6855969
C	10.1226333	-7.0403225	-7.4389085
O	10.6736066	-6.6066313	-6.4406107
O	8.1017016	-5.7866684	-6.8335765
C	6.9255953	-5.2606033	-4.8209521
O	6.9290451	-4.0711766	-5.0618138
N	6.1310789	-5.8338035	-3.8620581
H	6.2027092	-6.8313536	-3.6995797
N	-0.7185383	-2.7209366	-1.2211927
O	-0.2475854	-3.2893214	-0.2432535
O	0.0296559	-1.8115997	-1.8134047
O	-1.8276736	-2.9378870	-1.6801731
N	-0.8782327	2.4144031	0.9224440
O	-0.0717556	2.9891074	1.6165055
O	-0.5301997	2.1443173	-0.3306595
O	-2.0013939	2.0659469	1.2761359
N	2.4721726	2.1429495	-1.9246710
O	3.4372733	2.8358550	-2.0393379
O	2.4424338	1.0941369	-1.1818647

O	1.3636872	2.3697195	-2.5274426
Np	0.1674975	0.4594420	-1.6381280
N	0.6157162	0.1975938	-4.4633481
O	1.4520079	-0.2208846	-3.5901850
O	-0.4436714	0.7220510	-3.9523425
O	0.7915481	0.1067420	-5.6412691
O	12.1487080	-10.4648127	6.4163948

$[L_{II}\text{-}Np(NO_3)_4]$ (all nitrate monodentate)

C	19.2126132	-10.4041543	9.7564006
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C	19.2944223	-11.7909364	11.8097769
C	19.1059529	-12.8286678	9.5493372
C	19.2028303	-14.1780312	10.2627122
O	19.2950817	-15.2082190	9.3146547
C	19.3271276	-16.4682822	9.9138604
C	19.2227520	-17.5520987	8.8428446
O	18.5679613	-17.4009162	7.8215672
O	18.9723778	-12.7451609	8.3364117
N	19.8629623	-18.7209863	9.1432994
C	19.6585363	-19.9101458	8.3314825
C	20.9230057	-20.7074794	8.0071190
C	20.6854362	-21.7282631	6.8778240
N	19.6448055	-22.7218594	7.1546834
C	18.8491366	-23.1512178	5.9974633
C	17.3978493	-22.6336048	5.9893267
C	17.3391078	-21.1126647	5.8347747
N	16.0202074	-20.4947379	5.8987328
C	15.5191912	-19.9440572	7.0339451
C	14.2383391	-19.1051922	6.8522285
O	14.3004713	-17.8657307	7.4882689
C	15.2845565	-16.9869090	6.9833211
C	15.0053931	-15.5716719	7.5184909
N	15.8623525	-14.5961627	7.1073075
C	15.5811239	-13.2112781	7.4528618
C	20.1167908	-23.8223750	7.9915552
C	19.0090298	-24.5335099	8.7705615
C	19.5342104	-25.6976982	9.6189718
N	18.4985292	-26.3181163	10.4335051
C	18.7753313	-27.6909406	10.8430518
C	17.5026516	-28.4705685	11.1855834
C	17.7430200	-29.8341304	11.8397976
C	16.4165438	-30.5547448	12.1365008
N	16.4720369	-31.4804683	13.2638172
C	17.2464923	-32.6838054	12.9741388
C	17.8400875	-33.3597229	14.2168894
C	18.6623664	-34.5964420	13.8459905
N	19.4154307	-35.2105719	14.9414024
C	18.5702777	-35.8137541	15.9809402

