

# **Evaluation of two aza-crown ether-based multiple diglycolamide-containing ligands for complexation with the tetravalent actinide ions $\text{Np}^{4+}$ and $\text{Pu}^{4+}$ : Extraction and DFT studies**

Seraj A. Ansari,<sup>a</sup> Arunasis Bhattacharyya,<sup>a</sup> Prasanta K. Mohapatra,<sup>a,\*</sup> Richard J. M. Egberink,<sup>b</sup> Jurriaan Huskens<sup>b</sup> and Willem Verboom<sup>b,\*</sup>

## **Electronic Supporting Information**

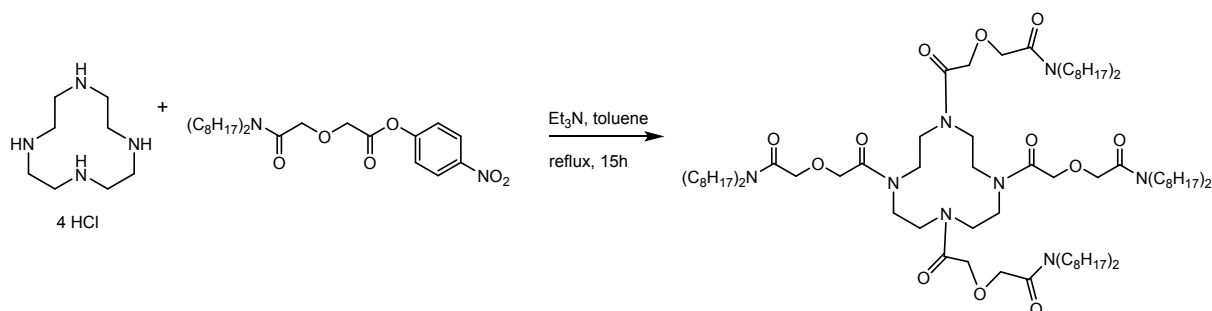
<b>CONTENTS</b>	<b>Page</b>
<b>S1. Experimental</b>	<b>2</b>
<b>S1.1 Synthesis of ligand</b>	<b>2</b>
<b>S1.2 Purification of radiotracer</b>	<b>5</b>
<b>S2. Results</b>	<b>6</b>
<b>S2.1 Solvent extraction studies</b>	<b>6</b>
<b>S2.2 DFT calculations</b>	<b>6</b>
<b>S2.2.1 Structures of free ligands</b>	<b>6</b>
<b>S2.2.2 Coordinates of optimized structures</b>	<b>6</b>
<b>References</b>	<b>16</b>

## S1. EXPERIMENTAL

### S1.1 Synthesis of **L<sub>II</sub>**

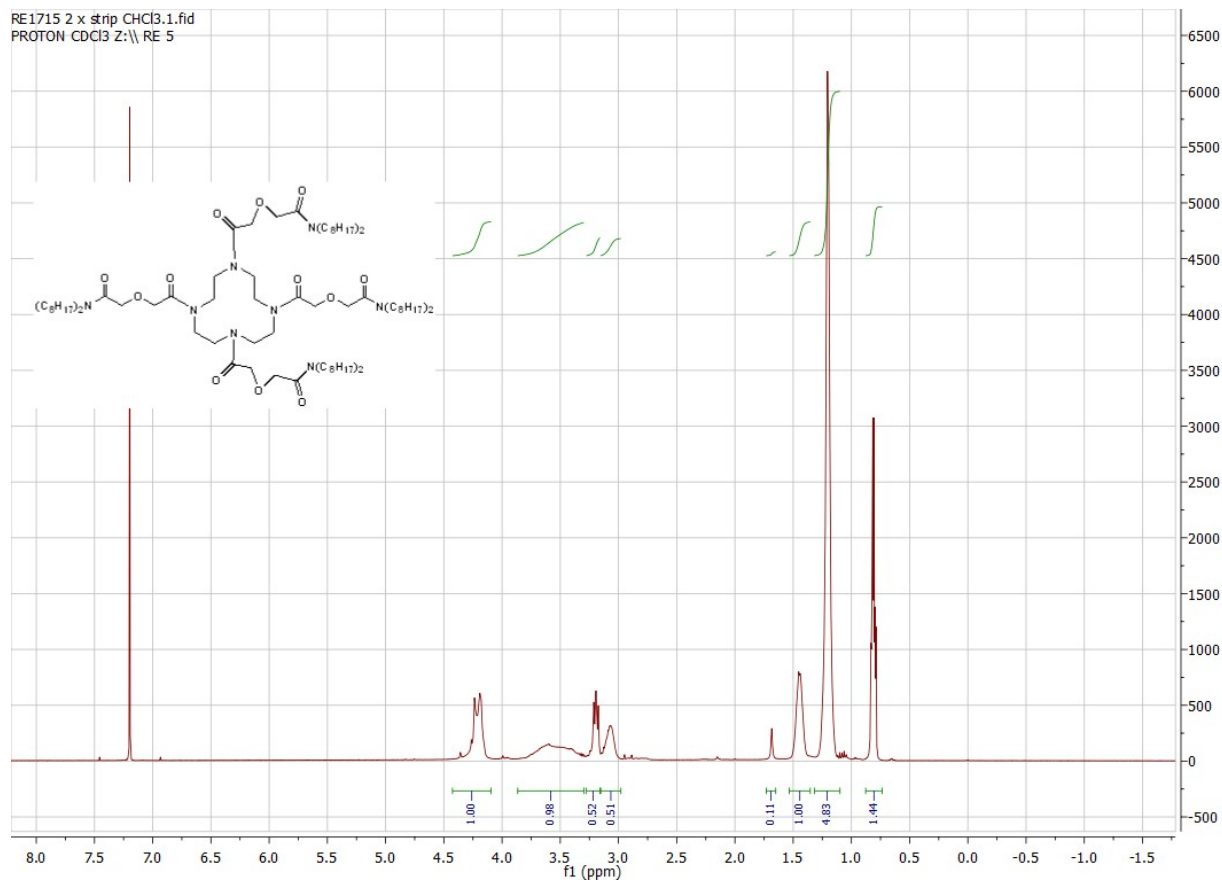
1,4,7,10-Tetraazacyclododecane tetrahydrochloride, triethylamine and Amberlyst A21 were obtained from Sigma-Aldrich and used without further purification. Triethylamine was stored on KOH. Toluene was purchased from Actu-all Chemicals and employed using a Braun MB SPS 800 dispensing machine. MeOH was obtained from Actu-all Chemicals. Et<sub>2</sub>O was bought from VWR and distilled before use. 4-Nitrophenyl 2-(2-(dioctylamino)-2-oxoethoxy)acetate<sup>1</sup> was prepared according to a literature procedure. All other reagents were of AR grade.

