

Theoretical study of plutonium nitrate complexes with amide derivatives

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SUPPORTING INFORMATIONS

1 Proton affinity of the ligands

The proton affinity of the ligands, the amount of energy produced by proton capture, have been also calculated at the same level of theory. The proton affinity of a ligand L is defined as the enthalpy change associated with the following gas-phase reaction:



A natural population analysis (NPA) was performed using natural bond orbital analysis (NBO) to determine atomic electronic charges.[2]

Intrinsic properties of the ligands, such as basicity and electronic properties are important parameters for understanding their ability to bind a metal ion. Atomic charges and molecular polarizabilities have been calculated for the different ligands are reported in Table 1. Atomic charges were determined from a Natural Population Analysis (NPA). The charges of the complexing oxygen atom are slightly affected by the lengthening of the alkyl chains, they vary from -0.61 to -0.63 for monoamides and from -0.63 to -0.65 for carbamides. Carbon and nitrogen electronic charges vary between monoamides and carbamides but do not vary significantly when changing the alkyl groups. The molecular polarizability shows a notable increase, from 8.9 Å³ for MMM to 15.9 Å³ for PEE. This rise was expected, since the increase in polarizability is equal to expected addition of polarizability for -CH₂- groups (≈ 1.8 Å³ per group). As polarizability increases, the dispersion forces are expected to become stronger. Thus, molecules attract one another more strongly which stabilize further the complexes.

Table 1: Electronic atomic charges (NBO charges q_O , q_N and q_C), molecular polarizabilities (α) and proton affinity (PA) for the different amide ligands

Charges	$q_O(e^-)$	$q_N(e^-)$	$q_C(e^-)$	$\alpha(\text{Å}^3)$	$PA(kJ.mol^{-1})$
MMM	-0.613	-0.409	0.653	8.9	0
MME	-0.614	-0.410	0.658	10.6	8
EMM	-0.617	-0.411	0.652	10.6	10
EEM	-0.618	-0.413	0.657	12.3	16
MEE	-0.621	-0.415	0.657	12.3	14
EEE	-0.625	-0.414	0.659	14.1	22
PEE	-0.623	-0.413	0.662	15.9	27
IEE	-0.628	-0.415	0.665	15.8	28
C4M	-0.631	-0.441	0.761	11.8	23
C4E	-0.652	-0.445	0.778	18.9	40

Intrinsic basicity has been evaluated through gas phase proton affinity and are reported in table 1. As mentioned, in the computational methods section, the energies are relative to the MMM protonation energy. For monoamides, the protonation energy shows an increase by substituting a methyl by an ethyl group, 10 $kJ.mol^{-1}$ in R_1 position and 8 $kJ.mol^{-1}$ in R_2 or R_3 position. As expected, proton affinities tend to increase with oxygen electronic charge

and with the size of the alkyl chain. Same thing is observed for carbamides, the protonation affinity increased from 23 up to 40 $kJ.mol^{-1}$ by changing methyl with ethyl groups. As reported in literature, for organic molecules the proton affinities tend to increase with the size and polarizability of the alkyl substituent.[1] One can expect that the ligands' complexation ability will follow the same evolution as the protonation, more favorable as the alkyl chains become bulkier.

2 The structural parameters for geometry I

Table 2: Selected interatomic distances (average values d in Å)^a and Hydrogen bond angle (α_{O-H-O}) calculated in $[Pu(NO_3)_6](HL_2)$ in geometry I in the gas phase.

Ligand	$d_{O_{Nit2}-O_L}$	$d_{Pu-O_{Nit1}}$	$d_{Pu-N_{Nit2}}$	d_{Pu-N_L}	$d_{Pu-C_{R1}}$	α_{HOH}
MMM	2.568	2.544	2.976	5.605	4.910	169.8
MME	2.598	2.541	2.972	5.536	4.905	169.4
EMM	2.603	2.526	2.992	5.411	5.176	165.3
EEM	2.595	2.514	2.959	5.386	5.129	163.0
MEE	2.566	2.544	2.978	5.720	4.897	170.1
EEE	2.589	2.537	2.968	5.703	5.167	163.4
PEE	2.594	2.537	2.974	5.839	5.122	163.4
IEE	2.551	2.537	2.969	5.682	5.996	158.4
C4M	2.592	2.529	2.957	5.427	5.793	171.8
C4E	2.573	2.540	2.972	5.584	5.947	168.2

^a O_{Nit1} denotes oxygen from nitrate ions which are not involve in hydrogen bond. O_{Nit2} denotes oxygen from nitrate ions which are involved in hydrogen bond.

3 Optimized coordinates of inner-sphere complexes

Pu-4NO3-2EEM			Pu-4NO3-2EEE			Pu-4NO3-2EME					
Pu	-0.01179	0.231195	-0.151277	Pu	-0.001133	0.306857	0.098261	Pu	0.001006	0.305512	0.133076
C	-3.341035	-0.776687	-0.215866	C	-3.405779	-0.698359	0.372123	C	-3.47391	-0.431739	0.38466
C	-5.683436	-0.448386	0.450793	C	-5.804001	-0.894264	-0.116986	C	-5.843214	-0.600961	-0.224066
H	-5.788536	-1.507412	0.222964	H	-5.74783	-1.852386	0.398176	H	-5.909217	-1.378688	0.530948
C	-3.435817	-2.266971	-0.058524	C	-3.548569	-1.54017	1.607218	C	-3.717976	-1.085752	1.714004
C	5.63819	-1.222689	0.335961	C	5.703327	-0.968617	-0.205393	C	5.622178	-1.393401	0.00561
H	6.122596	-1.893406	-0.378802	H	6.130319	-1.658748	-0.937986	C	3.445356	-0.268324	-0.105659
C	3.468974	-0.108663	0.020614	C	3.459458	0.028238	-0.251503	C	-4.21386	0.481016	-1.728425
C	-4.211164	1.450096	-0.200741	C	-4.288508	0.430561	-1.571808	H	-3.397144	1.184514	-1.579513
H	-3.642284	1.885001	0.622982	H	-3.513758	1.167529	-1.369429	C	3.525809	-2.677949	-0.216009
C	3.60779	-2.462739	-0.388235	C	3.682567	-2.332112	-0.687312	C	4.075131	1.081016	0.080809
C	4.018865	1.214316	0.465523	H	2.71902	-2.410826	-0.18521	N	-4.472449	-0.200696	-0.45878
N	-4.387307	0.013656	-0.022177	C	4.005122	1.378582	0.110084	N	4.179435	-1.374605	-0.101894
N	4.220722	-1.201602	0.002549	N	-4.457588	-0.405229	-0.381504	N	-0.009254	1.968713	-2.301178
N	0.033492	2.479168	-2.033728	N	4.257	-1.025201	-0.368565	N	0.254394	-0.36019	2.991849
N	-0.141737	-1.217008	2.426302	N	-0.239803	2.297682	-2.062128	N	-0.231675	-2.410789	-0.951046
N	0.161826	-2.048362	-1.969079	N	0.423211	-0.728275	2.826964	N	0.122099	2.966749	1.286671
N	-0.155152	2.465134	1.719124	N	-0.068114	-2.241263	-1.35339	O	1.091103	2.142958	1.360585
O	0.845422	1.681108	1.655905	N	-0.045724	2.776331	1.626932	O	2.212347	-0.357997	-0.295132
O	2.284669	-0.183183	-0.373407	O	0.987838	2.035784	1.55209	O	-2.310727	-0.114091	0.054226
O	-2.261041	-0.269339	-0.592733	O	2.235563	-0.100216	-0.482654	O	-1.020125	1.301103	-1.94232
O	-0.968857	1.718608	-1.930163	O	-2.27391	-0.287264	0.033409	O	-0.17114	-1.384369	-1.691469
O	0.218016	-0.846762	-2.365725	O	-1.176813	1.497503	-1.780811	O	-0.90265	2.518755	0.68103
O	-1.090569	2.189051	0.903656	O	-0.121161	-1.120116	-1.940975	O	-0.322613	-3.519077	-1.388897
O	0.238965	-2.97946	-2.713168	O	-1.05482	2.335528	0.990661	O	0.011256	2.654963	-3.276233

O	0.081316	3.40766	-2.779126	O	-0.091503	-3.281261	-1.94148	O	-0.790708	0.144984	2.4534
O	-1.126454	-0.601943	1.889932	O	-0.315118	3.117848	-2.924552	O	-0.188068	-2.173484	0.297264
O	0.01778	-2.190778	-0.712649	O	-0.678855	-0.241766	2.397263	O	0.999064	1.843923	-1.53043
O	1.008126	2.168721	-1.266082	O	0.012944	-2.177734	-0.085879	O	0.172865	4.062029	1.747108
O	-0.210116	3.378971	2.479712	O	0.803685	2.151785	-1.344534	O	0.308955	-0.611786	4.156087
O	-0.244731	-1.79232	3.466746	O	-0.064359	3.794068	2.242263	O	1.201558	-0.568233	2.187331
O	0.927125	-1.165105	1.761685	O	0.545867	-1.13252	3.942306	H	-6.256222	-1.000506	-1.151971
H	-6.445201	0.071836	-0.136364	O	1.349404	-0.744817	1.972888	H	-2.974654	-0.666217	2.392769
H	-2.43689	-2.602108	0.220842	H	-6.260109	-1.097837	-1.089275	H	3.331329	1.697154	0.588001
H	6.060475	-0.234346	0.160564	H	-5.230787	0.964158	-1.716013	H	-4.703799	-0.828315	2.103018
H	3.207161	1.713332	0.998134	H	-2.834017	-1.138764	2.327146	C	-3.539456	-2.601896	1.635832
C	-5.890896	-0.192845	1.932546	H	4.342172	-3.082395	-0.245891	H	-2.537865	-2.855444	1.285158
H	-5.147542	-0.725698	2.529116	H	6.05906	0.023552	-0.480202	H	-3.670985	-3.041078	2.62573
H	-5.811241	0.870473	2.166667	H	3.247049	1.858659	0.731299	H	-4.2639	-3.06603	0.961832
H	-6.884121	-0.530484	2.235302	C	-3.930848	-0.375544	-2.805593	H	4.944958	1.018012	0.735967
C	5.905194	-1.681102	1.757609	H	-4.682669	-1.138978	-3.022598	C	4.439336	1.721245	-1.258801
H	5.490168	-2.674409	1.939695	H	-3.863493	0.288922	-3.668798	H	5.177709	1.131281	-1.807814
H	6.980516	-1.72625	1.941727	H	-2.960556	-0.858292	-2.683882	H	3.55089	1.831674	-1.881258
H	5.46027	-0.995102	2.48106	C	-6.651666	0.092505	0.66501	H	4.858875	2.714041	-1.09049
H	-4.110303	-2.538786	0.754136	H	-6.232254	0.273449	1.656729	C	-3.874163	-0.479751	-2.851314
C	-3.853542	-2.938764	-1.365706	H	-6.719885	1.052426	0.149421	H	-5.115732	1.052615	-1.962077
H	-3.16417	-2.680246	-2.171092	H	-7.664533	-0.29675	0.787229	H	4.143424	-3.386356	0.3416
H	-3.840141	-4.023097	-1.248364	C	6.157226	-1.339054	1.194804	C	3.35645	-3.125602	-1.655626
H	-4.859177	-2.643073	-1.673962	H	5.813935	-2.337487	1.472501	H	2.562029	-2.615875	0.287813
H	4.84031	1.085852	1.170778	H	7.247741	-1.329984	1.250119	H	6.052199	-0.427369	-0.241491
C	4.447888	2.066436	-0.728667	H	5.769322	-0.635413	1.93382	H	6.01972	-2.125967	-0.699351
H	5.255918	1.595615	-1.294489	C	3.53679	-2.557438	-2.180704	H	5.934089	-1.679745	1.014369
H	3.604538	2.23362	-1.399226	H	3.120164	-3.548973	-2.367289	H	-6.45233	0.253995	0.084217
H	4.801161	3.038168	-0.380954	H	2.862199	-1.821117	-2.619629	H	-3.740268	0.077602	-3.779995
H	-3.665685	1.645486	-1.123183	H	4.500906	-2.493676	-2.691567	H	-4.665927	-1.216642	-3.010161
H	-5.194798	1.914529	-0.24919	H	-4.544789	-1.445823	2.03944	H	-2.940212	-1.002679	-2.641995
H	4.25777	-3.276971	-0.072353	C	-3.215895	-3.004673	1.32263	H	4.3178	-3.198951	-2.170359
H	3.47673	-2.511554	-1.472209	H	-2.204525	-3.101948	0.925383	H	2.720896	-2.429705	-2.205044
H	2.634556	-2.574088	0.086798	H	-3.273255	-3.583031	2.245846	H	2.882859	-4.108562	-1.684912
				H	-3.909267	-3.447569	0.603075				
				H	4.910709	1.291587	0.710666				
				C	4.254816	2.226555	-1.137213				
				H	5.006173	1.776379	-1.791182				
				H	3.331617	2.352999	-1.703338				
				H	4.610671	3.215607	-0.845386				