C	18.1532205	-34.8957890	17.1471472
C	19.2846199	-33.9755433	17.6228542
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C	19.8043170	-34.0374111	20.0238003
C	19.4693768	-33.5504316	21.4256966
O	20.5978553	-33.8540110	22.2036792
C	20.4888714	-33.5893972	23.5778128
C	21.7844673	-34.1034479	24.1990919
N	22.0628258	-33.8362376	25.4864780
C	23.2898991	-34.3624097	26.0855866
C	18.0158026	-25.4620409	11.5216781
C	16.5300373	-25.0870886	11.4483741
C	16.1814203	-24.0023738	12.4822766
N	14.7688702	-23.7297638	12.7244101
C	13.9968331	-23.3636992	11.5429345
C	14.4971630	-22.1172728	10.8072633
C	14.4943777	-20.8641324	11.6767019
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C	14.9421600	-18.4652466	11.4847117
C	15.4719220	-17.3615350	10.5626411
O	15.9382764	-16.2296716	11.2593028
C	14.9136118	-15.3510026	11.6465473
C	15.5128520	-14.1199905	12.3241208
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C	15.0862770	-12.0615347	13.5666112
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C	14.6940563	-24.9736459	14.9334316
C	15.1175622	-23.7064217	15.7115011
N	14.6191663	-23.6023371	17.0731379
C	15.0106200	-24.3995541	18.0706921
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O	13.8558697	-22.7973631	19.4649974
C	13.4054757	-22.4222827	20.7355171
C	12.9171404	-20.9710983	20.6877936
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C	11.9932395	-19.0734911	21.9012824
O	15.7609438	-25.3786371	17.9274462
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O	14.0478994	-15.3642856	8.2565049
C	17.0676835	-14.8151438	6.3163692
C	15.1577859	-31.7775471	13.8290105
C	14.4262625	-30.5627568	14.4176693
C	13.3224666	-30.9706408	15.3995491
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C	11.4334896	-29.5175802	14.8452971
C	11.3160989	-28.0296837	14.4785711
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C	9.5884366	-25.3435499	14.1891345
C	9.6088403	-23.8461587	13.8628929
O	10.6989330	-23.2235670	14.4914357
C	10.7600900	-21.8285768	14.4109304

C	11.8254114	-21.3451458	15.4162033
N	12.1070228	-20.0166639	15.4433406
C	13.1060928	-19.5306782	16.3914620
C	12.0070036	-30.0050633	17.2068761
C	13.0638128	-29.6194836	18.2515546
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N	14.4448062	-27.6668167	19.0762115
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O	15.1855086	-26.0692501	21.9753095
C	14.6808336	-26.5324309	23.1981640
C	14.0280433	-25.3689553	23.9507747
N	13.5409985	-25.6640309	25.2019993
C	12.9879585	-24.6012721	26.0227726
O	13.6642638	-28.4347250	21.0794196
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C	21.6635133	-36.9849088	16.5894688
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C	23.3760826	-37.3006152	18.3607925
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O	24.7520126	-38.4771422	19.9684202
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C	22.9736711	-39.5241340	21.2503826
N	22.3453997	-40.6374816	21.6622638
C	21.2383503	-40.5495548	22.6134466
O	22.6674966	-36.8015339	19.2454238
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N	19.4573140	-36.9996018	23.2885738
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O	24.7968145	-32.8205881	20.1929606
N	24.3830644	-33.9459899	20.0062885
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O	20.6774314	-34.8941441	19.8739687
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C	22.5187195	-41.9362326	21.0285025
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C	13.6022108	-26.9734670	25.8255199
O	14.4767930	-18.2283836	12.5981739
O	16.7220228	-13.9533605	12.4199167
C	13.1670061	-13.3706863	12.7587802
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H	19.4707896	-27.7292591	11.7161220
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H	19.9461080	-26.4668101	8.9439741
H	18.2368552	-24.9280290	8.0885506
H	18.5054327	-23.7861414	9.4062770
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H	16.6424902	-33.4247230	12.3973358

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H	15.9109143	-25.9843142	11.6121052
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H	18.2178701	-25.9442276	12.4993002
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H	21.6540532	-22.2153371	6.6233875
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H	22.4813169	-36.7281515	14.6197790
H	22.1390854	-35.2008296	15.4466174
H	21.1872987	-36.4042590	17.3876447
H	21.0640483	-37.9055580	16.4758049
H	25.0837589	-38.5750069	17.9106523
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H	24.7325200	-40.4633648	20.4230791
H	23.5036963	-39.9793231	19.2211868
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H	21.4519600	-41.1767789	23.4948316
H	21.0777233	-39.5144412	22.9271266
H	22.3388557	-42.7238358	21.7751687
H	21.7993520	-42.0718326	20.2009930
H	23.5359848	-42.0740374	20.6424134
H	23.6062977	-37.8433934	16.4362032
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H	17.6577383	-36.2648381	15.5330102
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H	12.4677276	-18.7028667	13.8261261
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$[L_{II}\text{-}Np(NO_3)_4]$ (three monodentate and one bidentate nitrate)