A solution of 4-nitrophenyl 2-(2-(dioctylamino)-2-oxoethoxy)acetate (3.16 g, 6.60 mmol), 1,4,7,10-tetraazacyclododecane tetrahydrochloride (0.5 g, 1.57 mmol) and triethylamine (1.30 g, 12.89 mmol) in dry toluene (45 mL) was refluxed for 15 h (Scheme S1). After removal of the solvent, the crude mixture was dissolved in Et<sub>2</sub>O (15 mL) and purified over a column with Amberlyst A21, using diethyl ether as the eluent. After removal of the solvent pure product was obtained as an oil (yield 81%). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ = 4.35-4.1 (m, 4H), 3.8-3.3 (m, 4H), 3.19 (t, 2H, *J* = 8.0 Hz), 3.15-3.0 (m, 2H), 1.55-1.35 (m, 4H), 1.3-1.1 (m, 20H), 0.9-0.75 (m, 6H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ = 167.9, 69.0, 46.9, 45.9, 31.8, 31.8, 29.4, 29.3, 29.2, 29.0, 27.7, 26.9, 22.7, 22.6, 14.1. ESI-MS: *m/z* 1530.0 [M+H]<sup>+</sup>; HRMS: *m/z* calcd for C<sub>88</sub>H<sub>169</sub>N<sub>8</sub>O<sub>12</sub>: 1530.2596 [M+H]<sup>+</sup>; found 1530.2616. As in the case of **L<sub>I</sub>**, in the <sup>1</sup>H NMR spectrum the signals of the DGA OCH<sub>2</sub> units and the methylene groups of the azamacrocyle are complex and broadened due to the hindrance of the movement of the DGA moieties by the azamacrocyle. The characterization data are presented in Figures S1-S3.



**Scheme S1.** Synthesis of 2,2',2'',2'''-(((1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrayl) tetrakis (2-oxoethane-2,1 diyl)) tetrakis (oxy)) tetrakis(*N,N*-dioctylacetamide) (**L<sub>II</sub>**).

$^1\text{H}$ - and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. ESI mass spectra were recorded on a Micromass LCT ESI-TOF mass spectrometer with LCT V4.1 SCN728 software from WATERS, Inc.