Pu-4NO3-2EMM

Pu	0.002342	0.158409	-0.058752
C	-3.388351	-0.571423	-0.093514
C	-5.680239	0.054749	0.529469
H	-5.799794	-0.993316	0.783005
C	-3.62345	-2.021151	0.224278
C	5.61149	-1.506815	0.490246
C	3.468782	-0.352636	0.153276
C	-4.100249	1.71688	-0.336516
H	-3.29193	1.774578	-1.06082
C	3.546512	-2.757608	0.056771
C	4.078226	0.993359	0.41747
N	-4.358134	0.328229	0.013636
N	4.186088	-1.467238	0.249752

Pu-4NO3-2MEE

Pu	-0.022837	0.143331	0.0027
C	-3.219048	-1.186571	-0.185638
C	-5.648029	-1.153869	0.112379
H	-5.573855	-2.238254	0.039412
C	-3.159643	-2.581485	0.356607
C	5.898249	0.110069	0.041116
C	3.465341	0.409967	0.180265
C	-4.427059	0.805233	-0.81862
H	-3.556176	1.348565	-0.455006
C	4.333553	-1.795334	-0.268501
C	3.63211	1.86482	0.482605
N	-4.38149	-0.558706	-0.287052
N	4.524929	-0.372834	0.008967

Pu-4NO3-2MEM

Pu	-0.00866	0.162253	-0.113876
C	-3.286615	-0.963126	-0.096134
C	-5.610039	-0.722276	0.644203
H	-5.394473	-1.603092	1.247479
C	-3.309371	-2.425679	0.219531
C	5.691268	-0.589299	0.678607
C	3.457193	0.197241	0.032316
C	-4.311133	1.204225	-0.231713
H	-3.936486	1.771002	0.624164
C	3.911895	-2.14072	-0.129244
C	3.816199	1.615167	0.347175
N	-4.367213	-0.216522	0.080047
N	4.334678	-0.783987	0.191608

N	0.242565	2.250444	-2.103498	N	0.127949	1.961583	-2.301281	N	-0.144826	2.525306	-1.850322
N	-0.285059	-1.075118	2.611467	N	-0.343815	-0.761927	2.784894	N	0.008155	-1.438004	2.37972
N	0.052645	-2.249509	-1.709625	N	0.534521	-2.431133	-1.268165	N	0.29077	-1.987635	-2.060368
N	-0.024956	2.536288	1.625485	N	-0.611246	2.684243	1.305953	N	-0.246975	2.26576	1.88574
O	0.92324	1.686848	1.645424	O	0.446852	2.018433	1.543984	O	0.802393	1.558308	1.751395
O	2.270103	-0.429331	-0.1879	O	2.321381	-0.079673	0.072926	O	2.314162	-0.082821	-0.389324
O	-2.268688	-0.2173	-0.523627	O	-2.17407	-0.616317	-0.570958	O	-2.24016	-0.436788	-0.532722
O	-0.815029	1.575185	-1.966304	O	-0.819	1.140049	-2.166731	O	-1.08622	1.685594	-1.791141
O	0.201507	-1.084867	-2.185938	O	0.557649	-1.33485	-1.903984	O	0.276487	-0.761002	-2.382758
O	-0.963142	2.25761	0.814088	O	-1.391108	2.142829	0.459779	O	-1.184552	1.975806	1.076916
O	0.073539	-3.232678	-2.386145	O	0.774813	-3.481631	-1.782338	O	0.434465	-2.863388	-2.857658
O	0.371879	3.114805	-2.913556	O	0.218654	2.71942	-3.217143	O	-0.176358	3.502592	-2.530983
O	-1.212121	-0.433117	2.007214	O	-1.309168	-0.388636	2.029471	O	-1.020978	-0.848034	1.903115
O	-0.119658	-2.292827	-0.448726	O	0.239047	-2.326852	-0.035164	O	0.141404	-2.213775	-0.816773
O	1.179047	1.927383	-1.294514	O	0.999636	1.917578	-1.365294	O	0.858325	2.238197	-1.111917
O	-0.03175	3.509171	2.310914	O	-0.850396	3.724541	1.831461	O	-0.342432	3.126678	2.702129
O	-0.449475	-1.561919	3.688086	O	-0.523939	-1.124563	3.906695	O	-0.039858	-2.085511	3.381398
O	0.797278	-1.14874	1.970888	O	0.789477	-0.716293	2.238709	O	1.057476	-1.280116	1.701571
H	-6.431346	0.321012	-0.218603	H	-2.116253	-2.862315	0.475442	C	-6.657651	-1.034225	-0.408937
H	-2.638744	-2.446461	0.415776	H	2.763542	2.201267	1.045876	H	-2.44293	-2.88707	-0.249512
H	3.277765	1.60635	0.834465	H	-3.666457	-2.660736	1.318759	H	3.092384	2.26498	-0.139312
H	-4.205893	-2.13312	1.140083	H	4.53843	2.089293	1.040429	H	-3.21796	-2.560605	1.300831
C	-4.283393	-2.755216	-0.941421	C	-4.480733	0.835692	-2.334132	H	3.746722	1.778955	1.426228
H	-3.682656	-2.659455	-1.847601	H	-5.312155	1.278533	-0.388564	H	-3.64474	1.37732	-1.073893
H	-4.372259	-3.817442	-0.709693	H	5.184828	-2.321597	0.169943	H	-5.314739	1.546515	-0.481809
H	-5.283116	-2.371367	-1.156614	C	4.223854	-2.091623	-1.752702	H	4.739254	-2.817861	0.074173
H	4.862747	0.929006	1.172427	H	3.437992	-2.123349	0.257762	H	3.632902	-2.221923	-1.180784
C	4.599126	1.636529	-0.867311	H	5.92262	1.149491	-0.284424	H	3.050767	-2.420856	0.478479
H	5.397241	1.047406	-1.326048	C	6.55478	-0.048935	1.400538	H	5.738667	0.351901	1.223707
H	3.790336	1.749848	-1.589665	C	-6.079909	-0.740805	1.508367	C	6.728076	-0.623193	-0.429317
H	4.995679	2.628853	-0.648322	H	-4.569582	1.868084	-2.677445	H	5.887527	-1.378407	1.409402
H	-5.009599	2.141113	-0.763682	H	-5.338828	0.277054	-2.717011	H	-5.979065	0.040959	1.334447
H	-3.815997	2.29019	0.549157	H	-3.566302	0.421185	-2.759204	H	-4.219955	-2.917946	-0.120784
H	4.041175	-3.487286	0.698869	H	5.120267	-1.775851	-2.292263	H	4.821097	1.876338	0.017236
H	3.63398	-3.084431	-0.983278	H	3.360899	-1.585793	-2.187913	H	6.566134	0.18642	-1.144137
H	2.495093	-2.696858	0.325334	H	4.097973	-3.164642	-1.908632	H	6.694344	-1.56778	-0.976131
H	6.054169	-0.518688	0.41597	H	3.643326	2.420751	-0.459311	H	7.730003	-0.513961	-0.009417
H	6.083004	-2.146823	-0.25953	H	-3.632256	-3.280254	-0.338808	H	-6.319388	-1.826806	-1.079564
H	5.822743	-1.922173	1.479698	H	6.543936	-1.090903	1.726507	H	-6.887663	-0.155934	-1.015274
H	-5.859354	0.655191	1.425551	H	6.041969	0.544748	2.159891	H	-7.582636	-1.362917	0.068981
				H	7.595456	0.278582	1.355504				
				H	6.449454	-0.457041	-0.713356				
				H	-6.177014	0.343429	1.589902				
				H	-5.357591	-1.068727	2.258319				
				H	-7.048819	-1.184266	1.746725				
				H	-6.394026	-0.844189	-0.624559				

Pu-4NO3-2MME			Pu-4NO3-2MMM			Pu-4NO3-2PEE					
Pu	-0.013094	0.133229	0.099292	Pu	-0.034034	0.196499	-0.301316	C	-3.792925	0.874782	-3.022861
C	-3.197462	-1.25818	0.035194	C	-3.278437	-0.972233	-0.097764	C	-4.090197	1.430917	-1.643348
C	-5.640134	-1.238316	0.180455	C	-5.523443	-0.71553	0.844428	N	-4.460916	0.390547	-0.682417
H	-5.531733	-2.249704	0.560352	H	-5.4048	-1.750624	1.148924	C	-5.878013	0.063938	-0.596133
C	-3.130803	-2.538367	0.809783	C	-3.275947	-2.437872	0.208493	C	-6.639026	0.964282	0.359886
C	5.891334	0.232498	-0.046079	C	5.557911	-0.466403	0.729659	C	-3.521965	-0.211755	0.036575
C	3.469372	0.487589	0.19236	C	3.408915	0.255537	-0.196194	O	-2.320436	0.083753	-0.150414