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C	19.7183172	-32.8558599	20.9045051
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C	14.5018939	-25.2491801	14.7482256
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C	11.8959920	-21.4374089	15.6098985
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C	13.3489151	-19.6681581	16.4176833
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H	15.7878724	-27.5503264	26.1188625
H	14.0074885	-27.6108084	26.0515951
H	14.9538358	-28.2098391	24.6811404
H	15.3755349	-27.2741252	18.1836593
H	10.2109633	-29.9595044	15.2973920
H	11.2727422	-30.1257531	13.9077219
H	11.1937761	-29.4486941	17.4001103
H	11.6169025	-31.1591690	17.3911084
H	15.4339223	-22.5670717	10.2602086
H	13.7841703	-22.1731588	9.7977583
H	13.4175920	-20.9918008	11.9749808
H	15.0208778	-21.4585752	12.5245644
H	16.4354373	-18.0557837	10.1845249
H	14.8213002	-17.3396767	10.0700700
H	14.3496268	-16.2458559	12.6438161
H	14.5186711	-15.3432619	11.1059161
H	14.9942429	-11.5724294	13.6497763
H	14.9181390	-12.6106279	15.1035743
H	16.4002453	-12.5942529	14.0973895

H	12.9099470	-14.1626891	14.0738584
H	12.9334985	-12.7437962	12.9926157
H	13.0626972	-14.3698394	12.3045344
H	15.3842548	-20.0946350	10.0391573
H	13.7142414	-25.7102579	15.3662869
H	15.3282322	-25.9771560	14.7364233
H	16.0291813	-23.7626228	15.1825414
H	14.4021527	-23.1002571	14.9934395
H	14.5137128	-25.0987577	19.6802675
H	16.1115917	-24.3570067	19.7183705
H	15.3385547	-22.7210029	21.2194070
H	13.6777507	-23.3053982	21.2063575
H	12.2813259	-19.2418136	22.6417394
H	13.9622333	-18.6384121	22.5629205
H	13.0347377	-18.8970351	21.0479797
H	14.7581247	-20.7705976	23.7748606
H	13.0738387	-21.3482458	23.8393167
H	14.3294954	-22.3469305	23.0661911
H	14.1768273	-23.1078855	17.1963930
H	12.8539763	-23.4851944	11.6683672
H	13.8007664	-24.4710870	10.5515686
H	12.8972391	-24.5981081	13.4795779
H	13.7398429	-26.0323798	12.8740384
Np	21.8472557	-35.7817229	21.4311413
N	24.2278188	-37.3147566	23.3542824
O	24.8784898	-38.3079831	23.1513205
O	23.1718032	-37.1174208	22.5309347
O	24.4179359	-36.4798929	24.2187392

[L_I-Pu(NO_3)$_4$] (all nitrate monodentate)

C	-3.7807437	-1.5799775	-2.4638566
H	-4.3685101	-2.4850004	-2.6900589
H	-4.4336403	-0.6982335	-2.5796667
H	-2.9382357	-1.5073294	-3.1635985
C	-1.4490692	-1.6993731	0.5726954
H	-1.8780593	-0.9211490	1.2293626
H	-1.7112076	-2.7060060	0.9435029
C	0.7059774	-1.6685354	1.6526598
H	0.4495765	-0.8734216	2.3760530
H	0.5773634	-2.6657733	2.1130967
C	4.5303895	-1.5654292	1.7864351
C	5.0558475	-2.8885486	1.2188836
H	5.0857745	-1.2600675	2.6876582
H	4.6455669	-0.7663834	1.0384502
C	6.4715428	-2.7465064	0.6232722
H	5.0387171	-3.6646958	2.0047536
H	4.3530800	-3.2176318	0.4375023
H	6.4637185	-1.9156705	-0.1036006
H	7.1777425	-2.4361582	1.4122861
C	7.5508861	-4.9312077	0.9116139
C	8.9976204	-4.6505068	1.3383694
H	7.5216190	-5.9181790	0.4210890