**Figure S1.**  $^1\text{H}$  NMR spectrum of **L<sub>11</sub>**.

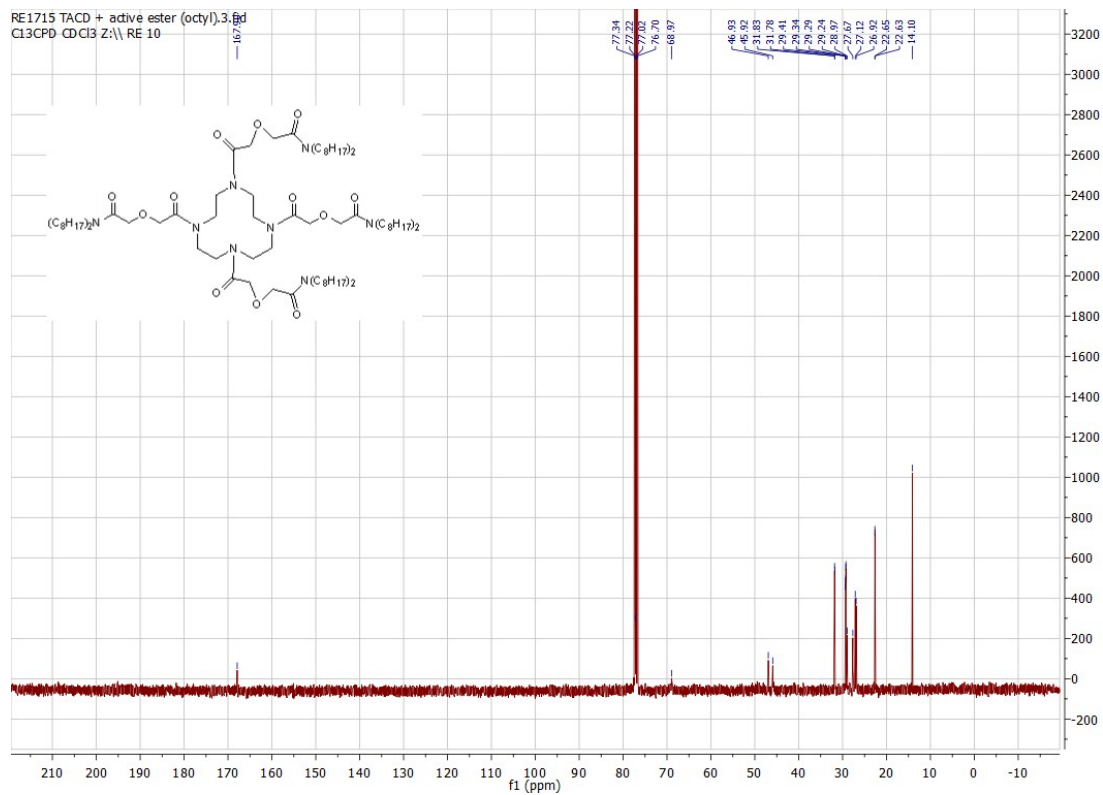


Figure S2. <sup>13</sup>C NMR spectrum of L<sub>II</sub>

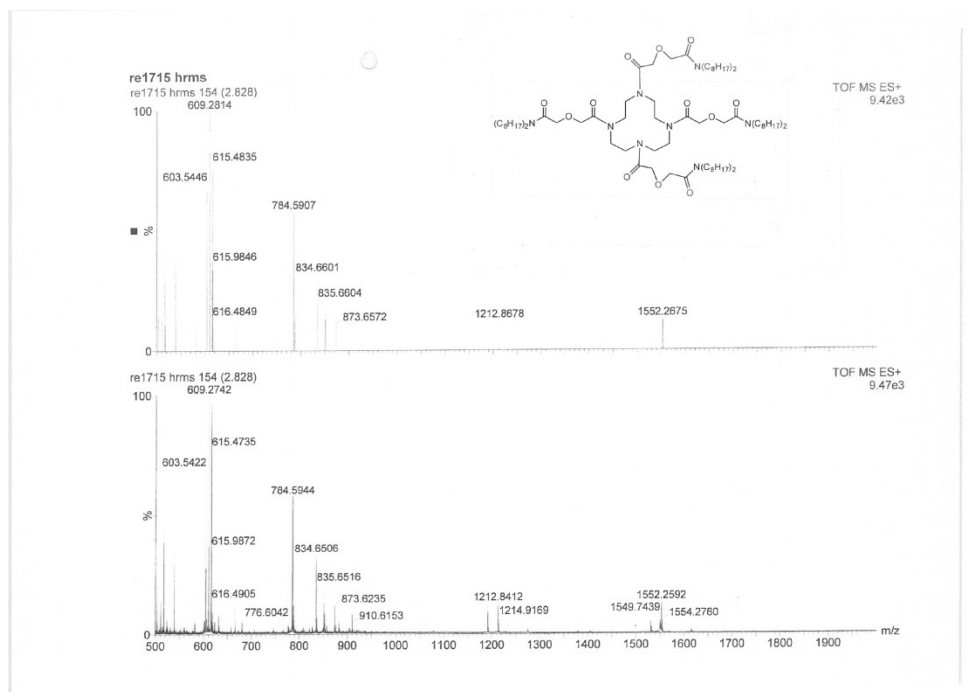
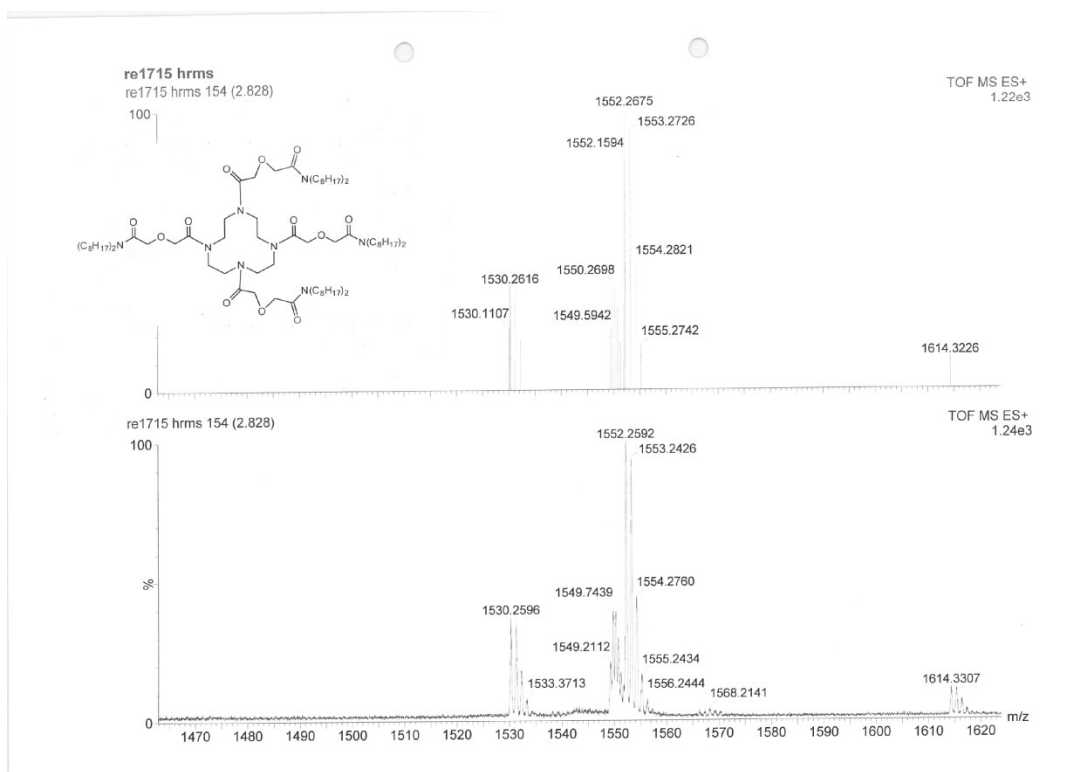


Figure S3a. HRMS ESI spectrum of L<sub>II</sub>.