C	-4.413212	0.578612	-0.957156	C	-4.336708	1.19311	-0.141327	C	-3.872875	-1.262132	1.047242
H	-3.556804	1.181253	-0.658521	H	-3.618929	1.398986	-0.931043	C	-3.669968	-2.671792	0.483775
C	4.390406	-1.731052	-0.07729	C	3.878589	-2.105561	0.052882	Pu	0.002032	0.252697	0.158411
C	3.624525	1.965061	0.368721	C	3.805108	1.694641	-0.069578	O	2.192033	-0.183459	-0.558547
N	-4.366193	-0.686788	-0.22115	N	-4.343394	-0.227572	0.167877	C	3.411551	-0.282799	-0.287936
N	4.541708	-0.281778	0.034713	N	4.251908	-0.707117	0.159247	N	4.085849	-1.343194	-0.711308
N	0.124377	1.660828	-2.409826	N	-0.280355	2.532659	-2.056857	C	3.379071	-2.4111	-1.418524
N	-0.321252	-0.432303	2.96721	N	0.072222	-1.35189	2.226068	C	3.283269	-2.157005	-2.911331
N	0.588984	-2.567222	-0.849718	N	0.188467	-1.962136	-2.247741	C	4.089594	0.820962	0.466443
N	-0.662062	2.801339	1.073577	N	-0.177876	2.330823	1.674714	C	4.512763	1.961052	-0.465285
O	0.409942	2.194711	1.394377	O	0.864861	1.621681	1.497709	C	5.518111	-1.522235	-0.516772
O	2.337509	-0.037899	0.193145	O	2.28132	-0.036899	-0.649648	C	5.849784	-2.352517	0.709785
O	-2.150232	-0.72233	-0.388267	O	-2.272886	-0.446495	-0.621763	O	-0.847958	1.857876	1.805736
O	-0.810389	0.846166	-2.181755	O	-1.214254	1.691467	-1.931032	N	0.173028	1.869606	2.564814
O	0.596268	-1.555835	-1.614153	O	0.147256	-0.737299	-2.573852	O	0.243777	2.547465	3.539885
O	-1.426557	2.140215	0.301283	O	-1.154421	2.028736	0.919127	O	1.1127	1.093796	2.19597
O	0.851785	-3.667528	-1.231669	O	0.271457	-2.842208	-3.047392	O	-0.853973	-1.099146	2.018721
O	0.210329	2.302831	-3.410803	O	-0.355156	3.50127	-2.745676	N	0.158474	-1.855743	2.216638
O	-1.292875	-0.174035	2.172538	O	-0.973015	-0.770002	1.775517	O	1.129288	-1.633476	1.446971
O	0.283771	-2.319459	0.36001	O	0.135337	-2.180806	-0.993178	O	0.162156	-2.699786	3.060099
O	0.989317	1.745756	-1.470462	O	0.766118	2.255878	-1.376356	O	1.113924	2.416785	-0.357523
O	-0.926328	3.893565	1.463722	O	-0.232006	3.203269	2.482475	N	0.153469	2.966502	-0.987599
O	-0.495186	-0.658952	4.124721	O	0.062161	-1.971736	3.246495	O	0.22651	4.069398	-1.435515
O	0.81196	-0.429976	2.417988	O	1.093765	-1.218105	1.502728	O	-0.876028	2.239625	-1.098264
H	-2.086676	-2.818596	0.922761	H	-6.39571	-0.633862	0.190103	O	-0.310202	-1.942228	-0.969643
H	2.698181	2.368504	0.770387	H	-2.376945	-2.871157	-0.223732	N	-0.325359	-1.506607	-2.16412
H	-3.575672	-2.417552	1.799145	H	3.052729	2.298587	-0.570294	O	-0.457277	-2.22868	-3.106985
H	4.449594	2.215062	1.035216	H	-3.246863	-2.593111	1.289652	O	-0.190121	-0.251675	-2.275488
C	-4.425449	0.378521	-2.460405	H	3.836457	1.985188	0.983565	H	-5.992739	-0.983605	-0.319989
H	-5.315715	1.096177	-0.623786	H	-5.337264	1.481947	-0.466341	H	5.901088	-2.006831	-1.418886
H	5.265126	-2.176495	0.403928	H	-4.062094	1.776025	0.74137	H	-3.223216	1.964027	-1.257928
C	4.266707	-2.199526	-1.514998	H	3.740202	-2.529597	1.049932	H	2.388877	-2.513924	-0.976354
H	3.512916	-2.020394	0.49942	H	4.673394	-2.649168	-0.462906	H	-6.282788	0.157801	-1.607059
H	5.899112	1.279597	-0.336029	H	2.947957	-2.201285	-0.496457	H	-4.926074	2.133591	-1.681577
H	6.413942	0.119866	0.908885	H	5.722734	0.590414	0.912548	H	-3.189199	-1.118612	1.885595
H	-6.094868	-0.617153	0.957284	H	6.338863	-0.839277	0.060714	H	3.923699	-3.336279	-1.21805
H	-4.519226	1.345374	-2.958178	H	5.638777	-0.997484	1.681374	H	5.999782	-0.546468	-0.468217
H	-5.264106	-0.246631	-2.777791	H	-5.705348	-0.112618	1.737777	H	3.359085	1.197362	1.18574
H	-3.493122	-0.077909	-2.793879	H	-4.1543	-2.943534	-0.194847	H	-4.638608	0.31015	-3.424091
H	5.142019	-1.920233	-2.106734	H	4.781424	1.889785	-0.514677	H	-3.5796	1.69588	-3.709714
H	3.378771	-1.776186	-1.98663					H	-2.916031	0.226963	-2.999396
H	4.175665	-3.286853	-1.543583					H	-6.27564	0.849968	1.383094
H	3.802221	2.434714	-0.602612					H	-6.535008	2.015065	0.082351
H	-3.658047	-3.341153	0.289426					H	-7.702198	0.715639	0.344156
H	-6.313885	-1.264495	-0.679106					H	5.37835	-3.336061	0.663195
H	6.438022	-0.32811	-0.805958					H	6.929419	-2.499024	0.782596
								H	5.506701	-1.861128	1.622209
								H	2.760988	-2.984101	-3.395792
								H	2.724874	-1.241981	-3.113588
								H	4.272515	-2.067852	-3.367438
								H	-4.890125	-1.143033	1.422144
								H	-2.660616	-2.743475	0.070168
								C	-3.869173	-3.734666	1.549533
								H	-4.360703	-2.840623	-0.350311
								H	4.945604	0.45317	1.034583

H	5.235341	1.59061	-1.201434
H	3.634927	2.297634	-1.021413
C	5.108201	3.12382	0.308061
H	-3.727496	-4.734408	1.134286
H	-3.152544	-3.606037	2.364273
H	-4.875124	-3.690426	1.976814
H	5.404208	3.929512	-0.366551
H	4.381998	3.531592	1.014982
H	5.993124	2.819132	0.874196

Pu-4NO ₃ -2IEE			Pu-4NO ₃ -2C4E			Pu-4NO ₃ -2C4M					
Pu	-0.012298	0.244985	0.0528	Pu	-0.000603	0.098493	0.259103	Pu	0.015438	-0.041705	0.178012
C	-3.415975	-0.821093	-0.243049	N	1.1284	-1.940804	-1.588875	N	0.990999	-1.374387	-2.285412
C	-5.798074	-0.270131	0.021685	N	-0.543403	1.134241	2.928778	N	-0.4282	0.112186	3.056563
H	-5.969563	-0.699604	-0.964915	N	-0.562577	-2.365973	1.74731	N	-0.412118	-2.868944	0.815806
C	-3.752331	-2.09061	-0.991398	N	-0.178098	2.730259	-1.026779	N	-0.22165	2.847605	-0.257034
C	5.690248	-1.248474	0.366017	O	-0.343662	2.550129	0.219827	O	-0.348726	2.30382	0.882191
H	5.86613	-2.23484	0.800457	O	0.291118	-1.050173	-1.937984	O	0.072733	-0.497646	-2.275855
C	3.539006	-0.223232	-0.282221	O	-1.213342	-1.980032	0.716633	O	-1.116654	-2.208196	-0.018894
C	-4.046492	1.189738	0.96992	O	0.07942	1.678095	-1.682243	O	0.047593	2.045355	-1.200645
H	-3.068944	1.060776	1.426338	O	-0.815139	-3.385457	2.310338	O	-0.602706	-4.024243	1.036086
C	3.64329	-1.626972	1.69118	O	1.572169	-2.741461	-2.357938	O	1.356446	-1.914825	-3.285944
H	2.800195	-1.021757	2.012897	O	-1.439063	0.630969	2.167458	O	-1.347529	-0.145229	2.20406
C	4.191444	0.537772	-1.41261	O	0.352623	-1.577962	2.112934	O	0.49372	-2.194742	1.384977
N	-4.371852	-0.024577	0.216562	O	1.457111	-1.904779	-0.367804	O	1.492897	-1.6228	-1.148036
N	4.264479	-0.982522	0.53261	O	-0.258538	3.807782	-1.536498	O	-0.348841	4.024099	-0.425765
N	-0.345049	2.184317	-2.1119	O	-0.792328	1.541374	4.01994	O	-0.642777	0.157653	4.226829
N	-0.340146	-0.723647	2.839014	O	0.614405	1.162237	2.423795	O	0.710409	0.315196	2.548699
N	0.388071	-2.018674	-1.792197	C	-4.557557	-2.166629	-0.227646	C	-5.211791	-1.336832	-1.101623
N	0.193368	2.736262	1.542964	H	-4.901445	-1.608072	0.641087	H	-5.610847	-0.970164	-0.158905
O	1.114532	1.854589	1.502393	C	-3.376691	-0.051299	-0.588476	C	-3.422553	0.275635	-0.634509
O	2.304825	-0.112754	-0.105502	C	-2.892768	-1.927462	-2.032768	C	-3.120364	-1.393619	-2.36551
O	-2.207611	-0.540272	-0.075247	H	-3.341663	-2.903112	-2.224752	H	-3.722857	-1.623932	-3.247376
O	-1.30557	1.463403	-1.719383	N	-3.777746	-1.263097	-1.075071	N	-3.955105	-0.69019	-1.411698
O	0.224737	-0.821612	-2.181356	O	-2.168038	0.301215	-0.652094	O	-2.180081	0.391919	-0.508444
O	-0.826108	2.463239	0.839912	H	-1.914125	-2.114941	-1.589399	H	-2.733522	-2.324116	-1.941623
O	0.588603	-2.920366	-2.550599	H	-3.869708	-2.928189	0.159034	H	-5.035272	-2.411388	-0.998171
O	-0.445365	2.9955	-2.978558	C	-2.755943	-1.171662	-3.337994	C	-5.514487	1.559293	-0.570939
O	-1.065271	0.198604	2.369036	H	-2.112597	-1.732744	-4.018185	H	-5.654604	1.134476	-1.562074
O	0.314669	-2.180203	-0.5373	H	-3.729435	-1.033505	-3.814662	C	-3.726218	1.99205	1.041022
O	0.755625	1.970502	-1.500266	H	-2.293595	-0.195566	-3.187825	H	-2.935586	1.483228	1.584531
O	0.290893	3.733857	2.185041	C	-5.715743	0.696797	-0.366324	N	-4.250103	1.138193	-0.007294
O	-0.445673	-1.133043	3.955435	H	-5.866617	-0.120531	-1.067575	H	-4.537363	2.220864	1.734865
O	0.515157	-1.186675	2.018749	C	-3.844388	2.084204	0.44648	H	-5.510783	2.649056	-0.6672
H	-6.276915	0.710713	0.008452	H	-2.892069	1.93459	0.945941	C	5.139198	-1.252424	-0.330933
H	-4.772905	1.254533	1.784851	N	-4.290271	0.800743	-0.092569	H	5.251731	-0.819065	-1.321511
H	4.387723	-1.611955	2.491731	H	-4.561268	2.375799	1.217032	C	3.454202	0.509175	-0.072065
H	5.930387	-1.341776	-0.69266	H	-6.012264	1.612894	-0.888626	C	3.581431	-1.279711	1.550251
C	-4.087432	2.440386	0.113118	C	-3.730699	3.167446	-0.611504	H	4.410041	-1.646923	2.159942
H	-5.079853	2.610533	-0.312445	H	-3.346481	4.083472	-0.15942	N	4.131896	-0.542349	0.429622
H	-3.83009	3.305565	0.726048	H	-3.040084	2.870679	-1.401557	O	2.24526	0.702459	0.215931
H	-3.363223	2.379182	-0.699466	H	-4.695225	3.400959	-1.068802	H	2.984274	-2.132013	1.215808
C	-6.408398	-1.131523	1.11177	C	4.762857	-1.685691	0.550652	H	4.81447	-2.289338	-0.455257
H	-5.978886	-2.135381	1.113629	H	4.793352	-1.799508	-0.530508	C	5.515084	1.656426	-0.757157
H	-6.242899	-0.693328	2.09801	C	3.423695	0.268307	-0.096327	H	5.937249	1.13715	0.099827

H	-7.485885	-1.222176	0.959274	C	3.586743	-0.319348	2.240358	C	3.34427	2.357228	-1.63211
C	6.577127	-0.2186	1.04045	H	4.120078	-1.078848	2.8133	H	2.33647	2.001673	-1.824633
H	6.337783	-0.128553	2.102047	N	4.079366	-0.431798	0.865462	N	4.099731	1.381152	-0.873887
H	7.625437	-0.512215	0.954211	O	2.26544	0.725686	0.122024	H	3.850339	2.52916	-2.584446
H	6.460399	0.766083	0.584194	H	2.529076	-0.580839	2.296825	H	5.651809	2.731112	-0.605237
C	3.189331	-3.044859	1.404581	H	4.127871	-2.501344	0.91564	H	3.276809	3.30918	-1.09493
H	2.77028	-3.480839	2.313044	C	3.839289	1.045718	2.84557	H	6.065269	1.368161	-1.657947
H	2.409677	-3.055721	0.642299	H	3.464217	1.068844	3.870192	H	6.108611	-1.25119	0.176425
H	4.017553	-3.67788	1.074771	H	4.907587	1.27497	2.859431	H	2.958108	-0.631725	2.161819
H	-4.820181	-2.290865	-0.90791	H	3.315576	1.82674	2.294077	H	-2.27946	-0.773141	-2.663011
C	-3.40996	-1.899666	-2.469248	C	5.459052	0.512012	-1.471934	H	-3.334047	2.930771	0.636415
H	-2.355654	-1.652723	-2.601341	H	5.928951	0.29996	-0.514653	H	-6.360623	1.276956	0.062831
H	-3.617376	-2.821073	-3.01657	C	3.247535	1.202578	-2.318041	H	-5.95608	-1.187231	-1.890004
H	-3.997071	-1.095459	-2.919219	H	2.226151	0.830509	-2.304874				
H	5.251655	0.289006	-1.446927	N	4.015994	0.52023	-1.278324				
C	3.561193	0.154262	-2.74813	H	3.678782	0.90789	-3.276849				
H	3.659452	-0.914981	-2.951708	H	5.755149	1.532252	-1.740557				
H	2.502404	0.410379	-2.768353	C	3.248938	2.714213	-2.17682				
H	4.058742	0.698526	-3.553365	H	2.629437	3.156352	-2.958945				
C	-3.009309	-3.272383	-0.375496	H	2.835729	3.013134	-1.21297				
H	-3.284234	-3.414514	0.672546	H	4.253722	3.133993	-2.267431				
H	-3.266581	-4.183917	-0.918552	C	6.151212	-1.811961	1.147288				
H	-1.929016	-3.136967	-0.42464	H	6.132904	-1.713932	2.234488				
C	4.075317	2.038786	-1.141048	H	6.560255	-2.797625	0.914567				
H	3.034359	2.358289	-1.149069	H	6.840509	-1.060118	0.757393				
H	4.514279	2.311823	-0.178554	C	5.951377	-0.441661	-2.546623				
H	4.605254	2.585828	-1.923671	H	7.037722	-0.364765	-2.629497				
				H	5.701017	-1.480515	-2.326783				
				H	5.531764	-0.199956	-3.524609				
				C	-5.72524	-2.834988	-0.927013				
				H	-5.400973	-3.406699	-1.798672				
				H	-6.210111	-3.533253	-0.241054				
				H	-6.475123	-2.114748	-1.260529				
				C	-6.587786	0.530184	0.866193				
				H	-7.637553	0.497418	0.5663				
				H	-6.363705	-0.387569	1.411698				
				H	-6.47151	1.365409	1.558972				