H	6.9156927	-5.0386293	1.8181062
C	9.5196970	-5.6549006	2.3695410
H	9.6315785	-4.6598693	0.4337900
H	9.0733229	-3.6269017	1.7474866
C	11.0091125	-5.4841970	2.6856219
H	8.9299858	-5.5619709	3.2990593
H	9.3607983	-6.6893900	2.0163380
H	11.5754136	-5.6313870	1.7517217
H	11.2037571	-4.4285128	2.9912252
C	12.9064257	-6.8059590	3.5081380
C	13.1368583	-7.8076738	2.3709427
H	13.5635396	-5.9159617	3.3570942
H	13.2506560	-7.2737949	4.4438750
C	14.6113776	-8.2042290	2.2312579
H	12.5284229	-8.7085109	2.5550705
H	12.7831553	-7.3822295	1.4142880
H	15.2359710	-7.3040114	2.0822136
H	14.9680018	-8.6996271	3.1467435
C	15.3727068	-11.2801363	0.0853891
H	14.6975533	-12.1511475	0.2191831
H	15.0212719	-10.7280898	-0.8140463
C	16.8865760	-12.6640205	-1.0321303
H	16.5131337	-12.3244873	-2.0241990
H	16.3165529	-13.5840279	-0.7804326
C	20.1113341	-14.4084422	-2.1180329
H	20.4673687	-14.3441269	-3.1619660
H	20.7125958	-13.7431835	-1.4872084
H	20.2452981	-15.4510015	-1.7743898
N	-3.2818683	-1.6580012	-1.0918461
N	18.7201689	-14.0022530	-2.0219509
C	-4.2629056	-1.9652271	-0.0639116
H	-5.1613204	-1.3475815	-0.2221399
H	-4.5628677	-3.0274810	-0.1031484
H	-3.8830658	-1.7426900	0.9400862
C	17.7749539	-14.8030359	-2.7735586
H	18.1440050	-14.9500892	-3.8035350
H	17.6303711	-15.8065979	-2.3272707
H	16.7940421	-14.3184753	-2.8476638
C	18.3852828	-12.9907054	-1.1447288
C	-1.9699690	-1.5191269	-0.8518961
O	-1.1702132	-1.2545316	-1.7622143
O	19.2118420	-12.3787916	-0.4994499
O	-0.0544829	-1.5520841	0.4779549
O	16.7062287	-11.6841337	-0.0586705
C	15.2511553	-10.4328054	1.3586635
C	2.1548293	-1.5051941	1.2082608
O	2.4274420	-1.2773746	0.0238008
O	15.4793289	-10.9040521	2.4557831
N	3.1102269	-1.6223062	2.1374132
H	2.8428421	-1.8690979	3.0836794
N	14.8484520	-9.1433795	1.1491579
H	14.7131565	-8.8252146	0.1971241