**Figure S3b. Zoomed in HRMS ESI mass spectrum of L<sub>II</sub>.**

### S1.2 Purification of radiotracer

Pu stock was freshly purified from the associated  $^{241}\text{Am}$  (from the decay of  $^{241}\text{Pu}$ ) by TTA extraction method carried out from 1 M  $\text{HNO}_3$ . The valency of Pu was adjusted to the +4 state using  $\text{NaNO}_2$  followed by selective extraction of the tetravalent ion by a solution of TTA (2-thenyltrifluoroacetone) in xylene (Merck).<sup>2</sup> The extracted Pu was back extracted using 8 M  $\text{HNO}_3$  and was used as the stock for the experiments reported in this study. For the production of  $^{239}\text{Np}$ , uranyl nitrate ( $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ) was irradiated in the DHRUVA reactor at a neutron flux of  $5 \times 10^{13}$  n/cm<sup>2</sup>/s for 5 days. Subsequently, the separation of  $^{239}\text{Np}$  radiotracer from the unreacted U and associated fission products was carried out by TTA extraction as reported before.<sup>3</sup>

## S2. RESULTS

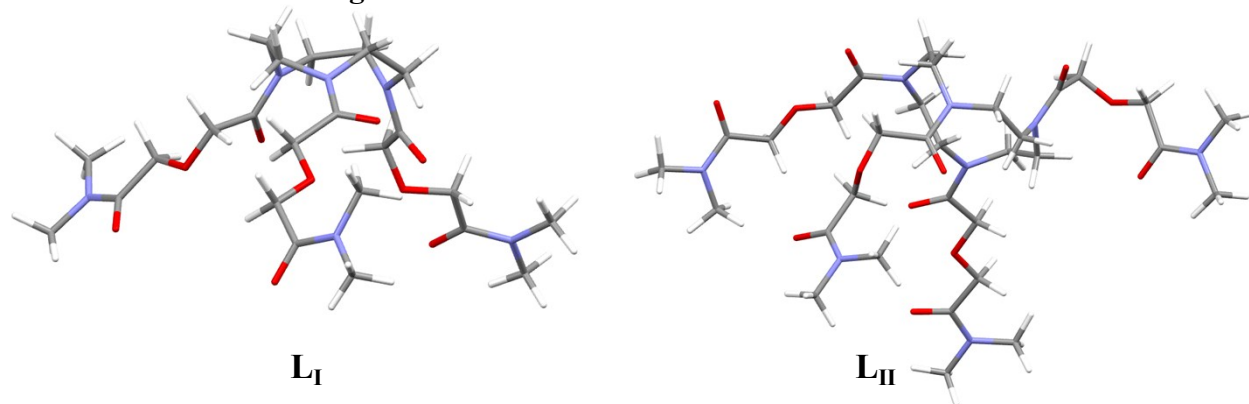
### S2.1 Solvent extraction studies

**Table S1.** Slope values of the  $\log D$  vs  $\log [\text{NO}_3^-]$  plots before and after nitrate complexation corrections as per the method cited in ref. 4.

Extraction system	Slope values of the $\log D$ vs $\log [\text{NO}_3^-]$ plots	
	Uncorrected	Corrected
$\text{Np}^{4+}\text{-L}_I$	$3.02 \pm 0.08$	$3.79 \pm 0.09$
$\text{Pu}^{4+}\text{-L}_I$	$3.07 \pm 0.12$	$3.84 \pm 0.12$
$\text{Np}^{4+}\text{-L}_{II}$	$3.08 \pm 0.11$	$3.85 \pm 0.15$
$\text{Pu}^{4+}\text{-L}_I$	$3.11 \pm 0.13$	$3.87 \pm 0.12$

### S2.2 DFT Calculations

#### S2.2.1 Structure of free ligands



#### S2.2.2 Coordinates in the optimized structures

##### $\text{Np}(\text{L}_I)(\text{NO}_3)_4$

O	-2.1145435	1.0382509	1.6581210
C	-0.9253308	0.8821691	2.0346798
N	-0.5644930	-0.1988680	2.7664918
C	-1.6324792	-1.1507111	3.1263000
C	-2.0285104	-2.1476757	2.0277739
N	-0.9860697	-3.0571719	1.5419563
C	-0.2606120	-3.8729606	2.5074415
C	1.0779330	-3.2586900	3.0688406
N	1.7302877	-2.2653108	2.2116471
C	1.8981710	-0.8800349	2.6858835

C	0.7252659	-0.2753743	3.4637945
O	-1.9536752	5.2057925	0.8509575
C	-0.7530994	5.3032339	0.4916073
C	0.1750118	4.1050397	0.6768504
O	-0.6154221	3.0704117	1.2455495
C	0.1178325	1.9022413	1.6092517
N	-0.2588119	6.4469543	-0.0211487
H	0.6043917	3.7576711	-0.2906701
H	1.0022040	4.3700512	1.3787690
H	0.6980635	1.5250462	0.7245743
H	0.8244196	2.1549393	2.4303889
H	1.0218854	0.7443345	3.7861343
H	0.5433215	-0.8219334	4.4117753
H	2.7862487	-0.8101969	3.3643313
H	2.1064254	-0.2542167	1.7950191
C	2.5241463	-2.7544646	1.1889257
H	1.7856371	-4.0985606	3.2394010
H	-0.9373288	-4.0777997	3.3671677
H	-0.0383897	-4.8619667	2.0660635
C	-0.7984073	-3.1286139	0.1623118
H	-2.4028376	-1.5981472	1.1416793
H	-2.8765204	-2.7493066	2.4378866
O	-1.2930377	-2.3129530	-0.6116738
C	-0.0341434	-4.3473901	-0.3845327
H	0.7025614	-4.7611927	0.3354866
H	-0.8080839	-5.1380182	-0.5861094
O	0.6360579	-3.9811849	-1.5726595
C	1.4070571	-5.0481105	-2.0621353
C	2.2641278	-4.5642599	-3.2461092
H	2.0896054	-5.4403225	-1.2623254
H	0.7486098	-5.8987479	-2.3806757
O	2.3409054	-3.3705817	-3.5428599
N	2.9507323	-5.5435091	-3.9337453
C	2.8750410	-6.9658460	-3.6331124
C	3.7145240	-5.1679866	-5.1164241
H	4.7806799	-5.4747734	-5.0112546
H	3.2966715	-5.6526363	-6.0301363
H	3.6564152	-4.0675559	-5.2273868
H	3.8545187	-7.4395039	-3.8652531
H	2.6741409	-7.1458238	-2.5583288
H	2.0923549	-7.4884785	-4.2357767
O	2.6343197	-3.9706319	0.9898050
C	3.3447787	-1.7569749	0.3290033
H	4.1912244	-1.3791199	0.9494593
H	3.7739148	-2.3719404	-0.4947233
O	2.6743175	-0.6155243	-0.1633996