4 Optimized coordinates of outer-sphere complexes

4.1 Geometry I

Pu-6NO3-2HL-GEOM1 MMM			Pu-6NO3-2HL-GEOM1_MME			Pu-6NO3-2HL-GEOM1 MEM					
Pu	-0.01093	-0.440413	-0.09975	Pu	-0.003507	-0.005158	0.015877	Pu	0.015545	-0.430533	0.098079
O	0.647886	2.006422	-0.268346	O	-0.212513	1.15404	2.221685	O	-0.750615	1.980351	-0.067452
O	1.750071	0.699701	-1.541141	O	1.172688	2.035375	0.860248	O	-1.838729	0.795092	1.330186
O	2.27306	2.793948	-1.451515	O	0.932433	2.881317	2.833775	O	-2.455983	2.830297	0.948229
O	0.335082	-1.734937	-2.152414	O	0.761456	1.592479	-1.922111	O	-0.349544	-1.46823	2.292254
O	2.046167	-2.984365	-2.580327	O	2.824808	1.841519	-2.514893	O	-2.027545	-2.718605	2.832967
O	1.868013	-1.956565	-0.686974	O	2.260962	0.360965	-1.05159	O	-1.821084	-1.944855	0.824911
O	-1.087386	0.683789	-2.036644	O	-1.452999	2.059631	-0.138986	O	0.988271	0.971205	1.90024
O	-3.079188	0.304755	-2.780581	O	-3.200367	2.285758	-1.389161	O	2.972054	0.778015	2.732475
O	-2.245672	-0.88677	-1.181661	O	-1.966317	0.515766	-1.512595	O	2.230874	-0.646888	1.286049
N	1.57768	1.871559	-1.101706	N	0.638558	2.062232	2.014222	N	-1.705582	1.90828	0.746103
N	1.442479	-2.265017	-1.845296	N	1.951402	1.278357	-1.851758	N	-1.424894	-2.078762	2.026702

N	-2.171123	0.0422	-2.035103	N	-2.241431	1.652868	-1.028334	N	2.097058	0.381736	2.0082
O	-0.637876	-2.826331	0.256344	O	0.209486	-1.164066	-2.194212	O	0.749685	-2.81897	0.076016
O	-1.648361	-1.424873	1.503012	O	-1.179337	-2.045728	-0.836833	O	1.742551	-1.54878	-1.316502
O	-2.152441	-3.522703	1.632805	O	-0.936393	-2.88857	-2.811632	O	2.344887	-3.61771	-1.144709
O	-0.394412	1.003839	2.17163	O	-0.771567	-1.613731	1.947924	O	0.424006	0.717346	-2.334276
O	-2.210703	2.117747	2.527393	O	-2.839305	-1.862455	2.526914	O	2.214999	1.844051	-2.77205
O	-1.853994	1.160021	0.629351	O	-2.262339	-0.368642	1.082483	O	1.813751	1.134946	-0.776531
O	1.175346	-1.492867	2.087785	O	1.446287	-2.071658	0.159643	O	-1.061805	-1.818761	-1.966445
O	3.154317	-0.899443	2.721084	O	3.19448	-2.298962	1.407965	O	-3.043128	-1.387215	-2.714886
O	2.147415	0.129707	1.115328	O	1.95368	-0.534696	1.543008	O	-2.112938	-0.118274	-1.240633
N	-1.505928	-2.641115	1.152479	N	-0.642578	-2.071126	-1.990507	N	1.641135	-2.713359	-0.808042
N	-1.479173	1.438247	1.794772	N	-1.960534	-1.29604	1.875115	N	1.477851	1.24088	-1.982275
N	2.161167	-0.766502	1.996797	N	2.232198	-1.666451	1.051607	N	-2.073938	-1.12403	-1.994788
H	4.257863	0.076188	2.203581	H	4.235384	1.290599	-2.011991	H	-4.195819	-0.388752	-2.349447
H	-3.556922	2.329765	1.784315	H	-4.250414	-1.297701	2.025528	H	3.536025	2.195104	-2.014875
O	4.843343	0.790215	1.770007	O	5.015754	0.79831	-1.592547	O	-4.811554	0.352218	-2.017976
C	4.967638	0.595019	0.49977	C	5.000687	0.905603	-0.302681	C	-4.987193	0.287689	-0.739903
N	5.202208	1.634483	-0.254368	N	5.543728	-0.061485	0.381363	N	-5.293207	1.388769	-0.110738
O	-4.355631	2.407771	1.150642	O	-5.020627	-0.791606	1.604818	O	4.303816	2.3678	-1.365229
C	-4.764533	1.248339	0.758116	C	-4.989143	-0.887109	0.31465	C	4.747183	1.267363	-0.85472
N	-5.361479	1.174393	-0.401012	N	-5.498802	0.087533	-0.385499	N	5.312429	1.323891	0.319963
C	4.8811	-0.779705	-0.060073	C	4.417014	2.107383	0.347625	C	-4.868259	-1.014021	-0.032939
H	4.730898	-1.49648	0.743572	H	4.025499	2.784862	-0.407413	H	-4.882605	-1.825349	-0.75773
H	4.045322	-0.864646	-0.756895	H	3.60239	1.831919	1.019522	H	-3.920648	-1.064838	0.511898
H	5.805019	-1.036392	-0.582146	H	5.183444	2.636238	0.918713	H	-5.683643	-1.156463	0.67519
C	-4.586586	0.055542	1.627882	C	-4.423369	-2.089888	-0.343792	C	4.632205	-0.006199	-1.61164
H	-4.106142	0.346359	2.55877	H	-4.223781	-2.862608	0.395075	H	4.415229	0.210402	-2.65563
H	-5.554915	-0.390194	1.864284	H	-5.115872	-2.479754	-1.091441	H	5.550284	-0.589038	-1.552981
H	-3.961493	-0.693654	1.139072	H	-3.482885	-1.843663	-0.84561	H	3.809596	-0.610375	-1.215845
C	5.36826	1.550152	-1.695419	C	5.634091	-0.052275	1.831802	C	-5.489768	1.435657	1.339665
H	4.487942	1.981958	-2.175886	H	4.880081	-0.729275	2.238762	H	-5.022308	2.362621	1.674654
H	6.256642	2.116634	-1.980293	H	6.628086	-0.394895	2.122259	C	-6.952411	1.378831	1.734833
H	5.482508	0.521524	-2.02027	H	5.477481	0.945476	2.22954	H	-4.917434	0.631638	1.797881
C	5.204358	2.988535	0.279191	C	6.028601	-1.277168	-0.281903	C	-5.362169	2.669282	-0.800369
H	4.456153	3.570355	-0.261365	H	5.824972	-2.097673	0.407425	H	-6.254458	3.199909	-0.467009
H	4.963811	2.974486	1.33652	H	5.423134	-1.435636	-1.172163	H	-4.476096	3.254171	-0.545461
H	6.190417	3.433224	0.130022	C	7.500857	-1.194224	-0.633474	H	-5.408395	2.518188	-1.873606
C	-5.880714	-0.066286	-0.950839	C	-5.532586	0.020451	-1.841747	C	5.82551	0.134183	1.002951
H	-5.895624	-0.853276	-0.204479	H	-4.540631	-0.20065	-2.234324	H	5.271997	-0.736105	0.656154
H	-6.897081	0.106525	-1.309279	H	-6.250119	-0.72765	-2.184827	C	7.320645	-0.044584	0.826327
H	-5.246561	-0.375234	-1.784269	H	-5.82999	0.995898	-2.216867	H	5.561399	0.256097	2.054417
C	-5.46109	2.322162	-1.290096	C	-6.01863	1.303257	0.247287	C	5.383353	2.566613	1.075335
H	-5.010558	2.054218	-2.247038	H	-5.595163	2.141751	-0.308375	H	4.661171	2.524041	1.893113
H	-6.513127	2.573062	-1.440921	C	-7.53418	1.341812	0.249738	H	6.388058	2.671459	1.485979
H	-4.938495	3.171619	-0.864147	H	-5.625582	1.343761	1.260072	H	5.162705	3.412023	0.432446
				H	-7.872222	2.277787	0.697629	H	-7.039707	1.462839	2.819386
				H	-7.948043	0.517378	0.833541	H	-7.415898	0.437777	1.431025
				H	-7.943633	1.291126	-0.76169	H	-7.523144	2.19704	1.291074
				H	8.11929	-1.017111	0.249404	H	7.87705	0.820797	1.191907
				H	7.68667	-0.397006	-1.354924	H	7.586895	-0.20172	-0.221109
				H	7.821591	-2.136961	-1.079995	H	7.652201	-0.916341	1.392911