N	7.0179905	-3.9392095	-0.0192440
N	11.5090445	-6.4245449	3.6812490
C	11.1098035	-6.1181818	5.0568086
C	10.1992986	-7.1704594	5.7054912
H	12.0085249	-5.9802904	5.6899677
H	10.5868966	-5.1446805	5.0806393
C	10.8404333	-8.5585668	5.8181246
H	9.9158397	-6.8143640	6.7136181
H	9.2667924	-7.2605148	5.1236721
H	11.0478858	-8.9512784	4.8126049
H	11.8016870	-8.4876398	6.3596912
C	8.4902026	-11.4158235	6.7378477
H	7.4689221	-11.4584072	6.3091199
H	8.9108504	-12.4406632	6.6784906
C	7.8786015	-11.7179536	9.0157979
H	8.2971730	-12.7472767	9.0191644
H	6.7896878	-11.8165754	8.8203327
C	7.7803916	-11.1273687	12.7984964
H	8.3586275	-11.8319921	13.4241242
H	8.3460508	-10.1943468	12.6926938
H	6.8235786	-10.9207130	13.3098294
N	7.5444805	-11.6791515	11.4748464
C	6.8138982	-12.9306582	11.4349035
H	7.4026368	-13.7619981	11.8682263
H	5.8817607	-12.8450501	12.0204734
H	6.5337364	-13.2092636	10.4125291
C	8.1134280	-11.0581657	10.3875508
O	8.7729078	-10.0393916	10.4769877
O	8.4950334	-10.9246104	8.0532637
C	9.3379429	-10.5163854	5.8312869
N	9.9947073	-9.5278377	6.4866860
H	9.8251424	-9.4568947	7.4873087
C	6.2154324	-4.4901783	-1.1056089
C	5.9633689	-3.4982437	-2.2457662
H	6.7617502	-5.3607823	-1.5077364
H	5.2328948	-4.8854531	-0.7581989
C	5.0799095	-4.1139835	-3.3376010
H	5.4511775	-2.5986765	-1.8739662
H	6.9282541	-3.1646578	-2.6651802
H	5.6035642	-4.9238833	-3.8701566
H	4.1772910	-4.5464929	-2.8795419
C	3.1979200	-1.3587415	-5.2129030
H	4.0911285	-0.9234621	-5.6994813
H	2.5939498	-1.9224325	-5.9482283
C	1.9190108	0.6745182	-5.3903155
H	1.4487626	0.2870133	-6.3140887
H	2.7267497	1.3829884	-5.6403542
C	-0.5615061	3.2474517	-4.0015421
H	-0.1743702	4.2466330	-3.7436203
H	-1.5324416	3.3623964	-4.5122475
H	-0.6952718	2.6632474	-3.0837903
N	0.3942971	2.5661432	-4.8716411

C	0.8722902	3.3138718	-6.0247751
H	0.0255731	3.8464104	-6.4851628
H	1.6345857	4.0571580	-5.7324135
H	1.2961761	2.6514192	-6.7890760
C	0.8454904	1.3487129	-4.5344883
O	0.3953523	0.7380547	-3.5525165
O	2.4147915	-0.3712240	-4.5985403
C	3.6190412	-2.3013187	-4.0958023
O	3.0129981	-2.3149939	-3.0178554
N	4.6298983	-3.1468044	-4.3390184
H	5.1680084	-3.0286194	-5.1896989
N	0.5531378	-3.9936461	-0.5734619
O	1.3102236	-4.3438478	0.3294232
O	1.0483307	-3.2538593	-1.5216319
O	-0.6283194	-4.3137704	-0.6338604
N	0.0273987	1.1602352	0.2961921
O	0.8252836	1.2786189	1.2216790
O	0.4901959	0.8813523	-0.8863060
O	-1.1859839	1.3095927	0.4221129
N	3.9373645	0.8454860	-2.8292574
O	3.7295053	1.9401009	-3.3387773
O	4.9530824	0.1837058	-3.0149435
O	3.0282163	0.3630944	-2.0303372
N	-0.3234041	-1.7447148	-5.0459187
O	0.2775604	-1.8756152	-6.1184552
O	0.3031974	-2.0952968	-3.9640894
O	-1.4697389	-1.3222727	-4.9767873
O	9.3926409	-10.7334333	4.6314403
Pu	1.1802765	-1.0077048	-2.0623932

[L_I-Pu(NO_3)$_4$] (two monodentate and two bidentate nitrate)