C	1.8795385	-0.8823053	-1.3155205
C	1.2227994	0.4270800	-1.7791634
H	2.5156861	-1.3122509	-2.1260677
H	1.0936039	-1.6442039	-1.1081233
O	1.3938513	1.4839232	-1.1448973
N	0.4505558	0.3448796	-2.9029538
C	0.1168635	-0.9053499	-3.5827903
C	-0.2539343	1.5260774	-3.3831638
H	0.0447920	1.7550790	-4.4321076
H	-1.3549229	1.3581512	-3.3662984
H	-0.0054968	2.3875379	-2.7360093
H	0.0785574	-0.7176293	-4.6787971
H	0.8653315	-1.7007753	-3.3991313
H	-0.8764913	-1.2813458	-3.2465716
H	0.8899481	-2.7834441	4.0503954
H	-1.3070344	-1.6745254	4.0490275
H	-2.5426995	-0.5673407	3.3832526
C	-1.1601932	7.5672976	-0.2875818
H	-1.3327868	7.6660002	-1.3832249
H	-2.1274885	7.3801808	0.2143206
H	-0.7113683	8.5072605	0.1007287
C	1.0950877	6.5720764	-0.5476616
H	1.7640830	5.7890982	-0.1425808
H	1.0931757	6.4988294	-1.6597409
H	1.5121013	7.5610367	-0.2572274
O	-2.7168085	2.9939384	-0.8202558
O	-4.5372401	1.8371410	2.8936998
O	-2.3574295	3.6722628	3.4179143
N	-2.5491547	3.6394743	-1.9987655
N	-5.2229767	1.2603088	1.9700293
N	-1.1285140	3.6130628	3.9153134
O	-6.0280561	0.3812888	2.1823379
O	-4.9629724	1.6977480	0.7709884
O	-1.5765806	4.3993954	-2.0734861
O	-3.3420398	3.3938836	-2.8891357
O	-0.4289554	4.6248899	3.8580061
O	-0.7680130	2.5346724	4.4133145
Np	-3.1839729	3.2192971	1.3313667
O	-4.6726416	4.8548418	2.3250381
O	-4.7368539	4.6938496	0.1603293
N	-5.1816344	5.2957235	1.2161827
O	-5.9917229	6.1918185	1.1741229

**Pu(L<sub>1</sub>)(NO<sub>3</sub>)<sub>4</sub>**

O	-2.1802435	0.9907317	1.6375336
C	-0.9935527	0.8228842	2.0149269



N	-0.6484210	-0.2536174	2.7636176
C	-1.7146688	-1.2184400	3.0904247
C	-2.0940008	-2.1940573	1.9659240
N	-1.0462255	-3.0985985	1.4809442
C	-0.3306685	-3.9225823	2.4470087
C	1.0007650	-3.3116615	3.0294779
N	1.6519484	-2.2983995	2.1953421
C	1.8172088	-0.9245527	2.7011989
C	0.6339653	-0.3344567	3.4749952
O	-1.9116359	5.1669913	0.9310198
C	-0.7359353	5.2343924	0.4924145
C	0.1673172	4.0101685	0.6170699
O	-0.6272994	3.0033854	1.2255920
C	0.0721538	1.8155803	1.5820179
N	-0.2462236	6.3634097	-0.0554325
H	0.5381581	3.6535940	-0.3710153
H	1.0404413	4.2468853	1.2731803
H	0.6355757	1.4224714	0.6944550
H	0.7891149	2.0463964	2.3994719
H	0.9220124	0.6823577	3.8150825
H	0.4431842	-0.8980257	4.4113666
H	2.6966793	-0.8705284	3.3922421
H	2.0367731	-0.2797680	1.8272255
C	2.4478769	-2.7636087	1.1631236
H	1.7122692	-4.1505012	3.1888641
H	-1.0172986	-4.1368650	3.2964619
H	-0.1018804	-4.9067153	1.9983987
C	-0.8522312	-3.1624107	0.1012376
H	-2.4532758	-1.6274234	1.0842015
H	-2.9501497	-2.8006271	2.3513510
O	-1.3482796	-2.3445872	-0.6696487
C	-0.0776802	-4.3717093	-0.4534668
H	0.6356600	-4.8070243	0.2767081
H	-0.8491205	-5.1526016	-0.6971936
O	0.6284481	-3.9794866	-1.6126635
C	1.4384679	-5.0257386	-2.0848104
C	2.3228297	-4.5129459	-3.2362792
H	2.1006409	-5.4078555	-1.2644556
H	0.8106332	-5.8877036	-2.4347213
O	2.3450753	-3.3215393	-3.5510158
N	3.0960648	-5.4591933	-3.8768145
C	3.1027020	-6.8792264	-3.5604491
C	3.9029671	-5.0515323	-5.0192934
H	4.9802720	-5.2765739	-4.8418526
H	3.5797218	-5.5859053	-5.9434046
H	3.7721993	-3.9609906	-5.1615197