Pu-6NO3-2HL-GEOM1_EMM

Pu	0.011834	-0.185364	0.134335
O	-0.317622	-0.6367	2.564117

Pu-6NO3-2HL-GEOM1_EEM

Pu	0.015377	-0.068545	-0.002057
O	0.301029	2.411746	0.238058

Pu-6NO3-2HL-GEOM1_EME

Pu	-0.034403	0.155396	-0.03007
O	-0.214946	-1.958186	1.307905

O	-1.791246	-1.481078	1.275385	O	1.591789	1.490422	-1.188321	O	-1.610933	-1.783945	-0.295261
O	-1.988365	-1.71154	3.415056	O	1.78508	3.603334	-0.784519	O	-1.703035	-3.497304	1.016586
O	-1.067156	-2.022593	-1.413877	O	0.690012	-0.960562	-2.353224	O	-0.8699	-0.106832	-2.48243
O	-3.08989	-1.884443	-2.161497	O	2.680845	-1.648457	-2.843501	O	-2.913475	0.257169	-3.089592
O	-2.167079	-0.222619	-1.143042	O	2.139619	-1.17514	-0.811918	O	-2.238069	0.765801	-1.107605
O	0.767637	-2.497177	0.75185	O	-1.126646	1.205239	-1.85777	O	1.05552	-1.802964	-1.193574
O	2.396715	-3.576503	-0.170941	O	-2.974416	0.6462	-2.825612	O	2.829275	-1.714652	-2.422887
O	1.801079	-1.630206	-0.896171	O	-2.04856	-0.649789	-1.364283	O	1.928917	0.087168	-1.640169
N	-1.388018	-1.296613	2.469348	N	1.243848	2.552183	-0.586413	N	-1.192973	-2.461846	0.692405
N	-2.113786	-1.395698	-1.591103	N	1.840538	-1.274059	-2.029943	N	-2.012557	0.304432	-2.256051
N	1.681051	-2.614911	-0.105702	N	-2.080937	0.410927	-2.051282	N	1.967052	-1.168578	-1.780935
O	0.351764	0.274366	-2.340738	O	-0.271147	-2.545528	-0.231899	O	0.152232	2.270915	-1.355841
O	1.809662	1.122513	-1.039366	O	-1.54063	-1.608864	1.202542	O	1.526249	2.083895	0.263692
O	2.068393	1.287446	-3.176166	O	-1.737678	-3.727023	0.82847	O	1.629787	3.813458	-1.02598
O	1.048163	1.659971	1.632559	O	-0.684449	0.822022	2.370021	O	0.83023	0.432458	2.436387
O	3.085047	1.632448	2.349876	O	-2.673374	1.531322	2.829712	O	2.877546	0.057081	3.017426
O	2.220082	-0.099575	1.394434	O	-2.103687	1.060129	0.803472	O	2.166724	-0.474853	1.052077
O	-0.754508	2.13368	-0.531696	O	1.173901	-1.339757	1.850952	O	-1.137401	2.111351	1.13381
O	-2.435342	3.199545	0.307537	O	3.037356	-0.775498	2.787462	O	-2.91339	2.006318	2.360015
O	-1.807566	1.298702	1.120835	O	2.060712	0.536281	1.374762	O	-1.977652	0.211971	1.602935
N	1.426462	0.909884	-2.232725	N	-1.202073	-2.679954	0.608564	N	1.120709	2.774165	-0.722885
N	2.126388	1.07715	1.811026	N	-1.821452	1.150235	2.024199	N	1.960659	0.004106	2.194557
N	-1.689626	2.252476	0.298672	N	2.121494	-0.537524	2.04104	N	-2.038328	1.470125	1.72834
H	-4.330406	-0.894655	-1.942462	H	4.085985	-0.969746	-2.315959	H	-4.247452	-0.13034	-2.213946
H	4.446544	0.92131	1.814395	H	-4.073228	1.614403	2.046207	H	4.221067	-0.348621	2.260719
O	-4.956734	-0.112935	-1.796059	O	4.682143	-0.23684	-1.980708	O	-4.798336	-0.640155	-1.548578
C	-5.045486	0.228677	-0.550805	C	4.933552	-0.324657	-0.709673	C	-5.006312	0.014131	-0.446345
N	-5.259471	1.489226	-0.286707	N	5.153554	0.800161	-0.093512	N	-5.150934	-0.695241	0.633485
O	5.094808	0.32792	1.320289	O	-4.828138	1.6627	1.374271	O	4.949076	-0.697461	1.648073
C	5.056016	0.525608	0.03932	C	-4.962034	0.547392	0.727035	C	5.014808	-0.025077	0.54195
N	5.204712	-0.512634	-0.733762	N	-5.416825	0.626339	-0.49262	N	5.425623	-0.667012	-0.514952
C	-4.938991	-0.790331	0.53112	C	5.044422	-1.669612	-0.071816	C	-5.157133	1.497393	-0.484025
C	-5.521364	-2.149774	0.165985	H	4.424429	-2.348093	-0.657786	H	-4.49983	1.862455	-1.273704
H	-3.873501	-0.886978	0.780406	C	6.490848	-2.165956	-0.054951	C	-6.603587	1.898666	-0.778952
H	-5.419537	-0.408265	1.430807	H	4.620722	-1.652791	0.93255	H	-4.801011	1.939257	0.446605
C	4.893015	1.902879	-0.517109	C	-4.667164	-0.744002	1.414147	C	4.706423	1.433232	0.537703
C	5.358837	3.013148	0.413201	H	-3.974316	-0.528886	2.226888	H	3.962672	1.618002	1.311762
H	5.438372	1.955679	-1.460604	C	-5.930534	-1.384964	1.990644	C	5.95667	2.265512	0.830136
H	3.83321	2.019597	-0.778165	H	-4.14082	-1.421955	0.743571	H	4.239326	1.722258	-0.402292
C	-5.369692	1.98459	1.082806	C	5.552797	0.898299	1.309034	C	-5.482225	-0.121661	1.927722
H	-5.370514	3.07045	1.041268	C	6.927925	1.516338	1.472129	H	-6.163461	-0.803041	2.437673
H	-6.298012	1.646608	1.547197	H	4.786435	1.493065	1.810831	H	-4.571132	0.001275	2.515917
H	-4.508965	1.675305	1.673769	H	5.516567	-0.089462	1.758748	H	-5.971969	0.841426	1.821406
C	-5.308157	2.498972	-1.336055	C	4.957032	2.06214	-0.804818	C	-4.904708	-2.144543	0.622959
H	-4.489964	3.203253	-1.17743	H	5.819349	2.290612	-1.433234	C	-6.164286	-2.941197	0.349528
H	-5.208716	2.031785	-2.309493	H	4.062217	2.000593	-1.419896	H	-4.133001	-2.350473	-0.1154
H	-6.261632	3.02717	-1.275795	H	4.824668	2.848826	-0.065594	H	-4.488085	-2.38495	1.60211
C	5.136416	-0.418736	-2.186273	C	-5.718402	-0.539749	-1.323983	C	5.63253	-0.034724	-1.808239
H	4.429025	0.345349	-2.500104	H	-5.421975	-1.437067	-0.788583	H	5.717939	1.042655	-1.712278
H	6.124346	-0.22	-2.609535	C	-7.183764	-0.609225	-1.708585	H	6.559866	-0.418864	-2.235072
H	4.777784	-1.376555	-2.558458	H	-5.077442	-0.465194	-2.205549	H	4.797073	-0.285128	-2.465043
C	5.379763	-1.858023	-0.200907	C	-5.614922	1.927144	-1.121626	C	5.649878	-2.116832	-0.476586
H	4.521387	-2.469666	-0.484659	H	-5.420264	1.817302	-2.187045	H	5.358544	-2.491625	-1.458789
H	6.288157	-2.285537	-0.630216	H	-6.63521	2.282075	-0.965111	C	7.086598	-2.47045	-0.146686
H	5.463115	-1.825495	0.879625	H	-4.91873	2.646327	-0.700003	H	4.966061	-2.540849	0.255973

H	4.738754	3.092323	1.305494	H	6.51936	-3.181662	0.340774	H	-6.670203	2.984253	-0.856067
H	5.289565	3.965024	-0.114333	H	7.12868	-1.543048	0.574592	H	-7.287356	1.574472	0.008354
H	6.396782	2.87267	0.720967	H	6.915349	-2.183044	-1.060491	H	-6.946396	1.470576	-1.722507
H	-5.427284	-2.811711	1.027043	H	-5.653652	-2.284074	2.541699	H	5.682952	3.320094	0.868558
H	-4.990744	-2.619497	-0.661644	H	-6.638586	-1.673052	1.211627	H	6.722826	2.142593	0.061702
H	-6.579039	-2.077959	-0.09569	H	-6.438314	-0.707535	2.679806	H	6.394448	1.992916	1.792048
				H	7.697312	0.916406	0.981153	H	7.786407	-2.036783	-0.864734
				H	7.168985	1.575807	2.534704	H	7.210101	-3.554401	-0.175866
				H	6.971785	2.528286	1.065835	H	7.354395	-2.12545	0.853172
				H	-7.349869	-1.498723	-2.318437	H	-6.553537	-2.727887	-0.647219
				H	-7.492514	0.255553	-2.298244	H	-6.947098	-2.732318	1.082815
				H	-7.828068	-0.674258	-0.828915	H	-5.933329	-4.006345	0.402115

Pu-6NO3-2HL-GEOM1_MEE			Pu-6NO3-2HL-GEOM1_EEE			Pu-6NO3-2HL-GEOM1_PEE					
Pu	-0.0143	-0.623832	-0.068723	Pu	-0.033257	-0.258743	0.101433	C	-4.809692	-0.840301	2.872803
O	0.806951	1.762892	-0.356531	O	-0.568511	1.518108	-1.598193	C	-5.949372	-0.993654	1.885038
O	1.786707	0.321485	-1.583275	O	-1.898486	1.449973	0.067544	N	-5.492176	-1.314364	0.529993
O	2.442356	2.379127	-1.626534	O	-2.272453	2.843332	-1.539829	C	-5.355876	-2.74537	0.220824
O	0.216522	-2.025093	-2.063853	O	-0.857405	0.341725	2.489776	C	-6.620221	-3.324799	-0.381543
O	1.828902	-3.411638	-2.450962	O	-2.849301	-0.120993	3.196299	C	-5.15427	-0.415298	-0.35348
O	1.753562	-2.28343	-0.608534	O	-2.095882	-0.972646	1.367504	C	-5.114283	1.04343	-0.065885
O	-1.054072	0.487092	-2.030146	O	0.769641	2.02025	0.813617	C	-5.498844	1.94135	-1.237263
O	-3.078317	0.198024	-2.726268	O	2.567667	2.417824	1.944196	C	-5.470905	3.403779	-0.826744
O	-2.289407	-0.970997	-1.08825	O	1.907241	0.391988	1.580636	O	-4.842698	-0.868943	-1.526994
N	1.702564	1.526699	-1.206631	N	-1.601968	1.976034	-1.046669	O	-2.988902	0.125311	-3.074034
N	1.290225	-2.616449	-1.744585	N	-1.940431	-0.246621	2.382412	N	-2.060725	0.250416	-2.283262
N	-2.175666	-0.08628	-1.984456	N	1.777404	1.645647	1.469052	O	-2.188198	0.963502	-1.256386
O	-0.80622	-2.951395	0.388825	O	0.522972	-2.046061	1.775437	O	-0.977075	-0.33234	-2.430054
O	-1.680914	-1.437121	1.605367	O	1.808485	-1.947097	0.078582	Pu	-0.065067	0.217802	-0.083945
O	-2.348502	-3.483085	1.807028	O	2.244181	-3.348695	1.663779	O	1.798893	1.879843	-0.111542
O	-0.254674	0.931414	2.152012	O	0.830554	-0.862278	-2.318598	N	1.492847	2.453856	-1.205643
O	-1.98483	2.180373	2.490565	O	2.804012	-0.32655	-3.019036	O	2.163498	3.326917	-1.673913
O	-1.730966	1.121787	0.62961	O	2.027821	0.474088	-1.175079	O	0.441606	2.022683	-1.748559
O	1.147518	-1.702718	2.112559	O	-0.840177	-2.539573	-0.639499	O	0.66302	-2.061796	-0.857131
O	3.191082	-1.269786	2.660668	O	-2.626754	-2.909216	-1.8004	N	1.65203	-1.701913	-1.549682
O	2.195878	-0.145605	1.111934	O	-1.958189	-0.894827	-1.398794	O	1.809142	-0.44982	-1.647111
N	-1.640596	-2.671521	1.289497	N	1.550484	-2.490571	1.200199	O	2.399479	-2.486594	-2.069629
N	-1.316067	1.423104	1.775981	N	1.888136	-0.241767	-2.194495	O	-0.552879	-1.581534	1.613508
N	2.179929	-1.051351	1.982561	N	-1.835631	-2.154029	-1.30308	N	-1.607789	-2.025445	1.094804
H	4.322848	-0.366609	2.149479	H	-4.188973	0.145848	2.251021	O	-2.25409	-2.910831	1.590562
H	-3.360908	2.42465	1.770125	H	4.070001	0.311776	-2.353546	O	-1.955607	-1.468048	0.011349
O	4.972726	0.342546	1.79816	O	-4.775787	0.683904	1.646218	O	-1.915874	0.86688	1.50618
C	5.100414	0.315896	0.515286	C	-5.061859	0.130027	0.508791	N	-1.756345	2.125334	1.438347
N	5.535202	1.405015	-0.059388	N	-5.424265	0.936942	-0.446687	O	-2.494832	2.890937	1.994029
O	-4.166776	2.478669	1.149393	O	4.801153	0.790708	-1.831937	O	-0.78434	2.496624	0.732049
C	-4.641331	1.301146	0.899653	C	5.173879	0.162065	-0.766086	O	2.03414	-0.569138	1.092283
N	-5.253131	1.1375	-0.240498	N	5.709106	0.884742	0.181474	N	1.954483	0.131192	2.129381
C	4.793082	-0.914482	-0.259455	C	-5.053033	-1.353987	0.377291	O	2.910293	0.184769	2.910159
H	4.643713	-1.753371	0.416309	H	-4.236522	-1.721569	0.999679	O	0.915932	0.767077	2.313826
H	3.87513	-0.778182	-0.837012	C	-6.380858	-1.957082	0.840185	O	4.832674	-1.008791	1.679883
H	5.604967	-1.152675	-0.94713	H	-4.815245	-1.647539	-0.644645	C	5.197073	-0.439557	0.579214
C	-4.500814	0.215373	1.905281	C	4.988544	-1.312141	-0.672344	C	4.978099	1.018268	0.388554
H	-4.168243	0.63858	2.850807	H	3.906765	-1.484884	-0.609876	C	5.625627	1.878436	1.477084
H	-5.4492	-0.297772	2.064203	C	5.578497	-2.068642	-1.858864	C	5.337599	3.351584	1.245676
H	-3.755037	-0.517045	1.581858	H	5.390637	-1.689663	0.264615	N	5.761608	-1.208879	-0.314787