C	-4.6938157	0.5953853	-3.0817371
H	-5.3041960	-0.1295576	-3.6435336
H	-5.2338495	1.5558603	-3.0380177
H	-3.7348390	0.7385354	-3.5914305
C	-2.9627512	-0.5742948	0.1318105
H	-3.4210320	0.0816691	0.8925974
H	-3.3849014	-1.5932565	0.1985432
C	-1.0770667	-0.9975719	1.5533162
H	-1.4202311	-0.2950570	2.3371973
H	-1.3931396	-2.0249400	1.8077556
C	2.6522789	-1.5195753	2.2956547
C	3.2285645	-2.7212967	1.5358043
H	3.0356690	-1.4761378	3.3276666
H	2.9426191	-0.5840301	1.7960042
C	4.6961124	-2.4640129	1.1195868
H	3.1592063	-3.6311705	2.1583286
H	2.6135302	-2.9015744	0.6392287
H	4.7068141	-1.6020136	0.4270605
H	5.2749443	-2.1432739	2.0043604
C	5.9598987	-4.5561832	1.4198868

C	7.3928774	-4.2080973	1.8473006
H	5.9662117	-5.5443854	0.9313116
H	5.3256675	-4.6846087	2.3240709
C	8.0464820	-5.2420061	2.7672569
H	7.9969473	-4.0836343	0.9316810
H	7.3921581	-3.2188746	2.3407803
C	9.4863502	-4.8666819	3.1338289
H	7.4408589	-5.3620801	3.6846162
H	8.0624312	-6.2336759	2.2811536
H	10.0520293	-4.7564260	2.1960643
H	9.4976329	-3.8578437	3.6095935
C	11.6176252	-5.8734161	3.7708800
C	12.0582718	-6.5083534	2.4480613
H	12.0490309	-4.8461243	3.8502249
H	12.0718700	-6.4468375	4.5933252
C	13.5854404	-6.5375082	2.2987777
H	11.6626558	-7.5353150	2.3858565
H	11.6293389	-5.9520431	1.5963258
H	14.0039784	-5.5329247	2.4903636
H	14.0215946	-7.2270535	3.0371526
C	14.9136798	-8.5367376	-0.6771177
H	14.7491259	-7.6586170	-1.3387913
H	16.0126272	-8.6818248	-0.5990040
C	14.9223294	-10.2270472	-2.2911807
H	15.9445043	-10.5696142	-2.0247439
H	15.0415206	-9.4809991	-3.1087727
C	13.9342009	-13.3074748	-4.3334044
H	14.5175351	-14.2346305	-4.1844424
H	12.9839194	-13.3870941	-3.7920666
H	13.7302733	-13.2031829	-5.4149770
N	-4.4573439	0.0864023	-1.7311693
N	14.6573691	-12.1549243	-3.8277003
C	-5.6425518	-0.3169397	-0.9885221
H	-6.3673157	0.5135661	-0.9665321
H	-6.1243294	-1.1839160	-1.4714203
H	-5.4046737	-0.5826797	0.0472632
C	15.9595751	-11.9241161	-4.4174998
H	16.6690623	-12.7372222	-4.1703174
H	15.8805141	-11.8792630	-5.5192408
H	16.4002973	-10.9784077	-4.0828786
C	14.0869292	-11.4064059	-2.8172904
C	-3.2075944	0.0050891	-1.2579122
O	-2.2341548	0.3929980	-1.9288704
O	12.9855709	-11.6454544	-2.3659614
O	-1.5661122	-0.6105167	0.2920496
O	14.2822612	-9.6772449	-1.1831115
C	14.4125392	-8.2786777	0.7503329
C	0.4398319	-0.9239296	1.4347960
O	0.9467455	-0.2784719	0.5010861
O	14.4223860	-9.1486651	1.5971710
N	1.1865126	-1.5144604	2.3655557
H	0.7265422	-2.1068956	3.0491121