H	4.1422174	-7.2699757	-3.6400382
H	2.7616010	-7.0688997	-2.5242166
H	2.4627316	-7.4701892	-4.2604772
O	2.5653382	-3.9754495	0.9428008
C	3.2589976	-1.7438999	0.3207444
H	4.0959660	-1.3603991	0.9506300
H	3.7023972	-2.3421687	-0.5076032
O	2.5737892	-0.6072992	-0.1630506
C	1.7967511	-0.8697632	-1.3290968
C	1.1789651	0.4477186	-1.8221473
H	2.4387758	-1.3244307	-2.1209458
H	0.9888332	-1.6102016	-1.1288040
O	1.3563335	1.5066900	-1.1935842
N	0.4295799	0.3698172	-2.9618862
C	0.0916966	-0.8793047	-3.6415546
C	-0.2417697	1.5596251	-3.4686137
H	0.0904746	1.7777824	-4.5098945
H	-1.3454883	1.4113476	-3.4816417
H	0.0014346	2.4211482	-2.8195994
H	0.0937256	-0.7017785	-4.7400101
H	0.8170396	-1.6881680	-3.4267244
H	-0.9208686	-1.2302682	-3.3367328
H	0.8036295	-2.8559875	4.0184956
H	-1.3979959	-1.7600064	4.0057935
H	-2.6319966	-0.6478387	3.3497903
C	-1.1266731	7.5132706	-0.2559391
H	-1.3421876	7.6438934	-1.3405163
H	-2.0760411	7.3398816	0.2832545
H	-0.6371867	8.4317409	0.1353062
C	1.0755976	6.4510850	-0.6648463
H	1.7497110	5.6558473	-0.2931660
H	1.0052124	6.3696604	-1.7740430
H	1.5324465	7.4320128	-0.4088812
O	-2.7657859	2.8987405	-0.7416652
O	-4.4907467	2.1139056	3.2424417
O	-2.1705333	3.4238120	3.4939525
N	-2.6589627	3.4904115	-1.9430748
N	-5.2283796	1.4552508	2.4288006
N	-0.9660283	3.8341041	3.8670388
O	-6.0624546	0.6478449	2.7734089
O	-4.9981394	1.7207026	1.1703329
O	-1.7598163	4.3321087	-2.0644463
O	-3.4230615	3.1245295	-2.8210121
O	-0.6509683	5.0115827	3.7003715
O	-0.2268772	2.9760734	4.3795744
Pu	-3.1748854	3.2185481	1.4206653

O	-4.5077046	5.0064260	2.3230355
O	-4.6401105	4.7176443	0.1775009
N	-4.9959999	5.4262951	1.1980679
O	-5.7149166	6.3947319	1.1133635

**Np(LII)(NO<sub>3</sub>)<sub>4</sub>**

N	1.1326661	-0.0947335	-1.5064286
C	0.4588210	1.0768691	-0.9425015
H	0.9935722	1.3540761	-0.0145138
H	-0.5773312	0.8248191	-0.6537234
C	0.4251426	2.3386013	-1.8311931
H	-0.3127922	2.2287994	-2.6493832
H	1.4108847	2.4931174	-2.3268231
N	0.1233555	3.5158184	-1.0257669
C	1.1546622	3.9982843	-0.0980007
H	1.2491650	5.0977795	-0.2377001
H	2.1211591	3.5337808	-0.3842783
C	0.8740616	3.7881847	1.4078304
H	1.6378401	4.3711322	1.9661055
H	-0.1249580	4.2151510	1.6258400
N	0.9021996	2.4100561	1.9362374
C	2.1580509	1.8799604	2.4986173
H	1.9514813	1.4355777	3.4989544
H	2.8337225	2.7402710	2.6589224
C	2.9425581	0.7989222	1.7147992
N	3.4577787	1.1097723	0.3637042
C	2.5707712	0.0394242	-1.8206712
H	2.8503560	-0.7987705	-2.4881495
H	2.7120943	0.9779449	-2.3939455
C	3.5127209	-0.0188756	-0.5990317
H	3.3095677	-0.9555615	-0.0414925
H	4.5493137	-0.1122388	-0.9796307
H	2.3380938	-0.1230103	1.6213944
H	3.8166923	0.5424604	2.3599190
C	0.5996304	-1.3360804	-1.4606840
C	-0.7995707	-1.5598825	-0.8756319
H	-0.9514625	-1.0285594	0.0911597
H	-1.5809389	-1.2145605	-1.5970465
O	-0.9106416	-2.9635026	-0.6648649
O	1.2335328	-2.3323037	-1.8823846
C	-2.0579096	-3.3559679	0.0832090
H	-2.9929478	-3.0576297	-0.4524986
H	-2.0686059	-2.8487890	1.0739691
C	-1.9814156	-4.8766254	0.1881000
O	-1.1266759	-5.4855086	-0.5141138
N	-2.8340148	-5.5454459	0.9819048