C	5.699334	1.518329	-1.508043	C	-5.88644	0.472788	-1.756813	C	5.812635	-2.661686	-0.115003
H	5.345458	2.514391	-1.779349	H	-6.720942	1.123912	-2.029955	C	7.080436	-3.105576	0.588028
C	7.134261	1.308605	-1.951387	C	-4.798703	0.5129	-2.811928	C	6.333097	-0.712434	-1.569933
H	5.021986	0.820993	-1.996845	H	-6.294823	-0.531029	-1.652485	C	5.325116	-0.665165	-2.700617
C	5.802257	2.610434	0.73431	C	-5.377353	2.392483	-0.250952	H	-4.306358	-0.254302	-2.099803
C	4.550328	3.434749	0.966201	C	-6.65397	2.930154	0.365115	H	4.1205	-0.493929	2.195468
H	6.249812	2.306125	1.679591	H	-4.507176	2.620533	0.361039	H	-4.083738	1.252705	0.242234
H	6.550331	3.180963	0.181031	H	-5.198044	2.826737	-1.234176	H	-5.73506	1.269521	0.800319
C	-5.78801	-0.154675	-0.672322	C	6.297812	0.323422	1.401564	H	3.893077	1.177317	0.386217
H	-5.439005	-0.922333	0.013475	H	6.798674	-0.61318	1.157211	H	5.315661	1.336231	-0.595733
C	-7.299895	-0.169462	-0.778475	H	7.082581	1.021981	1.699448	H	-6.607142	-1.814763	2.177119
H	-5.318806	-0.369939	-1.634954	C	5.289743	0.142703	2.518502	H	-6.570168	-0.098716	1.852422
C	-5.314816	2.24638	-1.203899	C	5.7073	2.350007	0.086363	H	-4.503006	-2.866321	-0.443092
H	-5.498343	1.791332	-2.176855	H	5.590299	2.721099	1.10561	H	-5.099305	-3.235427	1.160213
C	-6.372999	3.281008	-0.871076	C	6.968942	2.889425	-0.558058	H	6.784507	0.263486	-1.394001
H	-4.326796	2.705617	-1.240602	H	4.823696	2.650435	-0.472732	H	7.154329	-1.390702	-1.811813
H	7.207601	1.449222	-3.031142	H	-6.322084	-3.044106	0.78048	H	5.73297	-3.109203	-1.106948
H	7.482613	0.300449	-1.717472	H	-7.218457	-1.629183	0.220665	H	4.929994	-2.956114	0.449353
H	7.81161	2.02024	-1.474625	H	-6.598488	-1.686913	1.87498	H	-6.495757	1.670011	-1.600149
H	-7.625861	-1.161254	-1.096609	H	5.389959	-3.134443	-1.728984	H	-4.804325	1.792015	-2.067382
H	-7.663072	0.54842	-1.515946	H	6.657918	-1.920021	-1.934605	H	5.245	1.578747	2.456526
H	-7.772784	0.052675	0.180764	H	5.120962	-1.766216	-2.80087	H	6.706646	1.701517	1.491392
H	4.073763	3.716937	0.02619	H	7.864964	2.583255	-0.012904	H	7.974445	-2.804529	0.036836
H	4.811776	4.345191	1.508926	H	6.937888	3.980391	-0.562562	H	7.090238	-4.193796	0.671446
H	3.823095	2.879075	1.558956	H	7.055721	2.547935	-1.590544	H	7.134142	-2.68728	1.594065
H	-7.37134	2.842017	-0.833743	H	-6.807258	2.527269	1.367121	H	-6.846334	-2.85884	-1.34175
H	-6.372566	4.053351	-1.642674	H	-7.529012	2.693075	-0.244956	H	-7.480364	-3.195406	0.279921
H	-6.16684	3.761986	0.085235	H	-6.587412	4.016642	0.444221	H	-6.485342	-4.394993	-0.548034
				H	4.532824	-0.599051	2.260639	H	4.514442	0.033179	-2.487795
				H	4.764116	1.073002	2.738836	H	4.86737	-1.640255	-2.872506
				H	5.806027	-0.188632	3.421622	H	5.824541	-0.350027	-3.618909
				H	-3.980662	-0.165051	-2.56454	H	-4.158379	-0.00439	2.612165
				H	-4.381599	1.515585	-2.920909	H	-4.195713	-1.741841	2.910272
				H	-5.221288	0.2148	-3.773384	H	-5.218066	-0.661631	3.869489
								H	5.783341	3.961216	2.033693
								H	4.262442	3.542275	1.233175
								H	5.742684	3.691425	0.28902
								H	-6.182373	3.606454	-0.021619
								H	-5.728582	4.047041	-1.669692
								H	-4.478367	3.692825	-0.473608

	Pu-6NO3-2HL-GEOM1_IEE			Pu-6NO3-2HL-GEOM1_C4M			Pu-6NO3-2HL-GEOM1_C4E				
Pu	0.015829	-0.124627	-0.079689	Pu	-0.00009	0.449659	-0.000278	Pu	-0.006	-0.607593	-0.115992
O	0.227021	1.905856	1.387164	O	-1.571352	-0.649098	1.64689	O	-2.138429	-1.713724	0.592887
O	1.678655	1.766434	-0.168848	O	-1.608193	1.479085	1.671135	O	-0.929143	-0.939019	2.165958
O	1.787832	3.393071	1.24767	O	-3.002526	0.374526	2.898813	O	-2.808294	-1.891792	2.640485
O	0.968369	0.216918	-2.483342	O	-0.775732	2.673921	-0.733567	O	0.698398	1.218811	1.480749
O	3.001594	-0.267772	-3.037371	O	-0.00047	4.554082	-0.001318	O	2.269519	1.072561	2.954303
O	2.236468	-0.76244	-1.085178	O	0.775198	2.674457	0.731873	O	1.822175	-0.584993	1.642901
O	-0.93524	1.949124	-1.160508	O	-2.406446	0.390852	-0.830899	O	-1.891906	1.096425	0.392018
O	-2.595241	1.997966	-2.54233	O	-3.075973	0.231992	-2.877039	O	-2.210835	3.020094	-0.534011
O	-1.840137	0.123321	-1.777386	O	-0.977677	0.403143	-2.407449	O	-0.442623	1.866564	-0.966276
N	1.248687	2.400808	0.841132	N	-2.092319	0.406032	2.108552	N	-1.992021	-1.534134	1.837274
N	2.07601	-0.269816	-2.230991	N	-0.000343	3.362401	-0.001015	N	1.618552	0.586035	2.064293
N	-1.817629	1.383785	-1.857132	N	-2.16085	0.344721	-2.061834	N	-1.514173	2.01209	-0.371938

O	-0.210345	-2.1577	-1.530597	O	1.607877	1.478265	-1.672291	O	2.153711	0.602563	-0.897608
O	-1.644578	-1.984361	0.036879	O	1.571578	-0.649909	-1.646441	O	0.947264	-0.083538	-2.51233
O	-1.764019	-3.647259	-1.337103	O	3.003572	0.373068	-2.897917	O	2.893053	0.753264	-2.920103
O	-0.922779	-0.48194	2.331175	O	0.792281	-1.860938	0.71455	O	-0.748347	-2.288038	-1.829336
O	-2.92961	0.005179	2.952634	O	-0.000236	-3.739078	0.001368	O	-2.386246	-2.004695	-3.212197
O	-2.220755	0.527693	0.980518	O	-0.792291	-1.861375	-0.713505	O	-1.77743	-0.423014	-1.874167
O	0.983719	-2.191288	0.993762	O	2.406108	0.391717	0.830473	O	1.861344	-2.11338	-0.734551
O	2.718935	-2.245053	2.278818	O	3.076025	0.234998	2.876617	O	2.196523	-4.071548	0.115996
O	1.882756	-0.36451	1.617288	O	0.977532	0.404781	2.407195	O	0.465703	-2.900466	0.670082
N	-1.225695	-2.645826	-0.964573	N	2.09265	0.404994	-2.108467	N	2.002758	0.427436	-2.130816
N	-2.028004	0.017819	2.107382	N	-0.000076	-2.538117	0.000839	N	-1.663104	-1.597209	-2.346968
N	1.89096	-1.628424	1.659118	N	2.160644	0.346584	2.061473	N	1.535124	-3.080905	0.022467
H	4.342802	-0.038529	-2.108433	C	3.988922	-2.57983	-0.397688	C	4.600676	2.377077	1.086858
H	-4.241817	0.359285	2.263252	H	3.698934	-1.933533	-1.220802	H	4.391845	1.53255	1.734875
O	4.894701	0.548103	-1.509992	C	5.139319	-0.583054	0.454208	C	5.206729	0.566355	-0.458046
C	5.361722	0.030181	-0.418913	C	4.734846	-2.454099	1.932494	C	5.377231	2.862908	-1.228515
N	5.491716	0.850979	0.585515	H	5.442615	-1.946293	2.583655	H	5.777232	2.336316	-2.093223
O	-5.002798	0.778105	1.716203	N	4.718389	-1.835749	0.617985	N	5.137288	1.871804	-0.176303
C	-5.443262	0.115169	0.697739	O	5.262329	0.207029	1.485468	O	5.071947	0.15803	-1.691994
N	-5.662934	0.79812	-0.39265	H	5.044279	-3.494943	1.81837	H	6.172241	3.524124	-0.869845
C	5.850849	-1.391459	-0.379074	H	3.069704	-2.95433	0.056526	H	3.626183	2.823043	0.868557
C	5.054377	-2.334228	-1.270935	C	5.970483	-0.893672	-1.828654	C	5.482976	3.392427	1.784896
C	7.330497	-1.388015	-0.789706	H	6.195976	-1.90401	-1.497055	H	5.604181	4.304972	1.197951
H	5.760449	-1.744988	0.649739	C	5.557025	1.351984	-0.929576	H	5.015734	3.672301	2.730555
C	-5.805064	-1.338427	0.820767	H	4.988061	1.863983	-0.159971	H	6.478494	2.99827	2.002935
H	-5.887348	-1.752401	-0.184145	N	5.502078	-0.086602	-0.719833	C	4.164276	3.684882	-1.62189
C	-4.758831	-2.155173	1.568988	H	5.1148	1.571301	-1.902277	H	4.442978	4.354352	-2.438148
C	-7.1737	-1.420763	1.507571	H	6.890945	-0.442973	-2.207586	H	3.34508	3.053538	-1.96513
C	6.133382	0.500539	1.854483	H	4.450524	0.168157	2.088213	H	3.802492	4.305251	-0.800241
H	6.754591	1.359513	2.122175	C	-3.988622	-2.579613	0.398172	C	6.227389	-0.15408	1.659962
C	5.138818	0.192352	2.956287	H	-3.698638	-1.933098	1.221104	H	6.537545	0.888423	1.67722
H	6.811565	-0.335318	1.696259	C	-5.139225	-0.583014	-0.453636	C	5.197333	-1.782575	0.086966
C	4.998548	2.234514	0.482506	C	-4.736714	-2.454994	-1.931352	H	4.323862	-1.811837	-0.559999
C	6.024286	3.167505	-0.129534	H	-5.444897	-1.94736	-2.582194	N	5.466936	-0.380648	0.43391
H	4.072909	2.226584	-0.08921	N	-4.719009	-1.835975	-0.617171	H	4.910137	-2.280622	1.013408
H	4.74572	2.543659	1.49653	O	-5.262934	0.206685	-1.485096	H	7.145019	-0.745952	1.571682
C	-6.294625	0.236527	-1.590593	H	-5.046359	-3.495687	-1.816431	C	5.506577	-0.532623	2.941442
H	-7.041418	-0.498109	-1.290678	H	-5.069435	-2.953755	-0.056413	H	5.328196	-1.606892	3.002084
H	-6.841362	1.060769	-2.053392	C	-5.968888	-0.89234	1.829906	H	6.134084	-0.259624	3.792629
C	-5.290982	-0.348566	-2.565211	H	-6.194667	-1.902808	1.498876	H	4.541992	-0.034132	3.048186
C	-5.260077	2.208914	-0.482062	C	-5.555144	1.352818	0.929515	C	6.374791	-2.486559	-0.558832
H	-4.95849	2.376305	-1.516564	H	-4.985575	1.864187	0.159926	H	6.104834	-3.526363	-0.752463
C	-6.372271	3.150693	-0.065544	N	-5.50075	-0.085912	0.720493	H	6.635086	-2.019995	-1.509669
H	-4.378982	2.345369	0.140966	H	-5.113181	1.572367	1.902275	H	7.258549	-2.489973	0.083896
H	7.719862	-2.405849	-0.734711	H	-6.889131	-0.44129	2.208961	H	4.277361	0.560263	-2.167769
H	7.946427	-0.752458	-0.150357	H	-4.45229	0.166605	-2.08894	C	-5.096292	-0.349303	-1.338926
H	7.439034	-1.040099	-1.819245	H	3.742082	-2.433481	2.388585	H	-4.900822	-0.972198	-0.471064
H	-5.071022	-3.200933	1.56332	H	4.575099	-3.425359	-0.767184	C	-4.961462	1.412873	0.375856
H	-4.664921	-1.845994	2.611039	H	5.235865	-0.920277	-2.636035	C	-5.294532	2.060334	-1.94397
H	-3.780991	-2.101558	1.088477	H	6.59248	1.702391	-0.909074	H	-5.29038	3.036688	-1.463201
H	-7.270278	3.013329	-0.672889	H	-6.590415	1.703733	0.908419	N	-5.148376	1.045945	-0.893841
H	-6.038989	4.181966	-0.193409	H	-5.233955	-0.918647	2.637001	O	-4.45361	2.585189	0.651526
H	-6.634517	3.005982	0.983597	H	-4.574282	-3.425329	0.768068	H	-6.291231	1.92718	-2.377697
H	6.246025	2.88668	-1.159895	H	-3.74432	-2.434868	-2.388259	H	-4.211498	-0.44448	-1.971762
H	6.956964	3.178463	0.440215					C	-6.318858	-0.818603	-2.102592