N	14.0379357	-6.9853751	0.9929569
H	13.9439418	-6.3517115	0.2079491
N	5.3957031	-3.5734726	0.5026525
N	10.1680803	-5.8555848	3.9669715
C	9.7588103	-5.8048027	5.3711341
C	9.4605276	-7.1664513	6.0154758
H	10.5068345	-5.2586796	5.9874832
H	8.8356962	-5.2085371	5.4395144
C	10.6742844	-8.0554015	6.2817814
H	8.9549690	-6.9686765	6.9814934
H	8.7405973	-7.7103808	5.3807301
H	11.1616004	-8.3712713	5.3472753
H	11.4363774	-7.4924493	6.8569316
C	10.5165447	-11.5608189	7.8008167
H	9.5360437	-11.3162727	8.2662306
H	10.3369480	-12.3826177	7.0760080
C	11.1829397	-13.1520680	9.3765557
H	11.1664907	-13.9724347	8.6272514
H	10.1814803	-13.1491071	9.8621960
C	13.1829073	-14.9979964	12.0656826
H	13.7442784	-15.8970260	11.7507111
H	13.8774268	-14.1549460	12.1605616
H	12.7259449	-15.2078007	13.0497922
N	12.1671292	-14.6515481	11.0873841
C	11.1722053	-15.6722157	10.8286551
H	11.6191796	-16.5663246	10.3529404
H	10.7047703	-16.0009436	11.7747094
H	10.3705290	-15.3080295	10.1763476
C	12.2572090	-13.4353609	10.4407088
O	13.1240669	-12.6223243	10.6884875
O	11.4584468	-11.9295577	8.7689284
C	11.0769168	-10.3810510	6.9953488
N	10.2901852	-9.2635469	6.9929564
H	9.5213594	-9.2061539	7.6507824
C	4.8360836	-4.0643303	-0.7481084
C	5.8751908	-4.6901312	-1.6856723
H	4.0104043	-4.7977861	-0.5897656
H	4.3760425	-3.2039092	-1.2640682
C	5.2682552	-5.0885531	-3.0383648
H	6.6978884	-3.9749721	-1.8483441
H	6.3184374	-5.5868696	-1.2170250
H	4.3405004	-5.6669342	-2.8817036
H	5.0000615	-4.1856113	-3.6078329
C	7.8718939	-6.3070526	-5.5465725
H	8.7993437	-6.4178652	-4.9547222
H	7.3790480	-7.3024931	-5.5888250
C	8.7027474	-6.7592313	-7.7210159
H	8.6281012	-6.3096454	-8.7252324
H	8.1158641	-7.7043173	-7.7411628
C	12.2193097	-8.2641464	-8.0568397
H	12.3265848	-9.3569516	-7.9276241
H	12.8653993	-7.9537454	-8.8977727

H	12.5465326	-7.7585809	-7.1406908
N	10.8352632	-7.9057519	-8.3131431
C	10.2466542	-8.4905920	-9.5018684
H	10.8395175	-8.2316969	-10.3980795
H	10.2187203	-9.5944477	-9.4308426
H	9.2225622	-8.1395039	-9.6681645
C	10.1790105	-7.0936432	-7.4164194
O	10.7188766	-6.6547506	-6.4143706
O	8.1521692	-5.8365190	-6.8393346
C	6.9523935	-5.3024516	-4.8426735
O	6.9492474	-4.1158170	-5.0968407
N	6.1575613	-5.8699412	-3.8804951
H	6.2308801	-6.8659657	-3.7100079
N	-0.7616353	-2.6825650	-1.2465009
O	-0.2787829	-3.2628841	-0.2799969
O	-0.0243753	-1.7675302	-1.8342930
O	-1.8779612	-2.8954807	-1.6924528
N	-0.9009258	2.4219798	0.9892810
O	-0.0877275	2.9916351	1.6793898
O	-0.5605775	2.1493295	-0.2652062
O	-2.0227175	2.0757610	1.3468608
N	2.4114164	2.1779488	-1.9515728
O	3.3745641	2.8725096	-2.0755055
O	2.3943759	1.1283989	-1.2095170
O	1.2959285	2.4043727	-2.5359631
N	0.5620166	0.2493835	-4.4175106
O	1.3998158	-0.1702055	-3.5489785
O	-0.4947719	0.7701484	-3.9007042
O	0.7336418	0.1628142	-5.5966467
O	12.1185468	-10.4680125	6.3767774
Pu	0.1221549	0.5042433	-1.6058707

[L_{II}-Pu(NO_3)$_4$] (all nitrate monodentate)

C	18.8269732	-10.2769040	8.8525739
N	18.9157787	-11.5483638	9.5481800
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[L_{II}-Pu(NO_3)$_4$] (three monodentate and one bidentate nitrate)

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