C	-2.7573794	-7.0065521	1.0664219
H	-2.5716234	-7.3043661	2.1219490
H	-3.7202266	-7.4525764	0.7308192
H	-1.9314373	-7.3772516	0.4283613
C	-3.8615099	-4.9070312	1.8000717
H	-4.8694386	-5.2482561	1.4704870
H	-3.7239028	-5.2084995	2.8624999
H	-3.8187564	-3.8010073	1.7473415
C	-0.3079883	1.7542482	2.0215233
C	-0.3708158	0.3977327	2.7680913
H	0.4428590	-0.2945595	2.4659799
H	-0.2613774	0.5775302	3.8703374
O	-1.3371362	2.2168659	1.5153950
O	-1.5665307	-0.2981474	2.4806896
C	-2.7133081	0.2305229	3.1124651
H	-2.5994607	0.1805977	4.2284328
H	-2.8507344	1.2969139	2.8241342
C	-3.9401792	-0.5954973	2.6961030
O	-3.8265169	-1.6042137	1.9901368
N	-5.1612923	-0.1469094	3.1485491
C	-6.3639874	-0.8967668	2.8150127
H	-6.8315462	-1.3312978	3.7301942
H	-7.1110983	-0.2316160	2.3238479
H	-6.0872161	-1.7136432	2.1214052
C	-5.3635402	1.0066404	4.0131737
H	-6.1614442	1.6608991	3.5928027
H	-5.6813984	0.6942927	5.0369473
H	-4.4460420	1.6172625	4.1026688
C	-1.0505326	4.2548483	-1.0876352
C	-2.1449347	3.7271808	-2.0387399
H	-1.7704070	3.7642665	-3.0991853
H	-2.3568606	2.6472614	-1.8115829
O	-1.2004508	5.2760521	-0.4303794
O	-3.2945620	4.5089700	-1.8841358
C	-4.3050353	4.1323412	-2.7769450
H	-3.9700469	4.2685259	-3.8415811
H	-4.5626423	3.0432735	-2.6661913
C	-5.5593871	4.9904524	-2.4999363
O	-5.5748399	5.8214452	-1.6011405
N	-6.6493242	4.7538884	-3.3274742
C	-7.8827310	5.4811970	-3.0691190
H	-8.2227013	6.0196518	-3.9845312
H	-8.6986355	4.7898840	-2.7479736
H	-7.6831880	6.2117640	-2.2605043
C	-6.7180761	3.7270306	-4.3516152
H	-7.2275929	4.1303408	-5.2569378

H	-5.7104703	3.3918406	-4.6656751
H	-7.2951591	2.8305664	-4.0123359
C	4.3825549	2.1354508	0.2873737
C	5.1791684	2.3182874	-1.0290454
H	4.5126277	2.2618392	-1.9167153
H	5.6006875	3.3493958	-0.9691167
O	4.5623637	2.9406146	1.2077326
O	6.2089606	1.3722200	-1.2748409
C	7.3599711	1.4819341	-0.4720017
H	7.5943812	2.5553853	-0.2582777
H	8.1963013	1.0663268	-1.0786650
C	7.2363277	0.6824112	0.8516190
O	6.1774281	0.1198568	1.1356136
N	8.3519255	0.6204539	1.6566750
C	8.3053150	-0.1896322	2.8671563
H	9.0590404	-1.0106190	2.8211921
H	8.5178936	0.4340274	3.7663495
H	7.2919769	-0.6281857	2.9514124
C	9.6342620	1.2357439	1.3559622
H	10.3998455	0.4729235	1.0736559
H	9.5539736	1.9695755	0.5316318
H	10.0133366	1.7799410	2.2517273
O	-0.3351127	-5.8448393	-3.5334193
N	-0.9551682	-4.8237466	-4.0375931
O	-0.7355955	-3.7120948	-3.4075244
O	-1.6791464	-4.9025394	-5.0019967
O	1.3798408	-6.7135566	-1.2063377
N	1.1197398	-7.7453970	-0.3278342
O	1.9158569	-7.8898965	0.5815225
O	0.1250764	-8.4175054	-0.5674104
O	1.5265039	-4.1565023	0.3753460
N	1.0496879	-3.3496121	1.3109380
O	0.2631604	-3.8113682	2.1356756
O	1.4393418	-2.1681376	1.2962504
Np	0.7645372	-4.6946336	-1.7114568
O	2.5576950	-4.4619248	-2.9459572
O	4.1444428	-2.9277204	-2.9034660
O	2.7542097	-3.0081495	-4.5953010
N	3.1965652	-3.3891788	-3.5233058

**Pu(L<sub>II</sub>)(NO<sub>3</sub>)<sub>4</sub>**

N	1.1197824	-0.1413213	-1.4738262
C	0.4640311	1.0393792	-0.9050268
H	0.9875922	1.2945987	0.0355421
H	-0.5833147	0.8079676	-0.6400978
C	0.4731654	2.3127012	-1.7782227

H	-0.2319869	2.2178214	-2.6270828
H	1.4793214	2.4676658	-2.2303036
N	0.1477010	3.4827146	-0.9716508
C	1.1583613	3.9724109	-0.0251226
H	1.2331813	5.0749419	-0.1516988
H	2.1367281	3.5300020	-0.3040575
C	0.8635312	3.7411644	1.4742516
H	1.6113358	4.3299532	2.0481911
H	-0.1447558	4.1488600	1.6858599
N	0.9067777	2.3575499	1.9858394
C	2.1713916	1.8342293	2.5338923
H	1.9778727	1.3821170	3.5335701
H	2.8407627	2.6998264	2.6921812
C	2.9581350	0.7627940	1.7388684
N	3.4444839	1.0746037	0.3767256
C	2.5579674	-0.0323179	-1.7971496
H	2.8253487	-0.9016405	-2.4306264
H	2.7085500	0.8812848	-2.4074146
C	3.5050975	-0.0612455	-0.5775520
H	3.3119046	-0.9930616	-0.0088650
H	4.5416211	-0.1471259	-0.9613716
H	2.3650801	-0.1679961	1.6602438
H	3.8475813	0.5217988	2.3689889
C	0.5614883	-1.3713636	-1.4379219
C	-0.8340688	-1.5765088	-0.8390445
H	-0.9804193	-1.0293461	0.1197220
H	-1.6162287	-1.2381621	-1.5639205
O	-0.9462122	-2.9740686	-0.6078335
O	1.1676312	-2.3760060	-1.8843223
C	-2.1381906	-3.3664914	0.0650863
H	-3.0382123	-3.0473804	-0.5177266
H	-2.1964101	-2.8781148	1.0636545
C	-2.0872829	-4.8908243	0.1307064
O	-1.2609502	-5.4953549	-0.6049834
N	-2.9275220	-5.5678081	0.9335177
C	-2.8559850	-7.0308378	0.9805971
H	-2.7955807	-7.3561790	2.0420455
H	-3.7676291	-7.4748221	0.5201364
H	-1.9559335	-7.3770068	0.4352790
C	-3.9506155	-4.9423744	1.7661502
H	-4.9612011	-5.2728822	1.4329152
H	-3.8122932	-5.2632555	2.8227496
H	-3.9034732	-3.8358783	1.7340521
C	-0.2982649	1.6909502	2.0714328
C	-0.3455701	0.3240322	2.7998658
H	0.4563029	-0.3665785	2.4623502