H	5.62366	4.182488	-0.134628	H	-6.450143	-0.268805	-3.036492
H	-4.761906	-1.200135	-2.133885	H	-6.184457	-1.86933	-2.364982
H	-4.54015	0.386575	-2.858235	H	-7.243217	-0.728648	-1.526852
H	-5.813881	-0.687081	-3.461883	C	-4.250016	2.003458	-3.041596
H	4.531103	-0.682827	2.723526	H	-4.459588	2.799276	-3.759481
H	4.457921	1.026751	3.130141	H	-3.243299	2.154172	-2.654494
H	5.68362	0.003579	3.883585	H	-4.267163	1.05732	-3.584074
H	-7.122475	-1.005352	2.515896	C	-6.411749	-0.278329	1.418692
H	-7.473969	-2.46697	1.585628	H	-6.874964	-0.242668	0.435716
H	-7.949204	-0.883827	0.955881	C	-4.729718	0.994899	2.737981
H	3.998395	-2.354968	-1.008312	H	-3.731049	1.394184	2.57347
H	5.457659	-3.34118	-1.153148	N	-5.302724	0.671975	1.426752
H	5.144952	-2.070071	-2.327282	H	-4.606013	0.048584	3.265814
				H	-7.158369	0.105385	2.122748
				C	-6.051665	-1.701777	1.800854
				H	-5.702788	-1.772501	2.831089
				H	-6.943178	-2.326162	1.710259
				H	-5.26765	-2.121842	1.170586
				C	-5.567533	1.965644	3.548388
				H	-5.092324	2.130824	4.517421
				H	-5.650127	2.927409	3.040705
				H	-6.572743	1.582751	3.739297
				H	-3.609032	2.785426	0.125116

4.2 Geometry II

Pu-6NO3-2C4M_geom2			Pu-6NO3-2C4E_geom2			Pu-6NO3-2PEE_geom2					
Pu	-0.000047	0.435064	0.000032	Pu	-0.000012	-0.693854	0.000033	Pu	0.000026	-0.000212	0.000015
O	1.948067	-0.667515	-1.19015	O	2.555942	-0.642074	0.394068	O	-0.286056	-1.098704	2.238054
O	1.963984	1.460958	-1.243834	O	1.384629	-0.648386	2.168044	O	-1.411545	-1.968099	0.64985
O	3.591014	0.361085	-2.144264	O	3.533344	-0.517314	2.322621	O	-1.609832	-2.755671	2.652596
O	0.578532	2.662526	0.895191	O	-1.260216	-1.719393	1.933989	O	-0.361957	-1.623462	-1.966531
O	-0.000272	4.542793	-0.000847	O	-2.362379	-0.61153	3.428793	O	-2.207614	-1.885333	-3.060168
O	-0.578874	2.662081	-0.896085	O	-1.228738	0.40966	1.898738	O	-2.019444	-0.375005	-1.518869
N	2.537121	0.389537	-1.556357	O	0.898773	-2.921296	0.574618	O	1.358294	-2.132272	0.210784
N	-0.000223	3.350825	-0.000583	O	-0.00005	-4.801143	0.000294	O	3.230681	-2.54097	-0.787774
O	-1.9642	1.461314	1.24339	O	-0.898853	-2.92136	-0.574272	O	2.197023	-0.666498	-1.086019
O	-1.94806	-0.667176	1.190709	N	2.519381	-0.60351	1.679279	N	-1.119211	-1.976979	1.888204
O	-3.59119	0.3617	2.144209	N	-1.643139	-0.645044	2.468304	N	-1.53928	-1.33835	-2.232644
O	-0.591299	-1.879519	-0.885936	N	-0.00004	-3.608632	0.000209	N	2.294803	-1.818303	-0.56443
O	0.000048	-3.758634	0.000771	O	1.228767	0.409388	-1.898805	O	0.286116	1.098267	-2.238032
O	0.591276	-1.879183	0.886846	O	2.362339	-0.612034	-3.428754	O	1.411609	1.967668	-0.649831
O	-2.12975	0.385702	-1.425637	O	1.260151	-1.719671	-1.933801	O	1.609917	2.755209	-2.652586
O	-2.210044	0.277653	-3.586244	O	-0.911774	1.62545	-0.552977	O	0.361997	1.623028	1.966557
O	-0.321428	0.388042	-2.542296	O	0.000166	3.503719	-0.000318	O	2.207666	1.884952	3.06016
N	-2.53723	0.389978	1.556406	O	0.911831	1.625436	0.552743	O	2.019502	0.374597	1.518888
N	0.000032	-2.558014	0.000552	N	1.643126	-0.645403	-2.468242	O	-1.35825	2.131833	-0.210769
N	-1.561135	0.350523	-2.583312	N	0.000079	2.302004	-0.000196	O	-3.230641	2.54052	0.787794
C	-4.588036	-2.597598	0.690036	C	5.519674	2.597058	0.777286	O	-2.196967	0.666057	1.08604
H	-4.808976	-2.025604	1.587092	H	5.923166	3.464102	0.244497	N	1.119228	1.976579	-1.888173
C	-5.140927	-0.504525	-0.444967	C	5.677587	0.35024	-0.174114	N	1.539314	1.337908	2.232692
C	-3.931467	-2.233883	-1.64791	C	3.971627	1.839701	-1.050419	N	-2.294791	1.817835	0.564398
H	-4.120542	-1.597744	-2.510073	H	3.058952	1.87892	-0.455485	H	-3.511713	-0.038222	-1.524974
N	-4.651022	-1.741354	-0.482194	N	5.129351	1.565482	-0.184723	H	3.511804	0.037954	1.524915
O	-4.678084	0.426114	-1.223233	O	4.979531	-0.703518	-0.466734	O	-4.417695	0.399543	-1.372435

H	-4.291957	-3.240956	-1.870386	H	3.868715	1.001459	-1.736924	C	-5.052807	-0.058318	-0.347072
H	-3.56356	-2.961722	0.780867	H	6.318672	2.188144	1.394304	N	-6.047186	0.667901	0.092041
C	-7.138046	-1.094662	0.83362	C	4.366664	3.016082	1.672183	O	4.417834	-0.399639	1.372213
H	-7.077233	-2.032315	0.286763	H	3.979861	2.164949	2.234589	C	5.052802	0.058778	0.347012
C	-6.382877	1.235752	0.684396	H	4.727969	3.762177	2.383135	N	6.047343	-0.667018	-0.092437
H	-5.500337	1.826886	0.46261	H	3.540777	3.459029	1.115005	C	-4.672507	-1.37299	0.232152
N	-6.151804	-0.157402	0.345595	C	4.14662	3.114828	-1.850381	C	-5.143566	-2.54046	-0.645669
H	-6.590566	1.303545	1.753711	H	3.296546	3.210596	-2.527492	H	-5.050627	-1.478162	1.247712
H	-8.129261	-0.664886	0.669715	H	4.165265	4.006505	-1.220739	C	4.672118	1.373576	-0.231668
H	-3.681346	0.355114	-1.403206	H	5.058597	3.090832	-2.452145	H	5.050166	1.479257	-1.247201
H	-2.857813	-2.275821	-1.452806	C	8.012266	1.099783	-0.22269	C	5.142869	2.540834	0.646597
H	-5.263562	-3.452912	0.60298	H	8.687528	1.17706	0.634873	C	-6.896456	0.26392	1.210941
H	-7.020343	-1.289407	1.902886	C	7.394678	-1.200072	0.533497	H	-6.99035	-0.821235	1.215752
H	-7.235397	1.630584	0.12503	H	8.479978	-1.220239	0.43092	C	-6.38406	0.78129	2.541398
O	2.129647	0.386454	1.425601	N	6.96547	0.137272	0.10322	H	-7.892367	0.659281	0.998403
O	2.210102	0.278949	3.586229	H	6.991222	-1.949182	-0.147995	C	-6.323667	1.982072	-0.499108
O	0.321411	0.389069	2.542383	H	7.562386	2.078665	-0.364615	C	-7.265196	1.894188	-1.684242
N	1.561124	0.351584	2.583333	C	8.778262	0.719024	-1.47855	H	-6.752578	2.592122	0.297439
C	4.588605	-2.597687	-0.689901	H	8.112583	0.684372	-2.343248	H	-5.373236	2.432706	-0.778808
H	4.809986	-2.025904	-1.586983	H	9.552999	1.463738	-1.673168	C	6.896446	-0.262387	-1.211231
C	5.141055	-0.504345	0.444776	H	9.267007	-0.252118	-1.386479	H	6.990068	0.822794	-1.215625
C	3.931275	-2.233448	1.647763	C	6.996706	-1.500883	1.964956	H	7.892467	-0.657581	-0.998903
H	4.120285	-1.597265	2.509911	H	7.352652	-2.494575	2.244571	C	6.384104	-0.779368	-2.541861
N	4.651277	-1.741226	0.482189	H	7.434714	-0.777133	2.656353	C	6.324195	-1.98135	0.498179
O	4.677878	0.426471	1.222631	H	5.913062	-1.483275	2.087749	H	6.753225	-2.590972	-0.298632
H	4.29147	-3.240578	1.870443	H	4.010637	-0.639834	-0.171314	C	7.265764	-1.893689	1.683298
H	3.564109	-2.961678	-0.781072	O	-2.555978	-0.642084	-0.39405	H	5.373897	-2.432344	0.777748
C	7.138517	-1.094759	-0.833112	O	-1.384605	-0.648611	-2.167989	H	8.218344	-1.433784	1.409281
H	7.077452	-2.032328	-0.28614	O	-3.533311	-0.517562	-2.322657	H	7.474046	-2.897012	2.059187
C	6.383327	1.235706	-0.684591	N	-2.51937	-0.603638	-1.679262	H	6.819228	-1.315076	2.492896
H	5.500662	1.82686	-0.463353	C	-5.519377	2.597066	-0.77726	H	-8.21791	1.43464	-1.410092
N	6.152145	-0.15738	-0.345578	H	-5.922747	3.464182	-0.244497	H	-6.818769	1.315138	-2.493588
H	6.591511	1.303256	-1.753824	C	-5.677637	0.350226	0.174046	H	-7.473197	2.897416	-2.060539
H	8.129699	-0.665011	-0.668932	C	-3.971651	1.839465	1.050632	H	5.397174	-0.373393	-2.769806
H	3.681156	0.355213	1.402649	H	-3.058843	1.878313	0.455882	H	6.300002	-1.867432	-2.539492
H	2.85766	-2.275171	1.45239	N	-5.129311	1.565427	0.184787	H	7.072082	-0.491935	-3.33915
H	5.263982	-3.453073	-0.602413	O	-4.979663	-0.703598	0.466646	H	-6.299676	1.869332	2.538607
H	7.02117	-1.289659	-1.90239	H	-3.869119	1.0013	1.737295	H	-5.397249	0.375147	2.769563
H	7.235575	1.630702	-0.124924	H	-6.318408	2.1883	-1.394333	H	-7.07216	0.494349	3.338758
				C	-4.366228	3.015866	-1.672082	H	4.727881	2.422913	1.651603
				H	-3.979619	2.164678	-2.234537	H	6.233361	2.511291	0.751498
				H	-4.727317	3.762105	-2.382994	H	-6.234046	-2.510639	-0.750621
				H	-3.540244	3.458556	-1.114844	H	-4.728506	-2.423055	-1.650706
				C	-4.146414	3.114759	1.850372	H	-3.581968	-1.394024	0.304594
				H	-3.296442	3.210356	2.527634	H	3.581566	1.394328	-0.304052
				H	-4.164659	4.006352	1.2206	C	4.706115	3.871775	0.0599
				H	-5.058516	3.091131	2.451962	H	5.145699	4.034468	-0.927718
				C	-8.012246	1.099975	0.222557	H	3.620679	3.910772	-0.051905
				H	-8.687428	1.177376	-0.635059	H	5.014066	4.697071	0.704484
				C	-7.394852	-1.199902	-0.5337	C	-4.707224	-3.8713	-0.058438
				H	-8.480139	-1.220031	-0.430971	H	-5.146884	-4.033476	0.929231
				N	-6.965528	0.137373	-0.103325	H	-5.015403	-4.696756	-0.702709
				H	-6.991337	-1.949104	0.147653	H	-3.621803	-3.910577	0.053413
				H	-7.562278	2.078801	0.364584				
				C	-8.77839	0.71921	1.478324				