H	-0.2015455	0.4847642	3.9010671
O	-1.3342856	2.1519420	1.5787055
O	-1.5522903	-0.3612682	2.5372787
C	-2.6770767	0.1649242	3.2081081
H	-2.5296047	0.1054091	4.3196177
H	-2.8210964	1.2346626	2.9337968
C	-3.9199163	-0.6520694	2.8225807
O	-3.8375872	-1.6426391	2.0877200
N	-5.1202170	-0.2137690	3.3373955
C	-6.3346364	-0.9647455	3.0517133
H	-6.7450109	-1.4317540	3.9784010
H	-7.1139877	-0.2921479	2.6255367
H	-6.0925443	-1.7576073	2.3185512
C	-5.2754736	0.9101573	4.2496966
H	-6.1458025	1.5296889	3.9359227
H	-5.4590189	0.5673779	5.2967566
H	-4.3845106	1.5655268	4.2448088
C	-1.0285721	4.2168046	-1.0548509
C	-2.0954615	3.6987452	-2.0419123
H	-1.6872450	3.7412561	-3.0896963
H	-2.3192037	2.6180588	-1.8297136
O	-1.1995525	5.2298108	-0.3903393
O	-3.2443834	4.4865522	-1.9178434
C	-4.2189300	4.1443260	-2.8633579
H	-3.8319514	4.2963263	-3.9075226
H	-4.4996671	3.0580044	-2.7863494
C	-5.4700634	5.0192544	-2.6237549
O	-5.5220880	5.8070535	-1.6881846
N	-6.5124479	4.8514096	-3.5253771
C	-7.7302306	5.6217236	-3.3252283
H	-7.9666561	6.2299867	-4.2298523
H	-8.5989866	4.9518492	-3.1184419
H	-7.5696969	6.2932939	-2.4587466
C	-6.5448107	3.8929668	-4.6147135
H	-6.8606366	4.3931064	-5.5606182
H	-5.5509752	3.4407570	-4.7948729
H	-7.2706516	3.0661928	-4.4149160
C	4.3433529	2.1196950	0.2728806
C	5.1114290	2.3043963	-1.0599094
H	4.4365029	2.2032300	-1.9367876
H	5.4957019	3.3512610	-1.0285916
O	4.5242597	2.9377813	1.1819006
O	6.1724692	1.3911646	-1.2967733
C	7.3241326	1.5649022	-0.5059092
H	7.5159811	2.6513422	-0.3193048
H	8.1727721	1.1684134	-1.1085287

C	7.2412346	0.7910726	0.8363571
O	6.2186732	0.1672652	1.1255078
N	8.3512550	0.8206785	1.6511434
C	8.3395919	0.0534169	2.8898659
H	9.1553628	-0.7071974	2.8888692
H	8.4842424	0.7231899	3.7693682
H	7.3610654	-0.4585334	2.9713416
C	9.5908591	1.5194741	1.3542794
H	10.4256673	0.8024068	1.1642123
H	9.4910533	2.1756013	0.4691995
H	9.8852442	2.1616997	2.2169630
O	-0.5027622	-5.9243559	-3.4086371
N	-1.1761131	-4.9302320	-3.8839657
O	-0.9544925	-3.8080623	-3.2752402
O	-1.9506438	-5.0358010	-4.8079031
O	1.4346625	-6.6838320	-1.1781886
N	1.3571762	-7.7299956	-0.2905162
O	2.3764917	-7.9767116	0.3279104
O	0.2836833	-8.3143636	-0.2255955
O	1.4158170	-4.2391534	0.4254182
N	1.0282360	-3.3621907	1.3345345
O	0.2479265	-3.7374655	2.2069369
O	1.4842973	-2.2064827	1.2487991
Pu	0.6896306	-4.7144317	-1.6982848
O	2.2766219	-4.5076773	-3.1919143
O	3.8427090	-2.9545132	-3.2219633
O	2.6231059	-3.3208326	-5.0062585
N	2.9589908	-3.5245051	-3.8511743

## References

1. P.K. Mohapatra, M. Iqbal, D.R. Raut, W. Verboom, J. Huskens, S.V. Godbole, *Dalton Transactions* 2012, **41**, 360-363.
2. S. Bagawde, V.V. Ramakrishna, S.K. Patil, *J. Inorg. Nucl. Chem.*, 1976, **38**, 1669-1672.
3. P. K. Mohapatra, P. B. Ruikar and V. K. Manchanda, *Radiochim. Acta*, 2002, **90**, 323–327.
4. E.P. Horwitz, A.C. Muscatello, D.G. Kalina, L. Kaplan, *Sep. Sci. Technol.* 1981, **16**, 417-437.