H	-8.112787	0.684428	2.343075
H	-9.553062	1.463995	1.672926
H	-9.267234	-0.251872	1.386147
C	-6.997096	-1.50057	-1.96525
H	-7.35315	-2.494203	-2.244935
H	-7.435147	-0.776709	-2.656503
H	-5.913468	-1.483023	-2.088183
H	-4.010763	-0.639941	0.171259

Pu-6NO3-2IEE_geom2				Pu-6NO3-2EEE_geom2				Pu-6NO3-2MEE_geom2			
Pu	-0.000053	-0.001001	0.000269	Pu	-0.00003	0.000041	0.000029	Pu	0.000099	-0.000077	0.000131
O	0.586634	1.610326	-1.819105	O	-0.249841	0.83901	-2.351856	O	-0.252629	-2.407818	-0.659541
O	-0.626532	2.405585	-0.25552	O	-1.309751	1.94982	-0.873027	O	-1.188512	-1.004074	-1.961823
O	-0.050302	3.673162	-1.908276	O	-1.507207	2.489355	-2.956356	O	-1.429574	-3.120411	-2.326216
O	-0.377348	1.169007	2.271384	O	-0.250342	1.860376	1.763834	O	-0.082224	1.61457	-2.001131
O	-2.292793	1.586175	3.1795	O	-2.066282	2.35258	2.827494	O	-1.834076	2.668009	-2.703082
O	-2.152868	0.633732	1.239173	O	-1.97923	0.662797	1.475046	O	-1.901297	1.438937	-0.920121
O	1.928721	1.537261	0.631128	O	1.469494	2.014636	-0.46351	O	1.586778	-0.652763	-1.867888
O	3.546435	1.028361	1.971981	O	3.367847	2.438148	0.477953	O	3.529364	0.215347	-2.243
O	1.923361	-0.350886	1.613009	O	2.244814	0.663435	0.988138	O	2.311559	0.887922	-0.588909
N	-0.029667	2.613507	-1.355218	N	-1.03788	1.791138	-2.105761	N	-0.972024	-2.224338	-1.678278
N	-1.614568	1.157296	2.290027	N	-1.438417	1.675328	2.067534	N	-1.274685	1.94992	-1.929618
N	2.501639	0.754151	1.432296	N	2.395453	1.743047	0.339566	N	2.512259	0.151556	-1.602616
O	-0.586967	-1.611998	1.819777	O	0.249773	-0.838931	2.351917	O	0.252594	2.407698	0.659793
O	0.626151	-2.407319	0.256161	O	1.309694	-1.949735	0.873093	O	1.188839	1.004009	1.961891
O	0.050372	-3.674694	1.909242	O	1.507115	-2.489292	2.95642	O	1.429653	3.120361	2.326353
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C	7.392674	-0.090809	2.235467	H	6.844409	2.195644	0.09303	H	5.585426	-1.288926	-1.524536
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H	3.430356	-2.18865	0.166365	H	5.328742	0.317331	2.746335	H	6.930336	3.259114	-0.529491
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H	7.719119	2.430321	-1.380559	H	6.997668	0.407071	3.33796	H	-5.273025	-2.629869	0.543012
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H	-6.123776	-2.223021	2.120866	H	4.604944	-2.90987	-1.393764	H	4.994085	0.441799	2.710397
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H	4.550271	-2.205417	-2.195126								
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Pu-6NO3-2MME_geom2			Pu-6NO3-2EMM_geom2			Pu-6NO3-2MMM_geom2					
Pu	-0.00001	0.000021	0.000006	Pu	-0.000009	-0.000014	-0.000006	Pu	-0.000001	-0.000001	0.000001
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O	1.256203	-0.060712	-2.164882	O	-1.425824	-1.865892	0.87241	O	-1.925457	0.209505	1.668077
O	1.621718	1.642897	-3.443031	O	-1.65157	-2.395645	2.955358	O	-1.914028	1.356945	3.506281
O	-0.003921	-2.34993	-1.046123	O	-0.374346	-1.839279	-1.766921	O	-1.519539	-2.028136	-0.168231
O	1.686561	-3.693342	-1.140695	O	-2.227324	-2.220369	-2.812679	O	-3.45683	-2.080846	-1.12401
O	1.817799	-1.792878	-0.10842	O	-2.022042	-0.535404	-1.466456	O	-2.293997	-0.260172	-1.067045
O	-1.537886	-0.191434	-2.012127	O	1.339916	-2.106088	0.455697	O	0.283298	-1.559054	1.943092
O	-3.526161	-1.037325	-2.009298	O	3.215615	-2.63627	-0.477474	O	1.518365	-3.332694	1.941481
O	-2.355502	-0.942624	-0.195425	O	2.198073	-0.800151	-0.990671	O	1.258001	-2.159925	0.145386
N	1.109393	1.163506	-2.47369	N	-1.142175	-1.726283	2.104933	N	-1.330575	0.95058	2.546969
N	1.166631	-2.675459	-0.794624	N	-1.55091	-1.582431	-2.061317	N	-2.458188	-1.490458	-0.802624
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O	-0.396135	-1.82611	1.67235	O	0.296242	0.824774	-2.350438	O	0.141776	-1.183965	-2.281184
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O	1.537857	0.191472	2.01214	O	-1.339933	2.10606	-0.455711	O	-0.283298	1.559053	-1.943093
O	3.526143	1.037336	2.009313	O	-3.215631	2.636245	0.477465	O	-1.518359	3.332697	-1.941476
O	2.355486	0.942642	0.195438	O	-2.198092	0.800122	0.990653	O	-1.257995	2.159925	-0.145383
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H	-3.322827	1.855872	-0.054928	H	3.498349	0.206343	1.482593	H	3.422338	-0.051637	-1.635808
O	4.282918	-1.683985	0.35945	O	-4.404597	0.250844	-1.362898	O	-4.369987	-0.269387	1.416828
C	4.922866	-0.821793	-0.34839	C	-5.016203	-0.071468	-0.277541	C	-4.937328	0.35951	0.451009
N	6.018516	-0.346056	0.182777	N	-5.987284	0.717763	0.106584	N	-5.96763	-0.218446	-0.112775
O	-4.282931	1.683986	-0.35941	O	4.404618	-0.250821	1.362947	O	4.369986	0.269382	-1.416839
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C	4.460236	-0.438402	-1.706604	C	-4.647353	-1.320583	0.442867	C	-4.469703	1.705357	0.030915
H	4.488139	0.640976	-1.846662	C	-5.281885	-2.550482	-0.209698	H	-3.491956	1.919165	0.455321
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H	6.688127	0.588847	-1.553265	C	5.281827	2.550505	0.209701	H	4.38459	-1.773518	1.052543
C	6.564989	2.058917	0.0263	C	-6.83378	0.44289	1.252768	C	-6.717038	0.396453	-1.191063
H	7.888686	0.377368	-0.296076	H	-6.853276	-0.616903	1.487211	H	-7.771883	0.150941	-1.063808
C	6.370056	-0.729891	1.546303	H	-7.84922	0.759135	1.011648	H	-6.610022	1.477015	-1.181184
H	7.292353	-0.221348	1.816919	C	-6.250782	1.979522	-0.570497	H	-6.376176	0.005493	-2.153066
H	5.574219	-0.439269	2.232352	H	-6.420062	2.743797	0.188292	C	-6.367328	-1.574909	0.228129
C	-6.848061	-0.65687	0.478563	H	-5.39697	2.263875	-1.175909	H	-6.456107	-2.149584	-0.694535
H	-6.68795	-0.589156	1.553179	C	6.833794	-0.442689	-1.252745	H	-5.619464	-2.036925	0.862859
H	-7.888586	-0.377574	0.296074	H	6.853138	0.617109	-1.487189	H	-7.332137	-1.556554	0.73998
C	-6.564838	-2.059042	-0.026548	H	7.849283	-0.7588	-1.011654	C	6.717023	-0.396429	1.191073
C	-6.370012	0.729832	-1.546306	C	6.251032	-1.979392	0.570538	H	6.610033	-1.476994	1.181186
H	-7.292338	0.221335	-1.816908	H	6.420363	-2.743648	-0.188259	H	7.771865	-0.150891	1.063845
H	-5.574204	0.439191	-2.232381	H	5.397284	-2.263847	1.175988	H	6.376128	-0.005482	2.153069
H	-5.525295	-2.338733	0.151641	H	4.982643	2.63824	1.255432	C	6.367324	1.574918	-0.228142
H	-6.75066	-2.141738	-1.098739	H	6.373323	2.522791	0.165399	H	6.456028	2.14962	0.694513
H	-7.213312	-2.771438	0.486596	H	-6.37338	-2.522744	-0.165387	H	7.332169	1.556565	-0.739925
H	6.750758	2.141713	1.098494	H	-4.98271	-2.638201	-1.255432	H	5.619497	2.036904	-0.862937
H	5.525466	2.338633	-0.15197	H	-3.55945	-1.406369	0.40718	H	3.491965	-1.91917	-0.455321
H	7.213515	2.771236	-0.486883	H	3.559425	1.406347	-0.407159	H	-5.179089	2.462032	0.379086
H	3.43648	-0.766759	-1.868853	H	4.940676	3.444714	-0.312006				
H	-3.436643	0.767051	1.869118	H	6.486228	-1.005737	-2.122243				
H	6.517383	-1.808195	1.608694	H	7.140794	-1.887679	1.197944				
H	5.105489	-0.907715	-2.454999	H	-7.140524	1.887907	-1.197945				
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H	-5.105802	0.907255	2.455	H	-4.94075	-3.44471	0.311988				

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